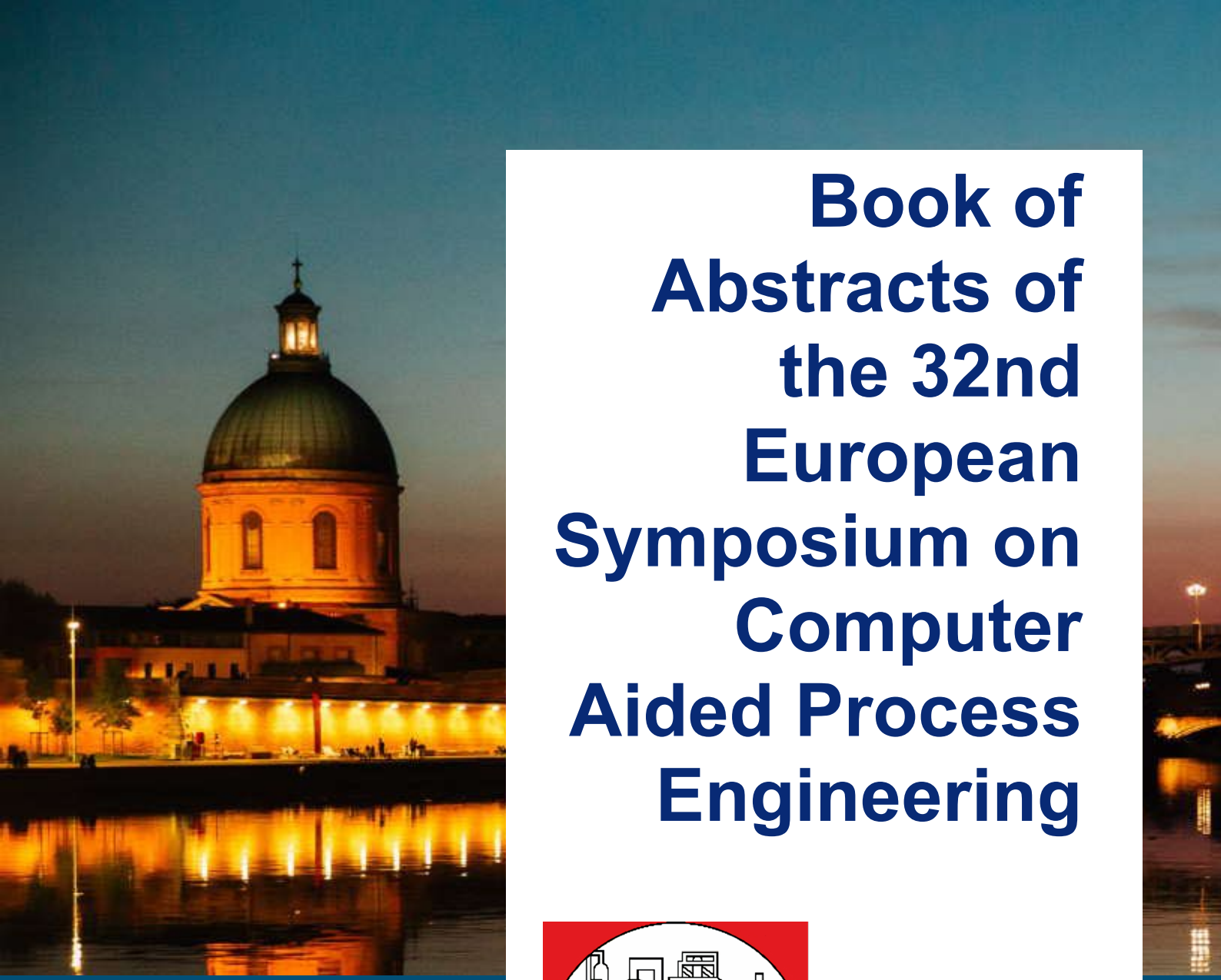

Book of Abstracts of the 32nd European Symposium on Computer Aided Process Engineering

ESCAPE 32
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Preface

This book of abstracts puts together all the contributions presented at the 32th European Symposium on Computer Aided Process Engineering (ESCAPE), held in Toulouse, France, from June 12th to 15th, 2022.

This 32th event of the ESCAPE series is conference organized under the auspices of the CAPE Working Party of the European Federation of Chemical Engineering (EFCE), and the Société Française de Génie des Procédés (SFGP).

The ESCAPE series is an opportunity for scientists, researchers, managers, engineers, and students from academia and industry, to share and learn about the exciting domain of CAPE and Process Systems Engineering (PSE). RSCAPE 32 congress provides an open forum to present and review the latest developments in CAPE and/or PSE.

While the ESCAPE conference has been organized annually since 1992, this is the first book of abstracts that compiles all conference submissions. However, the one-page abstracts have been expanded to a six-page version available in the Computer-Aided Chemical Engineering series (3 volumes dedicated to the 32th European Symposium of Computer Aided Process Engineering).

Like the previous editions, the main focus for ESCAPE-32 is on new developments that cover different aspects in process systems engineering, new applications of established methods, comparisons of alternative methodologies, but one of our goal was to give more emphasis on uncertainty towards sustainability (major theme of the congress). Another one was to give an audience to researchers in traditional fields of applications like modeling and simulation, product and process synthesis, planning and scheduling, control, artificial intelligence and education. The eight themes of ESCAPE-32 have been selected after in-depth discussion with the CAPE Working Party members. The themes include:

Modelling and Simulation
Coordinators : Iqbal Mujtaba, Jena-Pierre Belaud and Ludovic Montastruc

Product/Process Synthesis and Design
Coordinators: Grégoire Léonard and Laurent Cassayre

Large Scale Design and Planning/Scheduling
Coordinators: Antonio Espuna and Catherine Azzaro-Pantel

On Line Model Based Applications and Control
Coordinators: Miroslav Fikar and Nataliya Shcherbakova

Concepts, Methods and Tools
Coordinators: André Bardow and Pascal Floquet

Digitalization and Artificial Intelligence
Coordinators: Norbert Aspirion, Rachid Ouaret and Stéphane Negny

CAPE Applications Addressing Societal Challenges
Coordinators: Ana Barbosa-Povoa, Raphaële Thery-Hetreux and Marianne Boix

Education in CAPE and Knowledge Transfer
Coordinators: Eric Schaer and Vincent Gerbaud

The particular topics within these overarching themes have been formulated to allow researchers from CAPE-related sciences to present their results and exchange valuable knowledge and experience

This book of abstracts gathers 467 contributions from four continents (Europe, Americas, Africa, Asia). The papers have been reviewed and selected by the International Scientific Committee together with the help of Theme Coordinators. We are deeply thankful for timely and careful reviews by these Scientists, as well as their invaluable help.

As editors of this book, we hope that the contributions gather abstracts with different backgrounds and sensibilities, and we hope that this "melting pot" will give an illustration of the current research un the PSE field, will contribute to the progress of methodologies and approaches, and that it will favor improvements and the emergence of new ideas in computer aided process and product engineering.

June 2022

Ludovic Montastruc Stéphane Negny

ESCAPE32
Computer Aided Chemical Engineering book series

T1: Modelling and Simulation

T2: Product/Process Synthesis and Design

Qin, Hao (1); Song, Zhen (1,2); Qi, Zhiwen (2); Sundmacher, Kai (1,3)
1: Otto-von-Guericke University Magdeburg; 2: East China University of Science and Technology; 3: Max Planck Institute for Dynamics of Complex Technical Systems

T3: Large Scale Design and Planning/Scheduling

T4: On Line Model Based Applications and Control

T5: Concepts, Methods and Tools

T6: Digitalization and Artificial Intelligence

T7: CAPE Applications Addressing Societal Challenges

T8: Education in CAPE and Knowledge Transfer

Ludovic Montastruc, Stéphane Negny (Eds.)
Book of Abstracts of the 32nd European Symposium on Computer Aided Process Engineering (ESCAPE32), June 12th-15th, 2022, Toulouse, France.

Periodic Oscillations in Methane Reactor: Effects of the Main Operating Parameters.

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Abstract

Biofuels are widely considered as one of the most environmental-friendly energy sources. Among them, biogas from the anaerobic digestion of organic wastes stands out as an attractive way of reducing landfilling while producing energy. However, the CH_4 content in biogas usually reaches about 70% at most so that it needs to be purified (removal of trace components) and upgraded (removal of CO_2) before utilization. The most used carbon dioxide separation technologies are based on absorption, adsorption, cryogenic distillation, and membrane separation, all of them being high energy consuming (Zhang et al 2020). In this work, the upgrading process by biogas direct methanation is analyzed. Particularly, we envision using surplus electrical energy from renewable sources to produce via electrolysis the required hydrogen to be fed, along with the biogas, into the methanation reactor (Bareschino et al. 2020). Methanation enables the conversion of H_2 and CO_2 into methane, the result being simultaneous biogas upgrading and methane enrichment of the leaving gas. The process is carried out in an adiabatic fixed bed reactor with nickel-based catalysts, and a recycle loop is used for diluting the inlet reactants concentration to decrease the hot spot temperature. A predictive dynamical model of the adiabatic fixed bed reactor, assumed pseudo-homogeneous, is used to describe the main features of the methanation reactor (Bareschino et al. 2021). The effects on the feed temperature, reactor pressure, recycling ratio and feed hydrogen concentration are considered. In all cases, high CO_2 conversion efficiencies, even exceeding 95%, were predicted. However, multiplicity and periodic oscillations were observed in the numerical predictions, over a wide range of the investigated parameters. The main cause of the sustained periodic oscillation can be found in the positive feedback from the mass recycle coupled with the typical phenomena of fixed bed reactors, i.e. the inverse response. Although the maximum temperature reached during the oscillations is limited by the thermodynamic equilibrium, the system, as can be seen, oscillates with a period of about 10 minutes and in a range of 200°C. This behavior has to be avoided for catalyst stability. A detailed nonlinear analysis is performed, and the information can be useful for an effective plant design and an adequate plant control and operation.

Keywords: Biomethane, Power-to-Methane, fixed bed reactor, periodic oscillations, non-linear dynamics

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P. Bareschino, E. Mancusi, C. Tregambi, F.Pepe, M. Urciuolo, P. Brachi, G. Ruoppolo, 2021, Energy, 230, 120863
X. Zhang, J. Witte, T. Schildhauer, C. Bauer (2020), Energy Fuels 4, 1427–1436.

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Modeling, Simulation and Experimental Validation of Non-Isothermal Ceramic Drying

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Abstract

Drying constitutes an essential step in the ceramic industry. During this process most of the water that was added in a previous moulding step is removed. This step is characterized by significant complexity since heat and mass transfer are coupled processes and take place simultaneously. Accounting to the nature of the process, drying may be accompanied by dimensional variations which occur due to the moisture removal. However, products with differing shrinkage than the one expected are usually rejected being that they often do not meet the required quality standards or there is a high probability of breakage in the subsequent firing step. Furthermore, it is possible that breakage phenomena occur during the drying process itself, especially when the drying rates are not properly controlled. Consequently, drying is a quality defining process which makes the knowledge of the evolution of moisture content and linear shrinkage imperative.

In this work a non-isothermal model is proposed to predict the analysis of the water distribution and shrinkage of a ceramic tile over time. The main objective is to model, simulate and assess the drying behavior of a single tile which is exposed to the convective flux of air of known humidity, velocity and temperature. The proposed mathematical model is inspired by a moving boundary model which was originally presented by Adrover et al. (2019). More specifically, 1-D mass and heat transfer is assumed along the thickness of the tile. The mechanism of mass transfer inside the material is a combination of diffusion and capillary motion, whereas at the surface moisture is removed through forced convection by the blowing air. Based on this assumption, shrinkage takes place only on one dimension. The model is then validated by using experimental results which provide both dynamic and steady state measurements. Then the model can be used to accurately capture the drying behavior of a parallelepiped roof tile for two distinct case studies. Namely, the ideal-shrinkage case and the no-shrinkage case. The proposed modeling approach combines high quality results with low computational costs. Furthermore, the developed modeling method can be utilized to simulate drying for a wide variety of conditions or material properties, revealing the robustness of the model.

Keywords: Process Modeling, Ceramic Drying, Moving-Boundary Problem

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Numerical study on the solid residence time distribution in a counter-current screw extractor

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Abstract

The possibility of applying continuous counter-current extraction to extract Artemisinin from *Artemisia Annua* leaves was reported recently; Artemisinin is urgently needed as an efficient malaria drug (Triemer et al., 2018). The residence time distribution (RTD) of the solid and liquid phases are most important since they influence the reaction efficiency. This work is devoted to the numerical investigation of the solid phase RTD in a fully filled screw extractor by using computational fluid dynamics (CFD). A block-structured mesh is applied since it has been proved to be most accurate due to reduced numerical diffusion. The rotation of the screw inside a stationary housing is realized by the Sliding Mesh approach. The mushy phase is assumed as highly viscous liquid. To track it, a Passive Scalar model has been implemented in a frozen quasi steady-state simulation. Validation experiments have been performed by using dry leaves.

After adapting the inflow velocity of the solid phase and using the experimentally calculated axial diffusion coefficient for the Passive Scalar, a very good agreement between numerical and experimental residence times can be observed, with an error lower than 10%. Furthermore, the temporal distributions at three sampling points inside the screw extruder have been evaluated. Here also, a very good agreement has been found, proving that the numerical model can appropriately predict the solid RTD. Using a frozen quasi-steady state flow allows short computational times. This will enable future multiphase flow simulations even closer to the experimental reality.

As a next step the model will be extended to predict the RTD in the multiphase flow model including the liquid solvent. The numerical representation of the RTDs will then be used to parametrize compartment models (CM) in which the reaction kinetics can be taken into account with acceptable computational times. This mixed CFD/CM model will be used for the final optimization of the extraction process.

Keywords: computational fluid dynamics (CFD), residence time distribution, extraction

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Dynamic modelling of light and temperature effects on biomass growth and biohydrogen production by the photosynthetic bacterium *Rhodopseudomonas palustris*

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Abstract

Background: Parallel to the impending hydrogen economy, the simultaneous treatment of organic waste and biohydrogen synthesis by the photosynthetic bacterium *Rhodopseudomonas palustris* is a promising renewable energy technology. However, studies so far have been mostly laboratory based with upscaling of the bioprocess still being an open challenge. Therefore, this study investigates two different Photobioreactors (PBRs): schott bottle-based and vertical tubular-based PBRs and presents three original contributions to facilitate the biotechnology transfer across PBR scales and configurations.
Study Design: Firstly, a dynamic model is constructed to simulate the complicated influences of light intensity, light attenuation, and temperature, previously not unified for any photosynthetic bacteria to the best of our knowledge. Secondly, perturbation analysis was exploited to identify critical parameters influencing the model accuracy and reliability for across the scale extrapolations. Thirdly, two model parameters: *effective light coefficient* and *biohydrogen enhancement coefficient*, both linked to the PBR's transport phenomena were proposed for recalibrations during bioprocess upscaling predictions.
Major results: By comparing against experimental data, the upscaling prediction accuracy was thoroughly verified for the two investigated PBR scales. As well, the enhancement of biohydrogen production rate by improved culture mixing and gas removal was mechanistically described.
Conclusion: This provides important advances for the efficient design of novel PBRs and future online optimisation for biohydrogen production.

Keywords: Photobioreactor, Biohydrogen production, kinetic modelling, Purple non-sulfur bacteria, Upscaling.

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Reducing the experimental effort to design pharmaceutical tablet lubrication by model-based design of experiments

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Abstract

In oral solid-dosage manufacturing through direct compression, lubrication is used to enhance powder flowability and the ejection of the tablet from the die. However, lubrication can also negatively impact tablet quality attributes such as tablets hardness or dissolution. In order to facilitate the selection of an appropriate lubrication extent, different models describing the relation between compaction performance (quantified, e.g., by tensile strength) and process conditions may be used. In particular, the extension of the Kushner and Moore model proposed by Nassar et al. (2021) allows predicting tensile strength over a wide range of tablets solid fraction and powder blending time values. Despite its acceptance in the pharmaceutical industry, the main drawback of this model is that it requires considerable number of experiments for parameter estimation. This results into a significant consumption of active pharmaceutical ingredient (API), which may be scarce and considerably expensive during product development.
In this study, model-based design of experiments (MBDoE; Franceschini and Macchietto, 2008; Galvanin et al., 2007) is used to reduce the required experimental effort for the identification of the extended Kushner and Moore (Nassar et al., 2021) model parameters. We propose a novel MBDoE approach that is able to reduce parameters uncertainty while minimizing the number of required experiments (and, consequently, API consumption, labor, and time). We discuss the results with reference to both simulated and experimental systems.
Keywords: model-based design of experiments; pharmaceutical engineering; quality by design; pharmaceutical manufacturing

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A model-based approach to predict the flowability of directly compressed pharmaceutical blends from individual components

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Abstract

Understanding powder flowability is critical to the success of several unit operations involved in the manufacture of oral solid dosage (OSD) forms such as tablets and capsules (Prescott and Barnum, 2010). The performance of feeders, blenders, tablet presses and capsule fillers (Yadav et al, 2019; Muzzio et al., 2012; Osorio and Muzzio, 2013) depends, among other factors, on the flow properties of the formulation under development. Nevertheless, measuring and predicting powder flowability from the flowability of the individual components of the formulation is notoriously a difficult task (Seville et al., 2000), especially for powders with small particle size and uncontrolled size and shape distributions (Leung et al., 2017).
In this study, we take a well-established mixing rule model developed for equations of state of fluids (namely, the van der Waals mixing rule (van der Waals, 1873)) and show how the underlying model structure can be used to confidently predict the flowability of pharmaceutical blends from the individual components. We provide a theoretical rationale for the proposed approach by showing that, for cohesive pharmaceutical powders, the underlying dominant interactions between particles are van der Walls forces, thus resulting into a similar behavior at a particle level observed for certain mixtures of fluids. The modelling approach is validated with 35 different powder blends consisting of common active pharmaceutical ingredients (APIs) and common excipients used for directly compressed pharmaceutical formulations. Results show that, by measuring the flowability of the pure active pharmaceutical ingredient only once, the mixing rule model can be used to predict the flowability of any industrially relevant blend of the API without further experiments. For a new pharmaceutical product, this translates into a reduction of more than 80% on the number of flowability experiments and API consumption required during process development, hence resulting into a significant reduction of development costs and resources.

Keywords: quality by design; pharmaceutical manufacturing; mixing rules; Industry 4.0.

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Purification of MIBA by Continuous Distillation

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Abstract

MIBA (methyl isobutyryl acetate) is an intermediate used in the pharmaceutical industry and is generally produced in small scale batch processes making it expensive to produce. This study was to look at the potential for a continuous process for the manufacture of MIBA, with the aim to improve yields and hence reduce costs. The initial stage of the work has focused on the purification of the MIBA product, which is required at high levels of purity, that is typically in excess of 99 weight %. Vacuum distillation column models were built using both AVEVA PRO/II Simulation and AVEVA Process Simulation process modeling tools. The MIBA component was generated from SMILES using PropPred and the feasibility of separations were performed using the Ternary VLE tool. These initial studies suggested that high purities of MIBA could not be attained as the overhead product of the column. However, stage wise analysis of the distillation columns indicated maximum purity of the MIBA at trays below the column's condenser; and with a side draw to remove the MIBA purities of in excess of 99 weight % could be achieved. In conclusion, the study indicates that high purities of MIBA can be obtained by continuous vacuum distillation, with an appropriately positioned side -draw for the MIBA product. The results from AVEVA PRO/II Simulation and AVEVA Process Simulation match with the results from the Ternary plots tool available in AVEVA PRO/II Simulation. This study gives is a classical example of how Ternary Plots can be utilized to compliment the results from Simulation tools. Much of the thermodynamic and physical property data employed has, due to the paucity of data in the open literature, been generated by "fill" options. These data and the predicted performance of the distillation columns should be validated by experimental analysis. Once validated the model will be extended to include the reaction stages.

Keywords: MIBA, Distillation, Simulation, modeling, Ternary Plots.

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Modelling of Organophilic Pervaporation for Separation of Acetone-Butanol-Ethanol Mixture

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Abstract

The motivation of the research based on separation problem from fermentation industry, that is Acetone-Butanol-Ethanol solvent residue removal from its aqueous solutions. Pervaporation is a novel, promising technology for the separation of complex, azeotropic mixtures (Lipnizki et al. (2001)). Within this membrane category, organophilic pervaporation was investigated. In this work, laboratory experiments were performed with commercially available test membranes at different temperatures and pressures conditions. The separation factor, total and partial fluxes were determined as well. It was found that, the separation factor and fluxes were inversely proportional to the feed butanol concentration. The laboratory results were consistent with literature studies. Using partial fluxes, semiempirical pervaporation models were fitted. Rautenbach pervaporation model (Rautenbach et al. (1990)) and its exponentially improved model version (Valentinyi et al. (2013)) were investigated in the case of binary mixtures and ternary hydrophilic cases (Toth et al. (2015), Toth et al. (2018), Valentinyi et al. (2020)). The aim of this work was to extend the observations of organophilic pervaporation model to ternary mixture. It can be observed that, the exponentially Rautenbach model describes more accurately the transport process of organophilic pervaporation, than basic model. Thus, it is possible to implementation further studies in process simulator environment.

Keywords: Parameter estimation, Organophilic pervaporation, Acetone-Butanol-Ethanol mixture.

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Development of Deep Learning Architectures for Forecasting Distillation Columns Dynamic Behavior of Biobutanol Purification

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Abstract

Nonlinear identification of chemical processes is a central vexation towards the optimal operation and cost reduction of many industrial sectors. The forecasting of complex industrial processes is generally associated with computational packages that are capable of reproducing successfully and in relatively short computation time. However, dynamic perturbation and conditions of the process may affect the predictions of the desired variables. In recent years, Artificial Neural Network (ANN) has received special attention to a widespread application in the field of engineering, biology, energy, and finance. A key aspect of ANN is its ability to capture complex dynamics and adapt to the noise of the measurements. Within the ANN design, several factors play a major role in the correct prediction of the process, such as the number of internal layers, the number of neurons, the number of used features, the training algorithm, the activation function, the number of epochs, among many others. While ANNs have shown the ability to reproduce and simulate complex chemical processes, the ANN design itself has not been thoroughly investigated. In fact, its application for the downstream process in the chemical process engineering community is still very fragmented and based on black box software. Considering data sets of an intensified distillation column generated by Aspen Plus Dynamics at different operation conditions, here we bring clarity in the field with different architectures of ANNs to abstract the dynamics of both an intensified and conventional distillation process that separates an effluent coming from fermentation producing acetone, butanol, and ethanol (ABE) for spark-ignition purposes. The features for both distillation alternatives were the reflux ratio, the reboiler heat duty as well as the output parameters, were the purities of acetone, butanol, and ethanol. Our results highlight that a one-layer neural network can represent the dynamics of an intensified column to forecast the concentration of acetone, butanol, and ethanol. The best fits to the data sets were obtained using ADAM and RSMP as the training algorithms, however, poor predictions were obtained using the SGD algorithm. Based on the Akaike information criterion (AIC), we found that 5 neurons are the optimal criteria to have a good prediction and avoid overfitting. Remarkably, the linear activation function overperforms the tangent hyperbolic as activation functions. Ultimately, we found that the reflux ration and reboiler duty are key features to reconstruct the full dynamics of the intensified column.

Keywords: Artificial Neural Network, distillation, dynamic, intensification.

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Impact of the methanol synthesis kinetics on industrial production: an in silico assessment

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Abstract

Kinetic modelling covers a key role in process simulation and design. Recently the methanol sector is assisting an increasing enhancement due to its applications as fuel, solvent, and precursor as shown in Bozzano and Manenti (2016). The increasing number of patents, the market prospects, and recent research witness this renewed interest. However, despite this rate in developing and improving technologies, the kinetics modelling does not follow these trends. The methanol synthesis chemical paths, the intermediates, and the real role of the active sites is nowadays still unclear. However, process engineering requires reliable models to estimate the methanol synthesis rate, hence, to design and size the reactor and downstream equipment. Currently, the most used kinetics are Graaf and Vanden Bussche - Froment's models which in any case show some shortcomings and weaknesses. Starting from these premises, the need for updated kinetics is clear. This work aims at comparing and highlighting the impact of different kinetic models (1) original Graaf (or-GR), (2) Vanden Bussche - Froment (VBF), and (3) refitted Graaf (ref-GR) on the methanol synthesis configuration for different feedstocks through an in-silico assessment performed on Aspen Hysys V11. The general simulation flowsheet includes the single-staged PFR for the methanol synthesis, the condensation step (flash unit), and recycle loop for the unreacted syngas. The comparison with industrial data proves that ref-GR model predicts better than the original Graaf model, while the VBF tends to overestimate the methanol production. The validation exploits reliable industrial data published in the literature by Rahimpour et al. (2016), Chen et al. (2011) and Yusup et al. (2010). Finally, the prediction robustness has been performed including non-conventional feedstocks, as proposed in Leonzio (2020).

Keywords: kinetics, methanol synthesis, process simulation, comparative case study

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Optimal layout of modular multi-floor process plants using MILP

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Abstract

Off-Site Modular Construction (OSMC) research has been a growing research area over the past two decades driven by low productivity levels in construction (Bock, 2015). Productivity is higher in factories when compared to a stick-built site due to easier access to superior tools, methods and learning (Hosseini et al., 2018) (Jin et al., 2018). This has spawned the development of small, factory built, rapidly deployable and flexible process plants (Seifert et al., 2012) to take advantage of the gains in OSMC productivity. This is a rapidly growing area in Chemical process plant research (Bielenberg and Palou-Rivera, 2019). Research has shown that OSMC can provide 20% savings in cost and up to 50% savings in scheduling, providing benefits to risk and finance (Mignacca et al., 2018). Design process automation has been applied in earlier stages of the plant design. However, a layout optimization methodology has not been applied to OSMC industrial process plants. This paper proposes to develop and utilise a MILP mathematical layout optimisation model to help design and construct modular process plant. The main considerations are the module sizes for transport requirements and factory handling. Data from previous research was utilised and run through the new modular optimization model. The previous research layout results were compared to the new modular layouts process plant optimization to compare how modularization may affect the design of industrial process plants. The results demonstrate that building a plant in road transportable, factory built could enable equipment to be located closer together due to advanced factory manufacturing processes as assembly and tools are more accessible than building stick built plants. This proposition would need more assessments through detailed Computer Aided Design and analysis methods and proved through practical prototypes. Quality, inspection and safety are also higher in factories. Not considered here are the schedule reduction implications which have shown to be 20-50% in modular plants already built. The study also limited by the currently available dataset, and as such more appropriate data should be sought and analysed (also considering schedules). Also, further process plant considerations should be built into the model such as safety considerations and irregular and oversize equipment.

Keywords: MILP layout optimisation offsite modular construction industrial process plants

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Paving the way to multi-case optimization of a Rankine cycle for cogeneration in nuclear power plants

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Abstract

The current global climate scenario requires technical alternatives to reduce CO2 emissions in the energy field to meet the recent and very demanding decarbonization targets. A promising solution could be cogeneration in nuclear power plants, which would provide heat to some industrial processes and has strong benefits over fossil fuels, with no emission of carbon dioxide during power generation. Currently, these plants are in most cases, optimized only for electricity production, and this is the case for Pressurized Water Reactors in France. A significant asset of cogeneration units is that they can efficiently switch from single electricity production to heat and power production. In this context, the objective of this work is to assess the benefits of performance optimization for such a multi-case operation applied to a Rankine cycle during its design phase. The key for such an optimization is to minimize the exergetic losses that change from one operational mode to another. As a proof of concept of the multi-case optimization relevancy for a steam-water cycle, a seasonal variation of the heat sink temperature is considered as it induces several operating modes for the cycle, even for a single power production. The model of the system developed in the Modelica environment with the Thermosyspro library, is first presented. The formulation of the optimization problem involves dimensional parameters as optimization variables to maximize the global efficiency of the thermodynamic cycle. Three cases are then simulated: the cycle is optimized for the minimal condenser pressure, maximal condenser pressure and a seasonal variation profile of condenser pressure. Multi-case optimization allows improving the mean operating efficiency of the cycle in the considered heat-sink temperature range, compared to an optimization focused on a single operating point. The relative efficiency gain obtained for a narrow condenser temperature range is about 0.5 %. While the gain is modest, this demonstrates the interest for the concept of partial regimes modelling in support of a multi-case optimization, which should be rather emphasized for a cogenerating Rankine cycle, for which operational modes will be much more different. Further developments on the models and the study of a cogeneration case constitute a natural perspective of this work.

Keywords: Modelica simulation, Optimization, Cogeneration, Rankine cycle, CO_2 reduction.

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Dynamic modelling of non-isothermal open-cell foam catalyst packings: Sugar hydrogenation as a case study

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Abstract

Structured catalysts are playing an essential role in the design of more energy-efficient chemical reactors. For three-phase catalytic systems (solid catalyst, gas phase, and liquid phase), the even distribution of the gas and liquid phases is critical to ensure maximum product yield. Open-cell foams have been investigated as suitable alternatives for catalytically active reactor packings, because of their advantageous structural properties. The structures of pores and struts in open-cell foams provide high porosity (75-95%) and high specific surface area, allowing radial liquid flow and local turbulence which results in enhanced mass and heat transfer.

A comprehensive multiphase model for a trickle bed reactor with solid foam packings was developed in this work. Two-dimensional dynamic mass and energy balances in the three phases of heterogeneously catalyzed reaction systems were implemented. The mass and heat transfer resistances in the gas-liquid and liquid-solid phases and inside the pores of the catalyst were considered. The model was implemented and validated in gPROMS® Modelbuilder V7.0.7. The hydrogenation of arabinose and galactose mixtures on a ruthenium catalyst supported by carbon-coated aluminum foams was applied as an industrially relevant case study. The reaction kinetic parameters were estimated using the experimentally obtained conversions of arabinose and galactose in a continuously operating tubular reactor with a diameter of 11 mm and bed length of 33 mm, equipped with open-cell aluminum foam with a pore density of 40 PPI. The experiments were performed at different operating conditions, with temperatures between 90 and 120 °C and arabinose-galactose molar ratios of 1:1 and 1:2.

The kinetic parameters were estimated with confidence intervals within 10% error, indicating a good accuracy of the parameters, and the model results present a good adjustment to the experimental values. The model developed is suitable for other three-phase research in continuous catalytic reactors with solid foam packings.

Keywords: Open cell foam catalyst packing, Non-isothermal trickle bed reactor, Kinetics, Mass transfer, gPROMS.

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Optimising a wind farm with energy storage consideration curtailment and uncertainties

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Abstract

Energy storage technologies (EST) can facilitate the decarbonisation of energy systems and lead to more sustainable futures. Battery storage (BS) has been found to improve power quality in electrical grids (Das et al., 2018) – particularly with high renewable penetration – and hydrogen storage (HS) can also replace fossil fuels in heating, industry and shipping (Gielen et al., 2019). Operating these technologies alongside renewables allows for the optimal use of variable electricity sources (IRENA, 2019) and a means to use otherwise curtailed generation. However, any decision making and scheduling of EST must take into account uncertainties relating to renewable generation, curtailment and market prices due to their unpredictable nature.

In this work we present a scenario-based stochastic optimisation (SBSO) model to schedule a wind farm with BS and a hydrogen electrolyser (HE) considering curtailment and uncertainties in generation and market prices. We compare cases with BS only, HE only, and a combination of the two. This builds upon recent studies optimising wind-hydrogen systems under uncertainties (Xiao et al., 2020; Yu et al., 2019) by incorporating BS and modelling wind curtailment, which were not previously considered. We apply Markov Chain (MC) and Gaussian Process (GP) techniques to generate wind curtailment and electricity price scenarios, respectively, capturing their inherent uncertainties. The model then assesses the economic benefits of incorporating BS and/or HE alongside wind generation and their scheduling as a function of curtailed and non-curtailed wind. The results can be used to determine the suitability of such systems for the purposes of maximizing profits and making optimal use of curtailed generation.

Keywords: Wind farm, Battery storage, Hydrogen electrolysis, Curtailment, Stochastic optimisation

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Alternative Fuels to facilitate the Implementation of a Carbon Offsetting and Reduction Scheme for International Aviation

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Abstract

The aviation industry supports the world economy, contributing US$2.7trillion to global growth domestic product (GDP). However, aviation raises environmental concerns. Aviation has a 12% share of CO2 emissions within the transportation sector. Therefore, ICAO suggested the implementation of CORSIA as a market-based measures (MBM) to mitigate CO2. CORSIA scheme may increase the operational costs by setting a carbon price on every extra tonne of CO2 beyond the baseline limits. In order to reduce the operators' obligations, the integration of reduction measures such as Alternative Jet Fuels (AJFs) may reduce the cost associated with CORSIA's offsetting requirements. Optimization models may also be an effective tool to help operators select a suitable AJF that maximizes operators' profit under policy requirements. A multi-objective model based on the FLEET model for aircraft allocation was constructed with two functions to account for the cost of carbon and cost of fuel. The model was to select between fuels as algae, jatropha, biomethane, LNG, GTL, liquid H2, 50% SPK-kerosene blends, 50% LNG-Kerosene blends, and 50% liquid H2-Kerosene. The model required a validation using the total emissions obtained from producing and operating each one of the selected alternatives. The production emissions data were collected from ten different supply chains. The operational emissions data were obtained from emission indices. The results indicated that clean fuels could provide better alternatives for the operator under a carbon policy compared to Kerosene. The latter has the worst performance, specifically at a higher carbon cost.

Keywords: Sustainable Aviation; Alternative Jet Fuels; CORSIA; Aviation; Carbon Policies.

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Dynamic Surrogate Modeling for Continuous Processes Control Applications

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Abstract

With the increasing amount of data to be quickly analyzed in a limited time range, during the last decades, surrogate modeling has become a topic of major interest in process engineering. Initially conceived to fill the lack of phenomenological models, black-box models have gained more interest as effective tools to reduce the computational effort when dealing with complex systems and to enhance the solution of optimization algorithms (Bhosekar and Ierapetritou, 2018).
Among the surrogate model applications, scheduling and control problems are getting particular attention in the last years (McBride and Sundmacher, 2019). However, when dealing with dynamics, the majority of works proposed in literature concern batch processes to be modeled within the corresponding residence time interval (Shokry et al. 2020).
With the purpose to extend the established procedures to continuous operations, in this research work the surrogate modeling procedure of a non-isothermal CSTR reactor is discussed and analyzed in detail from a dynamics and control perspective. The modeling phase has been carried out for the temperature and concentration over the domain of the manipulated variable step perturbations vs time with different sampling size and techniques by means of the software ALAMO®. After the open-loop model was build and validated, the related closed loop configuration has been tested by means of a conventional PID controller implementation. The controller has been properly tuned on both models in order to compare the performances.
The obtained trends show good agreement with those obtained by the rigorous model both for open loop and closed loop performances. More importantly, the implemented surrogate model requires shorter calculation time due to the replacement of differential equations to be integrated with explicit input-output variable analytical correlations.
In conclusion, the proposed approach for dynamic surrogate modeling aiming at process control applications has proved to be effective and provided reliable variables trend compared with the rigorous model for continuous operations. Moreover, the study shows how the obtained system of explicit equations allows to reduce the computational time by an order of magnitude with respect to the differential system and to detect the best compromise between the algorithm performances and the solution accuracy.

Keywords: data-driven modeling, design of experiment, process control, ALAMO.

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Probabilistic machine learning based soft-sensors for product quality prediction in batch processes

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Abstract

Statistical machine learning algorithms have been widely used to analyse industrial data for batch process monitoring and control. In this study, we develop a three-step methodology to identify, visualize and systematically reduce data dimensionality for the construction of robust soft-sensors for end-product quality prediction. The approach first employs partial least squares to screen the entire dataset and identify critical time regions and operational variables, then adopts multiway partial least squares to construct a latent space descriptive of the existing batches. Nonlinear estimators are then constructed within the reduced latent space to estimate final product quality, each of which is able to express a given form of model uncertainty. Specifically, in this study, we explore the performance of Gaussian processes, Bayesian neural networks and heteroscedastic noise neural networks. Innovations of this approach include the ease of data visualisation and ability to identify major operational activities within the factory, as well as robustly predict end-quality. To highlight efficiency and practical benefits, an industrial personal care product manufacturing process was presented as an example and the different soft sensors were successfully constructed and cross validated. Furthermore, the accuracy, reliability, and interpretability of the soft-sensors are discussed and tested on a dataset generated from the same process, but within another plant.

Keywords: Machine learning, batch process, soft-sensor, dimensionality reduction, viscosity prediction, interpretability.

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Property Estimation Method for Cannabinoids and Terpenes Using Machine Learning

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Abstract

Nowadays, medical cannabis has great importance as a coadjuvant in the treatment of some pathologies as glaucoma, rheumatoid arthritis, HIV, Alzheimer's, asthma, cancer, chronic pain that is difficult to control, Crohn's disease, epilepsy, multiple sclerosis, insomnia and Parkinson's; additionally, cannabinoids and terpenes have important properties that need to be considered and studied in a deeper way to understand the way these compounds work. The main goal of this study is to develop a new hybrid methodology based on both contribution groups and machine learning algorithms. In this particular case, the study is focused on estimating properties of cannabinoids and terpenes whose experimental information is really scarce and in most cases not yet reported. To do so, a database of hundreds of thousands molecules which includes different thermodynamic properties have been considered. Our method is able to estimate different properties such as: boiling point, melting point, vapor pressure, viscosity, and vaporization enthalpy. Machine learning algorithms have been used to establish the contribution of every functional group and its prediction capability has been compared with other well known methods like the Joback *et al.* method (1987), *Gani et al*. (1994) among others. One of the major findings of the present study is the fact that the current estimation methods are not adequate enough for cannabinoids and terpenes, so there is an important need to find new and more precise ones that allow to improve the accuracy in the groups as well as to extend the predictions to a bigger set of chemical groups. This study clearly shows the importance and utility of the machine learning methods in one of the most relevant chemical engineering areas such as the properties estimation one. This study clearly shows the benefits of machine learning techniques in chemical engineering applications.

Keywords: Property Estimation Method, functional groups, Machine Learning, Neural Networks, Cannabinoids.

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Kinetic modelling of γ-linolenic acid production by *Cunninghamella echinulata*

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Abstract

Microbiological production of *γ*-linolenic acid (GLA) via a temperature-shift strategy has been found to shorten the batch cultivation period, improve GLA yields and reduce the operational cost. However, the underlining biochemical mechanistic phenomena are highly complex and challenging to model, thus hindering commercial upscaling applications of this fermentation technology. To bridge this gap, a dynamic model capable of simulating biomass growth, substrate consumption, and GLA biosynthesis of *Cunninghamella echinulata* for a wide temperature range was proposed for the first time. Haven identified the model parameters, the model's simulation accuracy was verified to be high using data from a small scale 1L bioreactor, it was found that the optimal temperatures for biomass growth and GLA production were respectively 37 ℃ and 14 ℃. Model aided upscaling to a 5L bioreactor with a two-stage temperature-shift strategy showed a 69.6% increment of GLA production and was verified experimentally. This presents important advances for the upscaling of GLA production biotechnology from laboratory scale to pilot scale.

Keywords: fermentation; kinetic modelling; *γ*-linolenic acid; temperature-shift; process upscaling.

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Development of a process simulation model for the pyrolysis of plastic waste (PET) with techno and economic analysis

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Abstract

The intensive use of plastic in daily life has accumulated an ample quantity of plastic waste. The waste management of plastic is challenging due to its un-degradable nature, increasing land, water and air pollution. Polyethylene terephthalate (PET) is one of the most important types of plastic used and has a big fraction in plastic wastes. The thermochemical conversion process such as pyrolysis is an important technique to convert the PET into value-added products such as char, oil and gas. This study develops a process simulation model for the pyrolysis of PET plastic for conversion into char, boil and gas. In addition, a techno-economic feasible model was also made using the tool present in Aspen Plus to understand the commercial viability of this process. The process flow sheet model is developed using the Aspen Plus V10® and the impact of temperature, pressure and residence time on the production of char, pyrolysis oil and gas. The process is optimized to determine the optimum condition to maximize product yield. The char, gas and oil productions are 0.489, 0.330, 178 kg/hr per kg PET, respectively at an optimum temperature of 400 □C. The cost of gas and oil is 0.065 and 0.0165 USD per kg PET, whereas the maximum cost of char was obtained 0.360 USD per kg. The CO2 emission was obtained -41.482 kg/hr per kg PET processing. This study provides a baseline for the sustainable utilization of the pyrolysis process for the PET conversion into value-added product.

Keywords: PET, Aspen Plus, Char, Pyrolysis, Techno-economic analysis.

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Monte Carlo Simulation of the Mechanical Processing of Bulk Materials with Fluctuating Compositions

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Abstract

The EU circular economy package requires increasing recycling rates of (mixed) municipal solid waste. Consequently, increased efficiency and effectiveness of (mechanical) treatment processes for these materials is crucial, and hence improved process understanding is desired. However, generating such an understanding through process models is challenging since the processes' performance depends on the material's composition, which is highly variable for waste streams. For example, the content of thin-film plastics affects the efficiency of screens by partially covering their perforation. Consequently, correlations of components' shares affect the screening performance for individual components. In this work, a Monte Carlo-based approach for modelling the mechanical treatment of fluctuating bulks is established and experimentally tested, using model materials and a lab-scale circular vibratory screen. The approach combines a process model with a multivariate probability density estimation of the material's composition through a Monte Carlo simulation. An experiment-based multi-linear empirical process model is used in this study. And the data for estimating the probability distribution of the composition are collected by continuous process sampling. The current focus of this ongoing work is on the method for describing the compositional probability density. First attempts, using analytical probability density functions (normal distribution on the simplex, and multivariate normal distribution) did not succeed. Hence, multivariate kernel density estimation is currently being examined as a distribution-independent, and thus more flexible approach. It requires a higher, but still reasonable number of samples in the case of three components. Currently, the handling or avoidance of invalid compositions when generating random data for the Monte Carlo step is being investigated: compositions are constrained by the simplex, i.e., all shares must be positive, and their sum must be constant. Subsequently, the simulation will be performed, and the resulting screening efficiencies will be compared with analyses of the total processing products. The results will show whether inherent assumptions - i.e., no axial backmixing, in analogy to plug flow, and hence invariance to the order of the compositions' occurrence - are applicable. In case of success, the method can finally be used for calculating process optima and the theoretical potential of dynamic adaptive process parametrisation.

Keywords: Monte Carlo simulation, kernel density, compositional data, mixed solid waste

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Determination of the burst pressure of pillow plates using finite element methods

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Abstract

Pillow plates represent an innovative type of heat transfer equipment and are characterised by a high degree of flexibility in terms of application and manufacturing. Due to the fact that manufacturing is usually carried out by means of CNC-controlled laser welding systems and a subsequent internal high-pressure forming process, geometric adjustments are very easy to realise, as the involvement of expensive forming tools is not necessary. However, this high degree of flexibility together with the geometrical complexity make the design of pillow-plate heat exchangers very difficult, while the required relationships for the determination of the maximum allowable operating pressure are missing. Therefore, an experimental verification according to regulations, such as AD 2000 (VD TÜV, 2009), is usually carried out, in which the allowable operating pressure is estimated as a function of the burst pressure. The latter has to be determined in time-consuming and cost-intensive bursting tests. For this reason, the aim of the present work was to perform a model-based determination of the burst pressure by means of structural-mechanical finite element simulations, which can be interpreted as a numerical reproduction of the experimental bursting tests. This was done by using the commercial finite element solver ABAQUS by Dassault Systèmes, which is well established in industry and academia. For validation reasons, BUCO Wärmeaustauscher International GmbH provided protocols of bursting tests for two completely different pillow plate geometries. Investigations carried out in a previous work (Zibart and Kenig, 2021) revealed that the thermal resistance of pillow plate heat exchangers can be reduced by up to 25% by using aluminium as the material of the plates instead of the commonly used stainless steel. As a next step, a structural properties analysis of aluminium-made pillow plates should be performed. Based on the finite element methods derived in the present study, the manufacturing feasibility of technically relevant pillow plates from aluminium was investigated. A parameter study was carried out in which the welding spot pattern and the sheet thickness were varied. The material chosen was the aluminium alloy EN AW 5083, which is widely used in process engineering and is characterised by good weldability and formability combined with high mechanical strength. The achievable burst pressures and the maximum realisable inflation heights of the pillow plates in the hydroforming process were studied in dependence on the geometry of the welding spot pattern and the sheet thickness of the plates.

Keywords: Pillow plates, Heat exchanger, Finite Element Analysis, Burst pressure

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A hybrid multi effect distillation and double reverse osmosis system for most economical brackish water desalination

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Abstract

Brackish water desalination was approved as one of the most promising methods to generate fresh water for the community in water-scarce regions. The current research proposes a hybrid multi effect distillation and thermal vapor compression (MED-TVC) and double reverse osmosis (RO) system for brackish water desalination for the Jordanian arid and semi-arid regions. In this regard, ten effects MED system was coupled with two permeate and retentate reprocessing designs of RO processes to desalinate brackish water. To carry out this proposal, an accurate model for the hybrid system developed by the same authors for seawater desalination has been used to conduct process simulation. The simulation introduces the main performance indicators including the fresh water productivity, fresh water salinity, specific energy consumption, and disposed brine flow rate for a given set of brackish water properties. These indicators are compared against the simulation results of the same hybrid system for seawater desalination to evaluate the operational, economic, and environmental perspectives of brackish water desalination via the proposed hybrid system. The results show the successfulness of producing fresh water from brackish water at a superior productivity and reduced specific energy consumption with a corresponding lower disposed brine flow rate into the environment compared to seawater desalination.

Keywords: Brackish Water Desalination; Multi Effect Distillation; Reverse Osmosis; Productivity; Specific Energy Consumption; Disposed Brine Flow Rate.

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Computational intelligence applied to the mathematical modeling of enzymatic syntheses of biosurfactants

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Abstract

Enzymatic esterification reactions of fatty acids with sugars generate non-ionic biosurfactants widely used in food, pharmaceutical and cosmetic industries, because of their high capacity to reduce surface and interfacial tensions. In turn, mathematical modeling can be a useful tool, in its different approaches, for the simulation and optimization of enzymatic processes. Particularly, neural and fuzzy approaches are still scarcely evaluated for data of producing sugar fatty acid esters. Thus, this study aimed at using these approaches to model data of enzymatic esterification of fatty acids (oleic and lauric acids) with xylose, catalyzed by immobilized lipase B from *Candida antarctica* (CALB-IM-T2-350) and CALB immobilized on silica magnetic microparticles (SMMPs) modified with octyl groups (CALB-SMMP-octyl) or octyl+glutaraldehyde moieties (CALB-SMMP-octyl-glu). Using Matlab Neural Network Toolbox, five artificial neural networks (ANNs) were trained to predict the reaction rate, one for each type of biocatalyst and acid, obtaining R-squared values greater than 0.97. Furthermore, as an additional effort in neural modeling, two new ANNs were fitted (for two of the biocatalysts), each one of them incorporating, in its inputs, an option referring to the type of acid. R-squared values above 0.98 indicated good predictive capability. To carry out the modeling study by fuzzy inference systems, the Neuro Fuzzy Designer tool from ANFIS (Adaptive Network-Based Fuzzy Inference System) of Matlab was used. Fuzzy models were built for each of the three biocatalysts under study (CALB-IM-T2-350, CALB-SMMP-octyl and CALB-SMMP-octyl-glu), considering as input linguistic variables the type of acid, the temperature, the reaction time and the substrates molar ratio, to predict the conversion of the esterification process. Gaussian membership functions and linear output functions were used, in a Takagi-Sugeno's fuzzy approach. The fuzzy systems parameters were fitted by a hybrid parametric optimization method. The results showed that the fuzzy model outputs were very close to the targets, with RMSE (root mean squared error) values below 0.006. Finally, to demonstrate the potential of fuzzy modeling to optimize processes, response surfaces were built for the conversion of xylose as function of different operating conditions. The fuzzy surfaces indicated that higher values of xylose conversion are reached after 45 h of reaction, temperatures above 50°C, and at substrates molar ratio of 1:0.2 (acid:sugar). Thus, the present work presents, in a broad way, the potential of computational intelligence tools in the study of enzymatic production of biosurfactants.

Keywords: biosurfactants, artificial neural networks, fuzzy logic.

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A Practical Guide to Coffee Roaster Modelling

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Abstract

Background

The process of converting the green arabica coffee bean into the cup of coffee one enjoys involves the roasting process, which brings to light an abundance of coffee flavours. The construction, design, and development of roasters and roaster technology alike is something a company located in South Africa, takes pride specialising in. There is a desire for the development of a predictive model which will accurately predict changes in the temperature profile of the coffee beans due to changes in the inputs to the system. The inputs are namely, the LPG flow rate to the burner, the drum rotation speed and the air blower speed. The model will be utilised in manually operated runs to preemptively adjust the inputs in order to shape the desired bean temperature profile, which is strongly correlated to the flavours produced. This paper will focus on the development of a model which generalises well to new sets of input features.

Study Design/Methods

The following paper investigates the modelling techniques applicable to the coffee roasting system based on theoretical first-principles (Schwartzburg, 2002) as well empirical (data-driven) methods such as linear regression, decision trees, random forests and neural networks implemented using the scikit-learn and tensorflow python libraries (G´eron, 2019). Comparison is made between models based on performance metrics such as RMSE on a validation set of input features.

Major Results/Findings

An empirical model provides superior results when compared to the performance of a first-principles model (performance based on RMSE between predictions and true temperatures). The empirical model devised predicts two characteristic portions of the bean temperature profile by accurately predicting the local minimum in measured temperature.

Conclusion

It can be concluded that an empirical model provides superior performance when compared to a first-principles model in predicting the bean temperature profile during coffee roasting. The methods shown can easily be applied to unrelated physical system modelling problems. It is suggested that with the development of an accurate model of the coffee roaster, the use of model based control algorithms such model-predictive control (MPC) be investigated.

Keywords: Coffee roaster, empirical modelling, machine learning, applied modelling

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Modeling and simulation of anoxic-aerobic algal-bacterial photobioreactor for nutrients removal

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Abstract

In recent years, microalgae-bacteria based technologies for wastewater treatment has generated a growing interest in scientific community. The increasing number of microalgae-based applications has contributed for development of new models. Mathematical models contribute to system optimization in terms of operation and control. Recently, the design and improvement of facilities for optimization of algae biomass yield and an adequate depuration of wastewater has received a great attention. In Alcántara et al. (2015), the operation of an innovative anoxic–aerobic algal–bacteria photobioreactor configuration with biomass recycling was proposed in order to promote nitrogen removal via denitrification. The goal of this work is modeling and simulation for first time the anoxic-aerobic algal-bacteria photobiorreactor for wastewater treatment proposed in Alcántara et al. (2015).

Process model and simulation has develop in dynamic simulation software PROOSIS®. The model was set-up and calibrated with data from a pilot plant treating synthetic wastewater, located in facilities of University of Valladolid. Data from different operating conditions were recorded. Parameter estimation via dynamic optimization in both reactors and settler is realized in order to fit model outputs to experimental data. Model validation is performed via simulation, comparing model outputs and experimental data.

The model proved to be effective in reproducing dynamic behavior of different measured variables. Model simulations have shown the capability of mathematical model to predict the removal efficiency of nutrients from wastewater. Removal efficiencies simulated are closely with experimental results ones. Removal efficiency for total suspended solids is over 95% for experimental and simulation results.

The model allows estimating the removal efficiency of nitrogen and carbon in this plant. Model application will allow, trough simulation, to predict the nutrient removal efficiency of this configuration, improve nutrient removal efficiency with other operating conditions, and significantly reduce the time spent on experimentation.

Keywords: Modeling, Optimization, Simulation, Wastewater treatment.

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Gaussian-Process based inference of electrolyte decomposition reaction networks in Li-ion battery failure

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Abstract

The electrification of the economy is essential for the reduction of carbon emissions to help mitigate climate change. The use of Li-ion batteries (LIBs) in EVs and stationary battery energy storage is helping to achieve this goal. LIBs have the benefits of high energy density and low cost, but they come with the risk of thermal runaway (TR). TR is a process in which a LIB decomposes exothermically, which can lead to fire and explosion.

Improving our understanding of TR is key to improving LIB safety. To achieve this, we aim to develop a more detailed model of LIB TR. Within this, we first develop a detailed reaction network (RN) of the theoretically possible reactions. Second, we make use of machine learning for robust parameter optimization of the complex RN.

Classical TR models consider four Arrhenius equations associated with the decomposition of battery materials. This oversimplification often leads to inaccuracies when compared to experiments. To build up a more realistic representation of the RN, we present a case study on the ethylene carbonate (EC) solvent component of the LIB electrolyte. We use a RN identified from literature for EC that contains 14 sub-reactions and corresponding activation energies. We aim to optimize the RN against experimental data to determine the frequency factors, and statistically most likely reaction pathway.

Obtaining the frequency factors for a large RN with a large variation in parameter magnitudes is made possible by using Gaussian Processes (GPs), a machine learning framework which encapsulates the systems behavior in a surrogate model. Training data is created by sampling the desired parameter space using Latin Hypercube sampling of the RN's full order model. The GP is cross validated ensuring it can accurately predict the experimental results given all the activation energies when compared to the RN. The GP is scrutinized by comparing its predictions to experimental data using a probabilistic error metric. Then, a robust parameter optimization is performed and the frequency factors which produce GP predictions closest to the experimental data are computed. This work provides a better understanding of this RN and provides a methodology that can be scaled to larger networks to aid development of more accurate LIB TR models.

Keywords: Thermal runaway, Gaussian Process, Li-ion battery, Reaction network analysis, Robust optimization

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Energy evaluation of processes for the production of hydrogen from biomass biodigestion under Aspen Plus

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Abstract

The energy sector is currently facing several major challenges, such as the increase in global energy demand and the acceleration of global warming, to which greenhouse gas emissions from the energy sector and transportation contribute significantly. Biomass, because of its abundance and CO2 neutral impact, appears to be an interesting alternative to fossil fuels, particularly oil. The production of hydrogen from renewable sources, in particular from biomass, stimulates the curiosity of researchers. In this work, different processes of hydrogen from biomass by anaerobic digestion were simulated and optimized under Aspen Plus software. The literature investigation allowed the identification of the different processes shown in figure 1. A mathematical approach for modelling the biodigestion based on a detailed kinetic system that represents the complex enzymatic reactions (Angelidaki et al., 1999). This predictive model can estimate the potential of methane produced from the different feedstock. Methane and monoxide conversion processes have been simulated using Gibbs energy optimization.

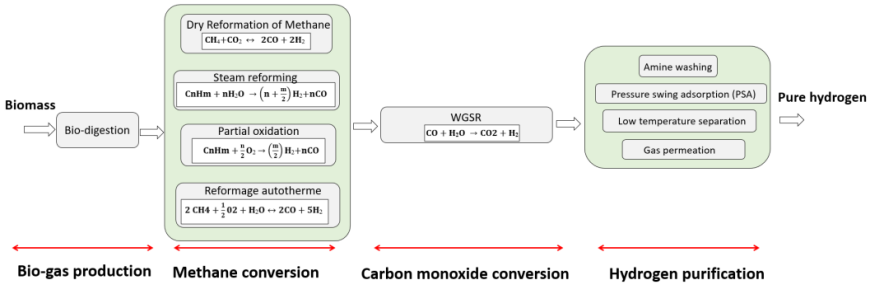

Figure 1: Combination of different processes for hydrogen production of from biomass

The results of the modelling show that the energy requested for the production of 1kg of pure hydrogen, varies considerably from one process to another. In some cases, the energy required can be six times greater than in others. All simulations have been validated with experimental results from the literature.

Keywords: Hydrogen, kinetic model, process simulation

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Development of dual loop organic Rankine cycles for high-temperature heating sources: Process simulation and analysis

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Abstract

The world energy demand has been increasing due to the growing population and industrialization. With the growing energy demand, the methods to generate power have been investigated thoroughly by academic researchers (Anastasovski et al., 2020). One of the potential methods to generate power is the organic Rankine cycle (ORC). The ORC utilizes heat to generate power through the turbine. This heat can be waste heat which is typically disregarded without utilization. The source of waste heat can vary from low to high-temperature waste industrial streams. In an ORC system, this waste heat is recovered by exchanging heat with working fluid (WF). This WF at high pressure and temperature is passed through a turbine to generate power. After power generation, WF is cooled, condensed, and then pumped to increase pressure. The WF is recycled back to complete the system loop. The parameters of the ORC system are opted based on the waste heat source and type, WF type, and mode of heat exchange. The most conventional type of ORC system is single-loop ORC (SORC) system. Several low-to-high temperature waste heat-based single-loop ORC (SORC) systems are operational worldwide, however, improving the plant effectiveness and competitiveness is still challenging especially for high-temperature waste heat sources. The SORC systems lack the potential of fully exploiting this high-temperature waste heat. The dual-loop ORC (DORC) systems can be a potential solution to this challenging problem. The DORC utilizes two loops of WFs integrated with each other to recover waste heat from a single heat source.

In this study, two DORC systems have been investigated, employing Benzene and Toluene as WFs in two separate loops to investigate the potential of utilizing high-temperature waste heat. The heat source considered in this study is biogas combusted flue gases. An intermediate fluid i.e., Therminol VP-1 is opted to exchange heat with biogas combusted flue gases and WFs because of its high thermal capacity, high-temperature stability, low melting temperature, low viscosity, low corrosion, high safety profile, and low environmental impact (Eastman, 2020). The chemical composition of Therminol VP-1 is 26.5% biphenyl and 73.5% diphenyl ether (molar percentages). Based on the process configuration, four cases have been established in this study. Case-1 and 2 are SORC systems employing pure benzene and toluene as WF whereas, case-3 and 4 employ DORC systems using benzene and toluene in separate loops. The difference between case-3 and 4 is self-recuperative and non-self-recuperative configuration. All these four cases are simulated in commercial process simulation software Aspen Hysys® v11. For an efficient and economical heat transfer, the minimum internal temperature approach

(~5℃) was taken as a process constraint (Qyyum et al., 2021). Identical simulation strategy has been adopted to simulate ORC utilizing n-butanol, i-butanol, methylcyclohexane, and toluene in Aspen Hysys (Qyyum et al., 2021). In another study, toluene based ORC system was simulated in Aspen Hysys (Mudasar et al., 2017).

The DORC systems have been analyzed with respect to energy generation and consumption and the results were compared with SORC systems. The net specific energy generation in case-1, 2, 3, and 4 are 322.1, 229.5, 366.2, and 389.3 kW. These results show that case-4 have the highest energy generation i.e., 389.3 kW followed by case-3 (366.2 kW). As compared to case-1, case-3 and case-4 depicted 14 and 21% more net energy generation, respectively. Whereas the case-3 and case-4 showed 60 and 70% more net energy generation compared to case-2. However, it is interesting to note the consumption of WF for ORC systems. The case-3 consumes largest amount of WF flowrate i.e., 9050 kg/h followed by case-4 (8855 kg/h). The specific net energy generation in each case (case-1 to 4) was calculated as 0.048, 0.038, 0.041, and 0.043 kWh/kg, respectively. The case-1 showed highest specific net energy generation followed by case-4. Further from configuration analysis, it is analyzed that the outlet heat source temperature, after heat exchange, is 218.6 ℃ (in case-2) followed by 187.1 ℃ in case-4, respectively. This high outlet temperature showed that there is still a large potential for waste heat recovery. The performances of case-2 and 4 can be further improved if this waste heat is recovered further. In process analyses, the economics of a process plays a vital role. The economics of a process can be analyzed through the area of heat exchanged which is calculated from the values of "UA" provided by Aspen Hysys® v11. High UA means large area and high cost. The values of UA for case-1, 2, 3, and 4 are 230556.9, 297172.1, 264748.5, and 358311.6 kJ/℃-h, respectively. Case-4 shows a high UA value because it utilizes two multistream heat exchangers (HXs) for heat recovery. Case 1 to 3 utilized one HX for heat exchange and amongst them, case-2 showed the largest UA value. In conclusion, amongst all cases, case-1 showed high performance owing to the highest net specific energy generation and lowest UA value. Among case-3 and 4, case 3 showed overall better performance due to low UA value and slightly lower generation i.e., 23 kW than case-4.

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Keywords: Organic Rankine cycle, Biogas, Waste heat, Aspen Hysys, Benzene

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Life cycle optimization of energy systems integrated with carbon capture and utilization

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Abstract

The fossil-based chemical industry should transition towards a low-carbon future aligned with the Paris climate agreement target. Notably, even though the European Union has adopted policies that lowered greenhouse gas emissions, the envisioned carbon neutrality goal by 2050 is still beyond reach. Thus, reducing the chemical sector's footprint could aid in achieving the climate mitigation target, which could be attained by replacing fossil-based resources with renewable carbon. Among the proposed alternatives, carbon dioxide (CO2) capture and utilization (CCU), which requires large amounts of energy often provided by an energy carrier such as hydrogen (H2)–, has received a lot of attention.

In CCU, the optimal design, location, and operation of the Energy System (ES) covering the energy demand strongly affects the performance of the low-carbon chemicals. However, current CCU assessments assume a power technology, e.g., wind or solar, overlooking energy storage and links with the power sector. Notably, CCU chemicals are often economically inferior to their fossil-based counterparts due to their high energy consumption. Furthermore, the variability and availability of renewable power to generate electrolytic H2 (eH2) is a barrier to the successful implementation of CCU. An optimal and cost-effective integrated design of ES-CCU systems, predominantly based on renewables, could help overcome these limitations. The designed ES could aid in coping with the power sources' inherent variability while reducing the CCU costs.

In an ES-CCU system, eH2 used to activate the CO2 could replace its carbon-intensive fossil-based counterpart. Furthermore, CO2 from direct air capture could substantially aid carbon removal –when consuming environmentally benign energy. Here we investigate the design of ES-CCU systems by combining network modeling, process simulation, and techno-economic and life cycle assessment. We develop a Mixed-Integer Linear Programming (MILP) model to design a reliable ES, considering strategic European locations, delivering the energy demand at minimum cost. We further integrate the ES with the production of eH2, CO2, and their transformation to methanol, which could indirectly benefit the sector's downstream applications. In particular, the mass and energy balances are retrieved from process simulations carried out in Aspen Plus V11, whereas raw materials and utility inputs are acquired from the Ecoinvent V3.5 database. Our analysis shows that the ES economic and environmental performance can significantly vary across locations and that an integrated design of the ES-CCU cluster is key to accurately assessing the feasibility and viability of CCU chemicals.

Keywords: Life cycle assessment; CO2 hydrogenation; Energy system optimization; Electrolytic hydrogen; Direct air capture.

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A comparative study of swarm intelligence and artificial neural networks applications in modeling complex reaction processes

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Abstract

To overcome the difficulties of simulating complex processes with unknown reactions and intermediates, this study investigated two artificial intelligence techniques, namely Swarm Intelligence (SI) and Artificial Neural Networks(ANN). The resulting models from ANN and SI were applied to both semi-batch and continuous flow reactors, comparing the model accuracy and applicability. The ANN inputs were concentrations and temperatures, and its outputs were reaction rates, which participated as the generation rates in mole or mass balances. The optimization of ANN hyper-parameters and the procedures to avoid the over-fitting were also performed. For SI, the integrated empirical model was Arrhenius equation and the detailed reaction networks were established initially. Through minimizing normalized mean squared errors of the modeling and experimental outputs, it gave the optimal kinetic parameters for the pre-built reaction networks. The information derived from the semi-batch reactors data by SI and ANN was applied to continuous flow reactors as well to make comparisons of their extrapolation abilities. The ANN-based model obtained the higher accuracy than the SI-based one in semi-batch reactors for the desired concentration predictions. However, the SI-based model was more accurate for temperature approximations in continuous flow reactors. The main reason for this phenomenon is that the training data was generated from semi-batch reactors and did not have the expected 4V's characteristics - Volume, Veracity, Variety and Velocity for the continuous flow reactors. The extrapolation capability of the ANN-based model is limited in a smaller range than the SI-based one. Moreover, the extra data processing was needed before the ANN training. The SI-based model requires more knowledge of the reactions and the primary reaction assumptions played an important role. It can be concluded that the trade-off between data and process knowledge determines the suitable method, which is helpful to develop the accurate and low computational models of complex reaction processes. The ANN-based model is recommended when the data is with the high quality in the applied space, where no deep reaction knowledge was required and computational costs were lower. Otherwise, the SI-based model should be employed, which provides more detailed information of the processes and was constrained by physical meaning parameters.

Keywords: swarm intelligence, artificial neural networks, hybrid models, semi-batch reactors, continuous flow reactors

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Combined optimization of start-up shut down and grade transition of a multistage continuous crystallization process

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Abstract

Over the last decade, continuous manufacturing has gained ground in the pharmaceutical and biopharmaceutical industries. However, and despite the advantages and opportunities commonly associated with this mode of operation, the later introduced a new set of challenges inherent to process dynamics, process and quality control, operating faults, and the lack of real-time measurements and effective optimization strategies. Most importantly, continuous pharmaceutical campaigns are anticipated to exhibit short operating windows. As a result, the impact of the start-up and shutdown on both cost of production and environmental footprint is extremely important. To unleash the full power of continuous manufacturing, it is important to develop agile and flexible plants. This requires the development of effective optimization and control strategies. In this paper, a punctilious and systematic model-based dynamic optimization strategy was developed to address the combined start-up, shut down and grade transition of a multistage combined cooling and antisolvent continuous crystallizer. A combined start-up and shut down optimization was achieved to maximize on-spec production which also corresponds to the maximization of the steady state operating window for a fixed total manufacturing schedule. It was shown that 5858 g of on-spec products can be obtained during an operating window of 800 minutes, which compared to the non-optimized scenario, corresponds to a 10% increase in production. In addition, the optimization of grade transition is also considered to improve the dynamic performance and flexibility of the process which is key in the case of multiproduct continuous manufacturing campaigns, where multiple bespoke pharmaceuticals can be produced on-demand without interruption or the need to restart the plant under new operating conditions. It was proven that a fast transition between two product grades, here product 1 corresponds to the maximum crystal mean size (417 μm) and product 2 corresponds to the minimum coefficient of variation and crystal mean size of 375 μm, can be optimally achieved which minimizes wastes and maximizes process efficiency and flexibility. The combined cooling and antisolvent crystallization of acetylsalicylic acid (ASA) in water and ethanol was used as a case study with a cascade of three MSMPR (mixed-suspension, mixedproduct removal) crystallizers. To address the optimization problem, several dynamic optimization strategies and discretization schemes were considered and compared. The dynamic optimization problems were solved using a hybrid optimization approach which combines a genetic algorithm and a sequential quadratic programming (SQP) method.

Keywords: Dynamic Optimization, MSMPR, Start-Up, Shut Down, Grade Transition

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Systematic dynamic modelling of heat exchanger network

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Abstract

Modelling and simulation are essential tools for the design of heat exchangers and Heat Exchangers Networks (HEN) (Roetzel et al. (2020)). Unfortunately many simulation approaches are based on the steady state model of the HEN. Dynamic performance of HEN has also to be explored in order to improve flexibility and controllability properties of HEN (Yang et al. (2021)). For this purpose, the authors propose a systematic way to compute the finite dimensional dynamic model of the counter current heat exchanger network based on the graph theory. This contribution focuses to the serial interconnection of heat exchanger. The proposed models are build from the elementary block composed of two compartments corresponding to the hot and cold streams. These compartments are separated by a wall without heat accumulation. The method is based on the graphic input-output representation of heat exchanger as shown in figure 1. This figure shows the cascade of two heat exchangers with i and j elementary blocks, resp. The convective input or output fluxes are the arrows of the graph. The heat exchanger block models (with energy accumulation) as well as the connections of input and output fluxes (grey nodes without energy accumulation) are the nodes. There are two graphes since there are the hot and the cold stream. The construction of the model is based on the adjacency matrix of the convective graphes based on the material balance and the energy one. With this method ready for simulation, dynamic models are obtained. One of the main advantage of this approach is its modularity. So it can be used for network retrofitting. Furthermore this modelling method gives structured matrices for which mathematical network analysis can be easily deduced and used for control purposes such as dynamic energy assessement approach. The method can be generalized to parallel interconnections in order to model collectors or distributors. The generecity of the proposed structured dynamical model can be implemented as a computer aided process engineering.

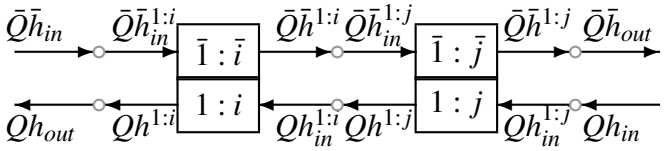

Figure 1: Interconnection of two heat exchangers with enthalpy flows, blocks and connections

Keywords: Heat exchanger network, Dynamic modelling, Graph theory

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Technical and economic assessment of a castor bean biorefinery to produce renewable aviation fuel: a computer-aided design

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Abstract

Due to pandemic, all economic sectors have been severely affected. Particularly, 2020 has been identified as the worst year in aviation history, and now this sector is facing its sustainable economic recovery; to achieve this, one of the alternatives relies on the use of renewable aviation fuel. The aviation biofuel can be generated from several types of biomass through different processing routes. All these routes are technically feasible, but the price of aviation biofuel is still greater than that for its fossil counterpart. In this context, biorefineries are an interesting processing scheme where the financial viability relies in several products; thus, it is a promising alternative to produce renewable aviation fuel.

Therefore, in this work the computer-aided modelling of a biorefinery scheme from castor bean plant to produce biojet fuel is presented. Castor bean plant includes stems, leaves, husk and kernel, and all of them are considered for the processing. The biorefinery scheme is studied in Aspen Plus V.10, including mechanical pressing of kernel, pyrolysis of press cake, gasification, pyrolysis and fermentation of residue (stems and leaves) and finally, transesterification and hydrotreating of vegetable oil. The fermentation stage produces bioethanol as intermediate product, which is the raw material for the alcohol-to-jet process; also, the gasification produces biohydrogen, used as reactive for the hydrotreating process. From this biorefinery scheme, products as biochar, biogases and bio-oil from pyrolysis, biohydrogen, bioethanol, biodiesel, light-gases, naphtha, green diesel and biojet fuel are obtained. The assessment of the biorefinery scheme involves the estimation of economic, environmental and energetic indicators. The economic indicators include the estimation of total annual cost (TAC) and the net gross profit of the products obtained; whilst as environmental indicator the counting of CO_2 emissions from electricity and steam requirements is considered. Finally, as energetic indicator the total energy invested in the processing and the total energy delivered by the products are compared. According to results, the main factors affecting the TAC are the steam requirements (48.6 %) and the raw material cost (22.5 %); while the biojet fuel represents 35.4 % of the net gross profit. Also, in this scheme are generated 4.97 ton CO_2 per kg of products obtained. Finally, 5.49 kW are invested per kW of energy delivered by the products. This biorefinery scheme can be improved by process intensification to further reduce the energy consumption.

Keywords: biorefinery scheme, castor bean plant, biojet fuel, computer-aided design.

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SiCN fibers as advanced materials for electromagnetic shielding in X-band: experiments and computational modelling and simulation

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Abstract

Materials prepared via the polymer-derived ceramic route have been increasingly studied for protection against electromagnetic energy to mitigate electromagnetic interference. Both experimental and computational evaluations of electrospun SiCN fibers applied to electromagnetic shielding are not yet reported in the literature. This work aims to evaluate the electromagnetic properties of SiCN electrospun fibers by experiments and computational modelling and simulation. Polysilazane and polyacrylonitrile were used respectively as the ceramic precursor and spinning aid. After electrospinning, the fibers were pyrolyzed at 1000 °C. The samples were named SiCN_0, SiCN_40, and SiCN_70 respectively for 0, 40, and 70 wt.% polyacrylonitrile. The scattering parameters, impedances, and reflection losses were collected under X-band (8.2-12.4 GHz) in a vector network analyzer employing the waveguide propagation setup. The experimental scattering parameters were converted through the Nicolson-Ross-Weir method together with the shielding effectiveness and numerical electromagnetic computational studies. Simulations of scattering parameters were performed, and introductory electromagnetic scattering calculations in free space were computed including the Radar Cross-Section (RCS) study. The relative complex electrical permittivity was approximately 3, 4.5, and 4 (real part) and 0.05, 0.22, and 0.1 (imaginary part) respectively for SiCN_0, SiCN_40, and SiCN_70. The SiCN_40 could experimentally store and lose more electromagnetic energy in the material, exhibiting a minimum reflection coefficient of -1.4 dB at 12.4 GHz. The computational simulation corroborated the better performance of SiCN_40 in reflection loss as well as in other electromagnetic spectral responses. Additionally, correlations between electromagnetic properties extracted from experiments and computational results from the RCS study were observed. The free space electromagnetic scattering of SiCN_40 showed better features when compared to the other samples. Owing to the microstructure and product design, SiCN_40 fibers demonstrated satisfying electromagnetic shielding properties in X-band. The computational experiments showed to be a new modelling and simulation approach to evaluate the electromagnetic properties of electrospun SiCN fibers. Further research will focus on material optimization and computational evaluation.

Keywords: complex permittivity, polymer-derived ceramic, radar cross-section, reflection loss, shielding effectiveness.

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Continuous-Time Surrogate Models for Data-Driven Dynamic Optimization

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Abstract

This work addresses the control optimization of time-varying systems without the full discretization of the underlying high-fidelity models and derives optimal control trajectories using surrogate modeling and data-driven optimization. Time-varying systems are ubiquitous in the chemical process industry and their systematic control is essential for ensuring each system to be operated in the desired settings. A vast number of techniques rely on approximations that utilize uniform and nonuniform discretization, leading to the solution of large-scale linear, nonlinear, or linearized problems. Yet, such problems are solely addressed using calculus of variations due to the inherent complexity of the approach and its applicability is commonly limited to linear ODE systems. For highly nonlinear problems, linear control schemes are often insufficient to portray an appropriate nonlinear control strategy for a given nonlinear process. In such cases, the full discretization of the time-varying problem is preferred to take a manipulated action at each discrete time point, which is computationally prohibitive. To overcome the stated challenges, we postulate nonlinear continuous-time control action trajectories using time-varying surrogate models and derive the parameters of these functional forms using data-driven optimization. Data-driven optimization allows us to collect data from the high-fidelity model without pursuing any discretization and fine-tune candidate control trajectories based on the retrieved input-output information from the nonlinear system. To this end, we test exponential and polynomial surrogate forms for the control trajectories and explore various data-driven optimization strategies (local vs. global and sample-based vs. model-based) to test the consistency of each approach for controlling dynamic systems. Path constraints are also considered in the formulation and handled as grey-box constraints. The applicability of our approach is demonstrated on a motivating example and a CSTR control case study with favorable results.

Keywords: Data-driven optimization, dynamic optimization, time-varying systems, optimal control, surrogate modeling

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Parameter estimation in dynamic metabolic models applying a surrogate approximation.

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Abstract

Dynamic Flux Balance Analysis (dFBA) models are widely applied in the system biology field. The model connects the cellular genome information to the cell's phenotype, therefore it can be applied to predict the effect of gene deletions or the inserting of new enzymes into the metabolic network. The dFBA model consists of a system of differential equations and an optimization problem that is performed to compute the internal flux distribution. Furthermore, kinetic equations (i.e. Michaelis-Menten) are used in order to model the uptake of substrates. The kinetic equations have some parameters that must be estimated from batch fermentation experimental data. When the dFBA model is inserted in a parameter estimation architecture, a bi-level optimization problem arises. As it is well know, bi-level optimization problems are hard to solve and suffer from convergence problems. A recent method to replace the dFBA optimization with a surrogate model was developed in our research group and applied to the simulation of a model predictive control of a bioreactor. Here, the recently developed surrogate dFBA model is applied to a parameter estimation problem. The approach was tested in a case study of a modified *Saccharomyces cerevisiae* that can use glucose and xylose as substrates. *S. cerevisiae* is the main microorganism for industrial alcoholic fermentation and research efforts have been applied in order to widen the range of substrates that can be used, such as xylose. dFBA models can be useful to propose genetic modification targets to improve yield and productivity. In order to achieve this aim, the kinetic parameters in the dFBA model must be well defined. Batch experiments using different mixtures of glucose and xylose on anaerobiosis were performed. First, the surrogate model was trained using Flux Balance Analysis simulations of the Yeast 8.3 genome-scale model. Thereafter, the kinetic parameters of the surrogate dFBA were fitted to the Batch experimental data. The surrogate dFBA allowed the parameters to be estimated in a single-level optimization problem. Furthermore, the sensitivities of the biomass and extracellular metabolites with respect to the parameters could also be computed. The analysis presented correlations among the parameter sensitivities, denoting that the parameters cannot be estimated uniquely, but just a combination of them. Also, the optimal time for the acquisition of data in experiments, could be deduced from the sensitivity analysis. The results indicate that the surrogate dFBA is an important tool for the parameter estimation and optimal design of experiments of dynamic metabolic models.

Keywords: Parameter estimation, Surrogate model, dFBA, Systems Biology, Metabolic Engineering

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A Benchmark Model to Generate Batch Process Data for Machine Learning Testing and Comparison

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Abstract

During production, batch processes generate batch data and time series values. The former contains start and end dates of the archived Manufacturing Execution System or Batch Control System procedures. Furthermore, attributes such as quality-related measurements may be stored in connection with a batch identification number. On the other hand, time series values are generated by sensors and controllers that implicitly contain information about delays, variability, start and end-points of the production (B¨ahner and Huusom, 2019). Even though it might not be contained in the aggregate batch data, time series values are valuable to build process models to support decision-making in planning and scheduling.

Due to the inherent repetitiveness of batch processes which are based on standardized recipes, there are reproducible behaviors among the data. For that reason, Machine Learning (ML) algorithms have been exploited for data analytics for batch processes. However, the practical use of these techniques is complicated by data noise, scarcity of quality data to train the algorithm, or process disturbances. In addition, the performance of an ML algorithm can be case-specific, complicating further the selection and tailoring of learning systems for a given setup.

This work presents a benchmark model of a batch process to generate data where active challenges, disturbances, and data noise are fully controlled. The process is viewed at the unit level following a single-path structure with filling, processing, draining, and cleaning operations. It is also considered that the vessel has three liquid and one solid raw material whose loads are valvecontrolled, and it is served by cooling water and medium pressure steam utilities. The simulation is limited to mass balances with chemical reactions and kinetics omitted since they are not relevant for the intended application of ML. Finally, scenarios were generated where up to 21 disturbances of different types, causes, or fault origins are injected (isolated or combined) in the simulated data for testing. The scenarios were grouped into six benchmark cycles (A-F) with increasing levels of complexity in terms of intensity and nature of nuisance in the data tackling some challenges for the application of ML methods.

Keywords: Batch Process, Machine Learning, Process Modeling, Data Generation, Hybrid Dynamic Simulation

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Global warming impact of electric city buses in Chile: Critical stages of their fabrication and use

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Abstract

The government of Chile has pledged that 100% of the city buses fleet will be powered by electricity by 2040 (Ministerio de Transporte, Gobierno de Chile, 2020). Since the fabrication processes of electric vehicles and electricity generation are not emissions-free, process analysis appears as a valuable tool to quantify their implications towards the optimization of the industrial processes in terms of better use of resources and recycling (Nordelöf, 2014). This work aims to quantify the greenhouse gas emissions and identify critical stages in the fabrication and use of electric and diesel city buses in Chile by simulation of: (i) metallurgical processes (aluminium, copper, and iron), (ii) thermoelectric power plants, and (iii) diesel production plants, which environmental impacts have been identified as critical in previous life cycle assessment studies (Nordelöf, 2014, 2019).

A total of ca. 617.5 kg of aluminium, 187.1 kg of copper, and 11 539 kg (10 622 kg) of iron are required for the fabrication of an electric bus (conventional bus). The results indicate that 2.5 kg $CO_{2,eq}$ (kg aluminium)$^{-1}$, 3.9 kg $CO_{2,eq}$ (kg copper)$^{-1}$, and 2.9 kg $CO_{2,eq}$ (kg iron)$^{-1}$ are generated, with the major contribution to emissions coming from the Bayer process, the Hall-Héroult process, the copper flotation and smelting processes, and the iron blast furnace. A natural gas power plant in Chile produces ca. 0.8 kg $CO_{2,eq}$ kWh^{-1}, which corresponds to ca. 0.8 kg $CO_{2,eq}$ km^{-1} for electric buses (energy grid: 48% thermoelectric power plants, 14% solar PV, 11% wind turbines, and 27% hydropower plants) (Comisión Nacional de Energía, Gobierno de Chile, 2020). The processing of crude oil in the United States (main supplier of diesel in Chile) produces ca. 1.5 t $CO_{2,eq}$ d^{-1}, corresponding to ca. 0.2 kg $CO_{2,eq}$ km^{-1} for conventional buses.

The analysis suggests the need of developing new metallurgical processes, replacing materials, and/or recycling strategies for the fabrication and use of electric city buses.

Keywords: city buses, metallurgical processes, electricity generation, diesel

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Optimization for sustainable hydrogen production path

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Abstract

There is a global burden to find sustainable ways to reduce greenhouse gases (GHG) emissions while meeting increasing energy demand. Hydrogen, a multipurpose energy carrier with application in various industrial and chemical processes has been identified as a key player in achieving this. There are several ways to produce hydrogen, however, 95% commercial hydrogen is produced via steam methane reforming (SMR) which emits CO_x as by-product making it environmentally unfriendly. Although carbon capture sequestration (CCS) can be applied, only about 90% CO_2 capture has been reported in the literature. Contrarily, burgeoning water electrolysis technology enables zero GHG emission depending on the source of energy applied. Nevertheless, with high cost of the emerging renewable energy as well as competing applications, electrolysis would need the support of fossil fuel to compete with SMR since it is highly energy intensive, consequently defeating the zero emission goal. This is why Methane pyrolysis (MP) is gaining much research attention. Methane pyrolysis is the thermal decomposition of methane (TDM) to produce hydrogen and solid carbon. In this study, the different TDM technologies are explored to develop an optimization model that considers energy efficiency, CO_2 emission and water consumption in production of hydrogen at a minimum cost on selecting a sustainable MP path that is comparable to prevalent technologies– SMR with and without CCS as well as water electrolysis- for further research. A MINLP optimization model for selecting a sustainable pathway to produce hydrogen in commercial quantity is formulated using associated data from the literature with respect to the different technologies considered. Sensitivity analysis is also performed to analyse the impact of the by-products produced from each technology. The model is implemented in GAMS. The findings from this work reveal an optimal production pathway for sustainable hydrogen production based on the process performance index considered. It also shows that the quality of carbon could greatly influence the commercialization of MP. Moreover, MP is flexible and can attain carbon-neutrality depending on the feedstock and energy source. With the supposition that MP low to zero CO_2 emissions and valuable solid carbon product features makes it sustainable, this study proposes a pointer to the optimal TDM technology that should be explored to compete with the current technology to meet hydrogen demand, and precedes a process simulation that explores the kinetics and thermodynamics for optimization.

Keywords: Methane pyrolysis, Hydrogen production, Thermal Methane Decomposition, Mixed integer nonlinear programing, Carbon.

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Model development of lactic acid evaporation process with multi effect evaporator and mechanical vaper recompression system

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Abstract

Lactic acid (LA) is a raw material for poly lactic acid (PLA) which used in food, pharmaceuticals, textiles, and various chemical industries. Evaporation process is essential to produce high purity LA after fermentation process. However, since the large amount of energy consumption is required in evaporation process, which accounts for about 50% of the total production cost, it is necessary to improve the energy efficiency of the evaporation process. Here, this work developed process using a Multi-effect evaporator (MEE) and a Mechanical vapor recompression (MVR) system to improve the energy efficiency of the LA evaporation process. The suggested process model with MEE reduced the steam consumption recovering the latent heat of secondary vapor and the steam and condensate from the final evaporator. Process model with MVR substituted the steam consumed in the evaporation with electricity by recompressing the vapor exiting the evaporator through a compressor. Through the simulation results, the energy efficiency was compared by analysing the consumption of steam, electricity and latent heat recovered from the secondary vapor. As a results, the steam consumption decrease from 99.381 to 37.913 ton/h according to increase of number of effects (1-8) and the electricity consumption of MVR is 11,115 kW.

Keywords: Evaporation process, Multi-effect evaporator, Mechanical vapor recompression, Process modeling

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Optimization-Based Framework for Robust Modeling and Design of Kinetic Systems

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Abstract

To understand the mechanism of a catalytic system, computational analysis is essential. Once a potential reaction mechanism has been identified, it typically involves (a) evaluating the energetics for the species and transition states using a computational chemistry method such as density functional theory (DFT), (b) relating these microscopic properties to macroscopic quantities such as reaction time. Microkinetic models may not match experimental data due to (1) inaccuracies in the energetic estimation, (2) inadequate catalyst models that are not representative of the surface environment. As a result of using experimental data, a more accurate model may be developed. If the model-experiment mismatch is resolved, a microkinetic model solution compatible with DFT assumptions may be identified. This work presents a generic optimization framework for solving parameter estimation and catalyst design problems in catalysis. Using a stochastic optimization method, Differential Evolution with Tabu List in conjunction with Aspen Plus, and considering experimental data, various activation energy and kinetic constants values were predicted. The sequential approach is a traditional approach to solving parameter estimation problems. Issues with the stiffness of the microkinetic model and the optimizer's capacity to tackle such highly nonlinear systems are common challenges. This proposal has the potential to use all the reactor models present in Aspen Plus, as well as being able to use all the kinetic models and solvers, avoiding numerical difficulty in optimization solution. This method has a number of advantages, including ease of implementation, which leads to physically realizable steady state solutions, and a reduced overall optimization problem in terms of the number of variables involved.
Initially, a dimerization reaction of isobutylene produced by the dehydration of 2-methylpropan-2-ol was considered. Since this reaction has been extensively studied, experimental data are available to validate the kinetic data obtained by the optimization process. Subsequently, this same technique is used to adequately predict two reactions of high interest: (i) the ethylene oligomerization and ii) the hydrogenation of long-chain alkenes for the production of linear hydrocarbons. The interest of these reactions is particularly because of the complexity associated with multiple reactions co-occurring and the direct application of this reactive process in producing jet fuel from ethanol. As a result of the proposed framework, it is possible to (a) compare and contrast competing dominant chemistries, (b) propose target energetics to maximize the desired performance of a catalyst. Additionally, the kinetic data associated with isobutylene dimerization and the oligomerization and hydrogenation reactions were adequately predicted, reducing the error between the experimental data and the data obtained by the simulation to less than 1%.

Keywords: optimization, kinetic data prediction, oligomerization, hydrogenation, biojet fuel.

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Hydrogen liquefaction process assisted by regasification of liquefied natural gas

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Abstract

Hydrogen is considered the fuel of the future and can change the energy share dynamics (Ayub et al., 2021); however, its low volumetric energy density questions its ability to challenge other energy storage system candidates. Like liquefied natural gas (LNG), liquid hydrogen is also considered a means for storage and transportation over longer distances, especially intercontinental transport. Hydrogen liquefaction is highly energy-intensive, equivalent to 25-35% of its heating value. Specific energy consumption (SEC) is believed as the performance gauging criteria for liquefaction processes. The minimum or ideal liquefaction load for a feed gas operating at 25 bar is approximately 2.7 kWh/kg_{LH2} (Stolzenburg et al., 2013), whereas the commercial plants operate at SEC in the range of 12.5–15.0 kWh/kg_{LH2} (Yin and Ju, 2020).

The boiling point of liquid hydrogen is –253 °C; helium is the only component with a boiling point lower than hydrogen. Such low temperatures require a tremendous amount of energy, approx. 20% of which is contributed by the interconversion of the spin isomers of hydrogen (Stetson et al., 2016). Normal hydrogen consists of 75% ortho-hydrogen and 25% para-hydrogen at ambient conditions. Para-hydrogen is the stable form at and near the normal boiling point of hydrogen. From the storage and transportation point of view, para-hydrogen is preferable because of the exothermic nature of the ortho-para conversion reaction.

Several liquefaction techniques, cycles, and refrigerants have been proposed over the past decades. Commercially, liquid nitrogen is used as a refrigerant in the precooling cycle, reducing the temperature to –193 °C. Recently, mixed refrigerants (MR), consisting of hydrocarbons, nitrogen, hydrogen, helium, and neon, have been studied with promising results (Qyyum et al., 2021). LNG is a relatively less explored option, whose invaluable cold energy is usually lost to seawater. Faramarzi et al. (Faramarzi et al., 2021) utilized cold energy from LNG regasification to supplement MR in the precooling cycle of an already published scheme. The SEC of the proposed process is 8.85 kWh/kg_{LH2}. In our earlier contribution (Riaz et al., 2021), LNG alone was used as a refrigerant in the precooling cycle. The SEC of that process was 7.64 kWh/kg_{LH2}; however, the required flow of LNG was relatively high. Therefore, a new configuration was developed and is presented here. The preliminary results are compared with the aforementioned studies considered as base cases.

The present study proposes a simple yet efficient and cost-effective integrated scheme wherein LNG's cold energy is utilized in the precooling stage alongside the existing mixed refrigerant (MR) cycle. The three-stage and cycles-based mixed fluid cascade configuration was used (Riaz et al., 2021). LNG was used as a supplement to the precooling MR cycle. The objective is to reduce the SEC and make a case for the

commercial acceptability of the process. For this purpose, the well-known commercial simulator Aspen HYSYS® v12.1 is used for the design and performance analysis. Refprop is used for ortho- and para-hydrogen, while PengRobinson is used for all other components. Aspen's built-in Mixed type optimizer optimized refrigerant flow rates, cycle suction and discharge pressures, and LNG flow rate to minimize SEC while meeting the minimum approach temperature constraint (1–2 °C). It was found that the overall refrigerant requirement has actually decreased by 21% compared to the base case (considering LNG flow as refrigerant). The SEC for the process is 7.7 kWh/kg, nearly 50% of the commercial hydrogen liquefiers. This value is slightly higher than our previous results but better than (Faramarzi et al., 2021). However, it is worth noting that the refrigerant requirement is much lower in the present study. An external optimizer may further improve the process variables and even reduce the SEC.
The potential benefits of the proposed integration are far-reaching. Further detailed thermodynamic analysis and economic impact assessment shall reveal its true potential.
Keywords: liquified natural gas, regasification, hydrogen liquefaction, hydrogen energy network, hydrogen economy.

Acknowledgments

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Optimal control system for products quality from a deethanizer column

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Abstract

Although the deethanizer process is very well known, the automatic control systems have a strong development and diversification. The research undertaken by the authors to develop an automatic system for products quality optimal control in an industrial column is included in this direction. The novelty of the research is the control structure, the objective function associated with the automatic system, the performance testing of the automatic system using the resources of the Unisim Design simulator.
The research starting point was an industrial natural gas processing plant, Halafawi et al. (2020). From this, the authors studied and developed an advanced control structure for the demethanizer column within the previously mentioned plant, Patrascioiu et al. (2021). The second column of the plant, the deethanizer column, raised many research problems, such as: adaptation of the pressure control system in order to use the Unisim Design simulator; process sensitivity analysis on disturbances/control agents - quality of separated products channels; elaboration of an objective function for the optimal control system; identification of the dynamic models associated with input-output channels; design of the dynamic simulator and tuning the PI controllers; validation through dynamic simulation of the proposed control structure. The resources used in the research were: constructive data of the industrial plant; literature data; Unisim Design simulator.
So far, the obtained results include: the elaboration of an equivalent structure of the deethanizer column and its simulation; elaboration and validation of the objective function associated with the column; design of the automatic system and its validation through dynamic simulation. The performance indicators used in the research were: meeting the products quality requirements in the conditions of column disturbances evolutions; minimizing the objective function associated with the column operation; achieving short response times and reduced steady-state and dynamic deviations.
The research carried out by the authors led to the development of an optimal control structure for the quality of the separated products in the deethanizer column. Steady-state and dynamic simulations validated the objective function and the proposed automation solution. The limitations of the structure elaborated by the authors were generated by the lack of industrial operation data and by the complexity of the industrial plant. Under these conditions, some of the elements developed in the research can only be theoretical. Future access to industrial operating data may lead to industrially applicable control structures.

Keywords: deethanizer column, optimal control, product quality, simulation.

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CFD model-based scale-up of a γ-valerolactone reactor

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Abstract

γ-valerolactone (GVL) is a promising new platform molecule used nowadays, mainly in the perfume industry. However, it also has excellent potential to be used as a green fuel. GVL can be produced by the catalytic hydrogenation of Alkyl levulinates (AL) and Levulinic Acids (LA), then the subsequent cyclization of hydroxyl alkyl levulinates. The feedstock can be various types of biomass since GVL can be produced from two of the main components of lignocellulosic biomass (cellulose, hemicellulose). Our study focuses on the modelling and simulation of a GVL production system. The reactions occur in a 300 ml laboratory-scale batch operated Parr reactor equipped with a gas entrainment impeller. The reactor's full 3D simulator, including a gas entrainment impeller, was created. The laboratory-scale model was used as a base point for the scale-up calculation. The CFD model of a pilot-size reactor was also implemented (300 L), and scale-up calculations were completed to achieve similar mixing conditions to the laboratory scale. GVL also served as a solvent, and 5% Ruthenium on activated carbon was used as a catalyst, extended using Amberlite IR120 for cyclization. The second reaction was used to test the scale-up calculation. The density of 1000 kg/m3 and dynamic viscosity of 2 mPas was used as material parameters. The primary aim of this work is to validate the scale-up of the laboratory GVL production reactor based on the velocity field calculated by the CFD simulations. This step is a necessary contribution to the industrial application of the process. The COMSOL Multiphysics turbulent k-ε model was used in a rotating reference frame to calculate the momentum balance. A time-dependent calculation was performed. The kinetic model was implemented from [1]. The non-catalytic step was used as a reference reaction to compare the two scales. The equation for calculating the impeller speed was: . Where D refers to the diameter of the impeller and n of the rotational speed (rpm – rotation/minute), 1 to the laboratory scale and 2 to the pilot scale. This equation is widely used in the scale-up of the devices with a centrifugal force field. The mixing between the two scales was compared using averaged velocity magnitudes and 1000 grid points from the whole reactor. The difference from the global average was plotted as a histogram to visualize the results. Figure 1 shows the results of the CFD model a) the average velocity field, a) in the case of the laboratory, b) in the case of the pilot scale c) the comparison of the average velocity histograms. The velocity fields look reasonably similar. However, let us take a closer look at the histograms of the velocity field. Quantity means the number 2 of node points for each

velocity interval. Some differences between the laboratory and pilot-scale can be seen. However, the difference is not significant, so it can be presumed that the operation of the vessel of the larger scale will be similar too. The next step can be implementing the whole reaction system and conducting a more detailed comparison of the two scales.

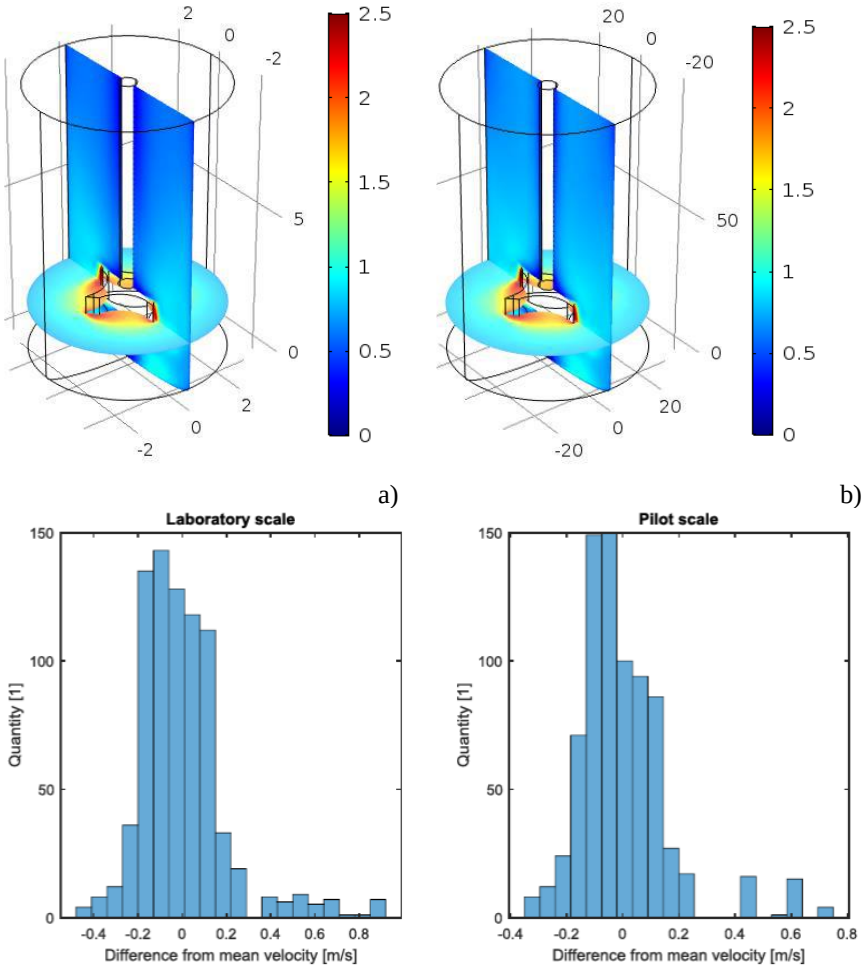

Figure 1 the results of the CFD simulation a) velocity field in case of the laboratory-scale device in m/s b) velocity field in case of the pilot-scale device c) comparison of the velocity histograms in case of the two scales.

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Comparison of droplet averaging method in pharmaceutical spray drying models

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Abstract

Spray dryers are an important unit operation in pharmaceutical manufacturing. In recent years, interest has grown in the formulation of powdered solid protein-based pharmaceuticals, because on the liquid form they have stringent storage temperature requirements and limited shelf life, which solid formulations aim to improve. Spray drying is one of the best candidates because of low energy requirements and good scale-up possibilities compared to similar technologies.

In modeling of spray dryers, the drying model is at the core, allowing the prediction of drying rates. Several drying models are reported in the spray drying literature, they differ in how they depict the falling rate of solvent evaporation: in the characteristic drying curve (CDC) approach, an empirical function is used to the limit the drying rate as a solid crust is formed; in the reaction engineering approach (REA), an empirical activation energy is used; and in more detailed models the droplet internal profiles, crust formation and porosity, are modeled. The latter type of model does not require empirical parameters but due to inclusion of properties that are difficult to measure they still require empirical input. In addition, when drying models are to be used in the design or in the scaling up of spray dryers, they must be implemented in one of two ways: either the average droplet-particle size is used, mostly the Sauter mean diameter (d32), or a discretization of the droplet-particle size distribution is used, in which case the average of the properties across droplet sizes is required to relate to experimental measurements. All the drying models and the averaging methods mentioned have been applied in pharmaceutical research applications with good success, but without comparison under the same conditions and considerations.

Here we compare the CDC and REA approaches and both averaging methods in terms of predictive power for the drying of a monoclonal antibody previously studied by Gikanga et al. (2015). We fit and validate the models to the operation conditions and resulting quality attributes reported in their work with a laboratory and a pilot scale spray dryers. The effect of model choice on the prediction of particle size, residual moisture, and degree of degradation is discussed. Recommendations regarding the choice of the model are presented for design and scale up applications, implications on others such as dryer optimization, soft sensing, and predictive control are also briefly discussed.

Keywords: Spray drying, droplet drying, drying model

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Process modelling of Direct Air Capture (DAC) of CO_2 using solid amine sorbents

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Abstract

This paper presents a fixed bed reactor system to capture CO_2 from ambient air via Temperature Swing Adsorption (TSA). The idea of CO_2 capture from ambient air, also referred to as Direct Air Capture (DAC), was first suggested by Lackner and coauthors in 1999 to mitigate climate change. CO_2 adsorption processes are often considered as the most suitable option for DAC and many laboratory and pilot scaled units have been developed over the last decade. In particular, there are 15 operational DAC plants globally capturing more than 9000 tCO_2/year (IEA, 2020). Some of the industrial pioneers are Climeworks (Switzerland) and Global Thermostat (USA) where solid sorbents are used to capture CO_2 while Carbon Engineering (Canada) has developed a liquid solvent DAC system. Also, some examples of active academia are Twente University and ETH Zurich where DAC systems with amine solid sorbents are studied while Arizona State University is developing Moisture Swing Adsorption (MSA). However, there is currently a scarcity of literature on simulation studies of adsorption processes in DAC context. Therefore, a model describing CO_2 mixture flow, mass and heat transfer with adsorption isotherm model is developed in Aspen Adsorption environment to study the performance of DAC processes with TSA. In the first part, a single adsorption column with the Lewatit VP OC 1065 (amine solid sorbent) is simulated to study both adsorption and desorption steps, and the model is validated with the literature results. Then, a full DAC model with TSA cycle is developed to capture 1 kilogram of CO_2 per day as a base case. Lastly, sensitivity studies on the model parameters (E.g. adsorption/desorption time, purge gas temperature, etc.) are conducted to evaluate their impact on the energy requirements, capital, and operating costs of the DAC system. A preliminary energy calculation shows energy requirements (considering the heat of reaction and sensible heat of sorbents) of 3.89 GJ/tCO_2 which is in the same magnitude as in the recent review paper of McQueen et al. (2021). An equilibrium loading of 1.06 mol/kg of CO_2 was obtained from the model as found from the works of Bos et al. (2019). Finally, this first identified modeling study of TSA-based Direct Air Capture will serve as a basis to analyze the feasibility of DAC system deployment and its relevance in comparison to CO_2 capture from point sources.
Keywords: Direct air capture, Carbon capture, TSA, Adsorption, Simulation

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Towards a model-based prediction tool for pest incidence in organic banana crops

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Abstract

Peru has an area of 197,837 hectares for organic agriculture (Castañeda, 2017) and is a major supplier of organic bananas to the American market (Machovina & Feeley, 2013), representing approximately 3% of the world's organic banana production. Most organic banana producers in Peru have small plots of land and are not able to produce enough to compete with industrial producers, fostering the formation of associations and consortiums. Nonetheless, they must face the presence of pests and diseases, which affect crop quality and productivity (Gaitán, 2020). Therefore, to achieve a correct pest management, the development of prediction tools is of paramount importance.

This contribution introduces data acquisition and modelling framework for the prediction of the banana pests' incidence. An IoT sensors-based data acquisition system collects weather variables such as temperature, relative humidity, and wind speed, which are uploaded in real time to a cloud storage space. The incidence of the red rust thrips (*Chaetanaphothrips signipennis*) is collected "manually" by periodic inspection at an association of small producers. The mathematical model was adapted from population growth functions and models of insect species development, and includes relevant microclimate parameters. The model parameters were estimated by cross-validation, calculating the RMSE and R-squared metrics to verify the well-fit.

The resulting model allows predictions to be made at various time intervals with an accuracy greater than 80%, improving decision-making capacity for agro-producers and enabling the improvement of pest management actions. Future developments will include the ability to predict optimal dates for spraying.

Keywords: Mechanistic modelling, IoT sensors, Precision agriculture, Organic banana, Red rust thrips.

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A novel approach for the modelling of trickle bed reactors

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Abstract

A frequently used solution for industrial multiphase exothermic catalytic reactions between gaseous and liquid components (e.g., hydrogenation, oxidation) is the trickle bed reactor (TBR), in which gas and liquid flow downward through packed beds undergo chemical reactions (Guo et al. 2008). The advantages of TBR with respect to other options are that there is no flow rate limitation imposed by its flooding limits, the liquid is more evenly and thinly distributed, their simplicity in operation, the low axial dispersion that can be achieved (enabling higher conversion and selectivity), and the often lower energy consumption compared with other reactor types (Degirmenci & Rebrov, 2015).
On the other hand, the behavior of TBRs is very complex and depends on mass & heat transfer, as well as on hydrodynamics (Qi et al., 2020). Thus, the rigorous modelling is highly challenging since numerous transport and reaction phenomena occur simultaneously in the reactor, with uncertainties in the catalyst heterogeneity, packing, fluid flow, and transport parameters elevating the complexity (Azarpour et al. 2021).
In this contribution, the development of a reactor model able to account for the local properties of the liquid flow in the packed bed at a particle scale, based on the work in (Schwidder & Schnitzlein, 2012) is introduced. The local liquid distribution is considered as a function of the operating conditions and physical properties of the three phases. Moreover, it accounts for the impact of local incomplete wetting on the conversion, and for the mass transport and the kinetics at both the particle and the reactor scales. The model is able to reliably predict the performance of catalytic TBRs, and, due to its flexible structure and the modular setup, it can be easily extended to incorporate other particle geometries, provided all model parameters characterizing the interactions are known.

Keywords: Trickle bed reactors; Multiphase reactors; Modelling; Multiscale analysis

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Alkaline Water Electrolysis Prediction Model For Biopharmaceutical Products

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Abstract

It is essential that the Cl- ions purity contained in NaOH solutions for the use of the biopharmaceutical production processes would be below 30 ppm to meet Good Manufacturing Practice (GMP) guidelines. The development of a commercially efficient process for purifying NaOH 50% aqueous solution of such purity is of interest in the related industry. This study describes a lab-scale electrochemical mathematical model for producing GMP grade NaOH aqueous solutions and a design of electrochemically efficient lab-scale production configuration. The model validation is carried out with experimental data for a different set of electrodes, membrane configurations, and temperatures [1]. The model calculates the theoretical open-circuit voltage via a thermodynamic analysis of the electrochemical purifying process and then outputs the expected voltage during operation by applying the Butler-Volmer equation [1,2,3]. A set of physical properties of the solution are obtained from well-known theoretical equations: concentrations from Henry's law and membrane diffusivity, permeability, and ionic conductivity from the Arrhenius equation, respectively. An experimental data fitting makes it possible to obtain a set of estimated values of critical process parameters and their data tendency at different temperatures. The conclusion shows about 90% accuracy of an electrochemical lab-scale mathematical model for producing GMP grade (Cl- ions below 30 ppm) 50% NaOH aqueous solution and an appropriate membrane-based purifying lab-scale configuration aqueous solution electrochemically high efficiency. Future work involves the model enhancement for applying to its commercial-scale production with an emphasis on optimization of electrochemical reaction time.

Keywords: Alkaline water electrolysis, prediction model, NaOH purification.

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Effect of air dynamics on the discharge of a pharma ceutical powder using the discrete element method

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Abstract

In continuous manufacturing of solid dosage pharmaceuticals, powder flow in silos or bins is critical to the process performance and end-product quality. The flow properties of powders vary with each material's chemical and physical characteristics, which include particle size and shape, bulk density, cohesive strength, and the material's behaviour under vacuum, atmospheric, and loading conditions. Often, due to cohesive and poorly flowing powders, it can be challenging to accurately feed, blend, and transfer between different manufacturing steps. Moreover, for fine particles, the strong influence of fluid-particle interaction can inhibit powder discharge.

Despite the increasing research in particle technologies for pharmaceutical applications, a general model to predict such powder flow behavior is still missing. Commonly used models are based on empirical approximations for coarse particles, multivariate predictions, and more recently, computational models such as Discrete Element Method (DEM). While DEM has been extensively used to predict powder discharge, it fails to capture the interstitial air effect. This is mostly resolved by the computationally intensive DEM-CFD coupling approach by Hesse et al. (2020). In this contribution, a leaner approach is proposed by introducing a relation that can be directly applied to the DEM results to obtain an accurate prediction.

The DEM methodology is exemplified by an application case of discharge dynamics in a laboratory silo for a free-flowing powder (SuperTab 11SD®). The implementation stages included bulk calibration of DEM input parameters. Subsequently, a comparison between experimental and numerical discharge rate values of a cylindrical laboratory-scale silo for a set of aperture sizes was performed. Lastly, a correction term to include the effect of interphase drag was implemented to rectify the mismatch between the discharge rate prediction by DEM and experimental values.

The developed DEM model allowed the visualization of flow profiles, flow uniformity, and estimation of residence time distribution values. The comparison between numerical and experiment discharge rates showed an overestimation of the effect of air impediment. This highlighted the critical importance of a relation to account for air interaction in DEM discharge rate predictions. The implemented relation proved to adequately correct the predicted DEM discharge rates for different aperture sizes in a laboratory-scale silo. However, the general applicability of this model for different powders and silo shapes remains to be verified. Moreover, assumptions in terms of the selected particle representation (size, shape) need to be further revised.

Keywords: Fine particles, Discrete Element Model, Computational Fluid Dynamics

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Biorefinery Modelling Is In Tatters, And Here's Why

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Abstract

Today, the design of biorefineries is following the traditional chemical process design. This approach reflects that biorefining-specific models are not established. Most biorefinery concepts are still in the experimental design phase, thus remaining limited and far off the expected industrial standard in their commercial and sustainable capabilities.
Models are a key factor in achieving a cost-effective design and operation. They are also essential for understanding integrated biorefining and how feedstock and operating conditions affect performance. Without rigorous holistic models, parameter estimates and process designs are rather speculative and a reliable identification of the dynamics is improbable. Correspondingly, the absence of reliable predictive models causes uncertainties, which put investors off and generate significant development bottlenecks in design, optimisation and control. We therefore reason that models are the jack of all trades in biorefinery design and operation, targeting not only commercial feasibility and operational safety but also social and environmental sustainability. This is further reflected by the study of Corona et al. (2018), in which maximizing product yields proved to be the most important environmental optimisation parameter for green biorefineries, even more important than reducing energy consumption. The secret to sustainability hides, after all, in the optimisation of processes.
According to the analytics of scopus, less than 17% of biorefinery-related publications in the last 20 years dealt with topics of modelling, while the overall share in chemical engineering publications is almost 24%. This lack of modelling activities in the biorefinery community is significant and induces some concerns. In cynical terms, biorefineries are designed on the backbone of industrial chemistry and not on the research and development systematics being established over the past century.
The aim of this contribution is to review the current state of biorefinery modelling, derive the presumed root causes, and outline the extent of the issues at hand. Based on this assessment, the future for biorefinery modelling is discussed, covering the challenges and preferred characteristics of the required holistic models, and their potential benefits for research, development and process integration. Channeling the rather large biorefinery community towards systematic approaches for process design and assessment, towards a condign research, may be virtually impossible; however, this discussion is long overdue.

Keywords: biorefinery, modelling, simulation, process control, process design

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Simulation of a Fischer-Tropsch reactor for jet fuel production using Aspen Custom Modeler

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Abstract

The reduction of CO_2 emissions is a key topic in the world energy transition. Fischer-Tropsch (FT) technologies can contribute to lower our CO_2 emissions to the environment by transforming captured CO_2 into a wide array of hydrocarbon chains when coupled with hydrogen. Under optimized conditions, the reaction yields a high concentration of C_{12}-C_{15} chains which in turn could be further upgraded into jet fuel. Thus, difficult to electrify sectors of the economy such as the aviation sector could have a defossilized supply of fuel. In this context, the objective of our research is to design, install, operate and optimize a FT reactor that would serve as core of a future Power-to-Jet Fuel pilot-scale implementation at the University of Liege (UL). In the present paper, a FT pilot implementation is simulated in accordance with the electrolysis capacity currently available at the UL. The first step was to select from the literature the kinetics and the stoichiometry that accurately depicted the FT reaction. In this study, the kinetics reported by Iglesia et al. (1993) and the stoichiometry proposed by Hillestad et al. (2014) were selected and implemented in a simulation model developed using Aspen Custom Modeler (ACM). This model was then validated by simulating computational, lab and pilot FT implementations reported in the literature by König et al. (2015), Vidal et al. (2018) and Tomte (2013). Once validated, the parameters are used to simulate a FT pilot reactor having an inlet of 0.6 kg per day of H2 and 8 kg per day of CO. In future work, the ACM model of the FT reactor will serve as input for a more complex process model of the Power-to-Jet Fuel production chain, further improving conversion efficiency.

Keywords: Fischer-Tropsch, Jet-Fuel, Aspen Custom Modeler, Simulation.

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Techno-economic-environmental analysis of a microbial oil production integrated into a bioethanol sugarcane biorefinery

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Abstract

Biodiesel and bioethanol play an important role as renewable liquid fuels. The production of these biofuels generates low-value by-products, such as sugarcane bagasse (usually used for heat generation). This bagasse can be processed to produce a sugarcane bagasse hemicellulose hydrolysate (SCBH) that contains fermentable sugars, mainly xylose. Oleaginous yeasts (eg., *Rhodotorula toruloides)* can grow in this SCBH producing microbial oil (MO) which can be used as raw material for biodiesel production. This strategy arises as a promising approach to exploit a synergy between bioethanol and biodiesel production processes within a biorefinery. Since techno-economic-environmental analysis (TEEA) can identify bottlenecks, providing insights concerning feasibility and sustainability of processes, in this work TEEA was applied to a study case consisting of a MO production from SCBH integrated into a first-generation (1G) bioethanol plant. The 1G section of the plant – processing $4x10^6$ t of sugarcane per season (240 days) - produces bioethanol and bioelectricity generating a surplus bagasse, which is sent to the MO production. The conversion of bagasse into SCBH was achieved with a diluted acid pre-treatment. NPV and global warming potential were chosen as the economic and the environmental metrics, respectively, for evaluating the process options simulations. Models of the integrated plant have been implemented in the EMSO simulator. The main result of this study had the plant producing 74.8 m^3/h of bioethanol, 2.8 t/h of MO, and 86.3 MW of bioelectricity. The integrated process exhibited a positive economic performance (net present value equals to US$ $19.7x10^6$ and internal rate of return of 11.8%) indicating that the microbial oil production from sugarcane is feasible. From the environmental perspective, the 1G process always had a higher environmental footprint than the integrated process.

Keywords: microbial oil, biorefinery, techno-economic analysis, modelling and simulation.

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Modeling the hydrodynamic sizing and rating of reactive packing in Aspen Plus

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Abstract

Reactive distillation is the integration of reaction and thermal separation in one piece of equipment. Structured catalytic packings have been developed for this application, but their simulation and design are often limited to manufacturer software. Studies in the literature that rely on process simulation using Aspen Plus typically assume that the reactive distillation equipment has trays partially filled with catalyst, and do not take into consideration the pressure drop across the column. This simplification, in turn, affects the temperature profile and the reaction kinetics of the column, which might lead to simulation results that would be unfeasible, due to catalyst degradation. In this work, a custom model was developed for hydrodynamic modeling of the Katapak-S packing in Aspen Plus. The model was validated using literature data on pressure drop and holdup for the water-air system and the esterification of lactic acid with ethanol over Amberlyst-15, showing a good fit between the literature data and the model results. Therefore, the model offers a more representative description of reactive distillation columns and serves as a tool for the holdup, pressure drop, and diameter sizing in Aspen Plus simulations.

Keywords: Aspen Plus, structured packing, Katapak, reactive distillation.

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Simplified Model-based Design of Plate-fin Microdevices for Uniform Flow Distribution at High Flow Rates

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Abstract

The application of microdevices in the chemical process industry has gained significant importance in recent years. It is well known that microdevices are more efficient than conventional devices in heat and mass transfer, due to the increased exchange surface and the reduced diffusion length. The production capacity of a micro chemical plant can be often increased by external/internal numbering-up. Such micro chemical plant requires a structure that is capable of distributing fluid to all parallelized microchannels. The structure, known as the manifold, helps to guide the fluid through many microchannels. The performance of manifold will be dependent of pressure drop and flow rate inherent to the design. The poor uniformity in flow distribution reduces the selectivity of reaction products. With regard to the flow analysis of microdevices, Computational Fluid Dynamics (CFD) can provide the detailed information about flow and pressure distributions, but it requires a considerable computational time. It means that the indiscriminate application of CFD to a design problem of microdevices wouldn't be practical. Hence, a simplified model is desirable in order to efficiently investigate the influence of design parameters on the microdevice performance. In our previous work, Pressure Drop Compartment (PDC) model was developed (Tonomura, et al., 2019). A combination of PDCs can estimate the flow rates at each location in the microdevice and is used at initial design stage to determine the good shape of the microdevice with the desired flow distribution. However, the PDC model does not apply to every case, because it cannot express the flow inertia in microdevices, especially at higher flow rate.

In this research, the PDC model is extended by adding the effect of flow inertia. After combining the extended PDCs, mass and momentum balance equations of an incompressible flow are formulated. The extended PDC model is different from the original PDC model in taking into account momentum. A comparative study of the flow distribution in a variety of manifold designs was carried out. These results demonstrate the effectiveness of the extended PDC model. In addition, the extended PDC model is applied to the design problem of a stacked plate-fin microdevice with uniform flow distribution. In this design, the stacked plates take the role of the microchannels in the plate and the vertical pipes take the role of the manifolds. The validity of the design result was confirmed through CFD simulation. It can be concluded that the developed PDC model has potential for being widely applied to various microdevices.

Keywords: Shape design, Microdevices, Simplified model, CFD model

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CFD-based study of fluid flow and transport in fixed bed compact reactors

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Abstract

Currently, functional chemicals are manufactured exclusively by the batch method, and a large amount of waste containing organic solvents is discharged, and energy is consumed to dispose of the waste. In recent years, it has been reported that functional chemicals are synthesized by a flow method utilizing an immobilized catalyst having high selectivity (Tsubogo et al., 2015). It is expected that the use of such a flow method will increase in the future in place of the batch method. In a reaction process with an immobilized catalyst, compact reactors such as microreactors, which are expected to enable rapid mass and heat transfer due to the large specific surface area between different phases, are often used. However, research on fixed bed compact reactors is not sufficient compared to conventional reactors, and their design methods have not been established. Although catalyst development is being actively carried out, the performance of the developed catalyst will not be fully exhibited without consideration of appropriate reactor design. It is important to rationally solve the engineering problems of the fixed bed compact reactors such as temperature control and pressure loss reduction, based on the models, which can quantitatively express mass and heat transfer as well as fluid dynamics.

When analyzing the flow and transport in a conventional reactor, a model that assumes a piston flow and regards the fixed bed as homogeneous porosity is often used. On the other hand, in the case of a fixed bed compact reactor, which is often used for reaction processes involving a large amount of heat of reaction, a model with high prediction accuracy of heat transfer is required to realize strict reaction control. Considering that heat transfer depends on flow, a model that can analyze local flow and transport is required. Therefore, it is useful to analyze the fixed bed compact reactor based on CFD simulation, which can express the discrete porosity distribution in consideration of an individual shape of catalyst carriers.

In this study, the flow and transport characteristics of a fixed bed compact reactor were analyzed by CFD simulation. How the packing methods of spherical catalyst carriers, reactor diameters, and catalyst carrier sizes, which are important design variables, affect the conversion and selectivity of a model reaction was investigated. One of the simulation results shows that the generation of flow perpendicular to the axis of the reactor leads to the improvement of the reactor performance. In addition, we performed CFD analysis of the reactor using a honeycomb structure, which is thought to have a higher ability to remove heat of reaction.

Keywords: CFD simulation, Compact reactor, Packed bed, Fluid dynamics, Heat transfer

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Multicomponent, nonisothermal VOC adsorption modelling for pharmaceutical effluent purification: effect of operating conditions on bed performance

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Abstract

Volatile organic compounds (VOC), exhibiting high volatility at standard conditions, represent a class of solvents employed for upstream pharmaceutical manufacturing, accounting for almost 90% to the overall process mass contribution for the development of active pharmaceutical ingredients (API) (Constable, 2007). Despite well-established processes, solvent use is problematic as organic gas releases threaten both environment and human health, exacerbating climate change and respiratory conditions (Dobre, 2014).

Multicomponent, nonisothermal adsorption is preferable among widespread VOC control methods (e.g. membrane separation, absorption and incineration), due to its ability to treat large volumetric streams with low organic pollutant loading. Fixed-bed columns with activated carbon beds can selectively adsorb VOC from gas effluent streams. However, these beds can be quickly and irregularly saturated, due to simultaneous feeding of variant solvent loading and composition mixtures. The consequent increase in the frequency and outsourcing cost for bed adsorbent regeneration harms operating (thus total) process cost.

This paper presents the development and implementation of a dynamic, non-isothermal axisymmetric adsorption model (under both adiabatic as well as non-adiabatic conditions) to describe multicomponent VOC adsorption. Recent literature studies (Fournel, 2010; Tefera, 2013; Knox, 2016) either focus exclusively on axial modelling neglecting radial gradients, or forego the investigation of the effect of heat balance boundary conditions. The aim of this contribution is to highlight the effect of key operating parameter changes (mixture composition, porosity, ambient temperature, column geometry) under varying heat transfer scenarios of VOC adsorption, to form a basis for column usage optimisation.

Keywords: Volatile Organic Compound (VOC), dynamic simulation, adsorption.

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Hydrogen Separation via Continuous Hydrate Formation

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Abstract

According to the International Energy Agency, hydrogen is one of the pillars to reach Net Zero by 2050. Forecasts indicate a market size of 200 Mton in 2030, of which 35% will be blue hydrogen (IEA, 2021). This work analyses the separation of carbon dioxide from a reformer outlet mixture, via continuous hydrate formation in a microstructured NetMIX device (Lopes et al, 2019). Hydrates are crystalline structures, typically composed by water and gas molecules (Ballard, 2002). They are usually formed when a gas contacts directly with water at low temperatures and high pressures, above saturation conditions. This formation process is exothermic and the required heat removal for a continuous production is achieved using the NetMIX technology. A simulation model for this process is developed in a framework which integrates the Python software environment with Aspen Plus software. Compression and cooling of the reactants to the hydrate formation conditions at the reactor upstream is modelled in Aspen Plus. In the Python software, the heat and mass balances associated with the NetMIX reactor are performed, including an existent Gibbs Energy Minimization algorithm developed by Ballard (Ballard, 2002) for the prediction of hydrate/liquid/vapor equilibrium. This procedure was adopted since the NetMIX reactor model, and the hydrate thermodynamic equilibrium parameters are not included in the Aspen Plus library and Aspen Properties database. Validation of this approach was performed by comparing the results obtained using the Python algorithm with predictions from Aspen Plus (for the vapor-liquid equilibrium), and results published in literature (for vapor-liquid-hydrate equilibrium). The model developed was then applied to a case study, which considers a stream of 250 ton·h^{-1} of CO_2, containing 60% (mol:mol) of hydrogen and 40% (mol:mol) of carbon dioxide. whose results show a recovery near 62% of CO_2, with 0.4 GJe·tonCO_2^{-1} of electrical demand and 2.7 GJt•tonCO_2^{-1} cooling demand.

Keywords: Hydrogen separation; NetMIX device; Hydrates.

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Combined particle model and experimental approach for predicting pyrolysis with palm kernel shells

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Abstract

Biomass pyrolysis can transform organic residues into energy and valuable chemicals, aiding the transformation of agro-industries into biorefineries. For pyrolysis to be integrated into biorefineries, a better understanding of the complex interactions between biomass components is needed. This is particularly critical for the development of reliable models for pyrolysis process design and scale-up (Bridgwater, 2018). Different modelling strategies have been used to describe pyrolysis. However, biomass components interactions are not fully understood and they are difficult to quantify, leading to poor agreement between predicted and experimental results. This work explores the combination of a pyrolysis particle model with experimental data to improve predictions on biomass conversion. A mechanistic model is developed to describe biomass pyrolysis in a shrinking particle. Biomass is considered as a mixture of cellulose, hemicellulose and lignin. The model is implemented and solved in gPROMS. The experiments considered residual palm kernel shells (PKS) as feedstock. Gravimetric analysis is used to determine PKS moisture and extractives content. The cellulose, hemicellulose and lignin content is determined with high performance liquid chromatography and UV-Visible spectrophotometry. A synthetic sample of cellulose, hemicellulose and lignin is prepared to resemble PKS composition. Pyrolysis of both PKS and the synthetic sample is evaluated using thermogravimetric analysis (TGA). The results highlight the complexity
of pyrolysis and the importance of having experimental data for supporting pyrolysis modelling. Although the model is able to predict pyrolysis conversion, it performs better for individual components than for mixtures. TGA results highlight the effect of biomass components interactions in pyrolysis, and a 20% difference in conversion is reached between PKS and the synthetic mixture. The agreement between predicted and experimental results improves when the model includes information from PKS pyrolysis. This work represents a step forward for understanding the role of combined modelling and experimental strategies in describing complex processes like pyrolysis.

Keywords: biomass pyrolysis, mechanistic model, TGA, palm kernel shells

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Methanation of CO_2 byproduct from an ammonia plant with green hydrogen

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Abstract

The methanation of carbon dioxide with hydrogen, to yield methane, aids in reducing carbon emissions, if hydrogen originating from electrolysis operated with green energy, is used. The Haber-Bosch process consumes natural gas as feedstock and delivers a concentrated carbon dioxide stream as side product, leading to it being highly synergistic with the methanation process. Borealis and voestalpine operate energy intensive industries in Linz, Austria and recognize a high potential of methanation to support industrial symbiosis. The voestalpine steelworks produce hydrogen rich coke oven gas; potentially being usable as hydrogen source for methanation.
Process simulation software like Aspen Plus is of vital importance in validating new industrial approaches and was used extensively in this work. Studies on both thermodynamic equilibrium and kinetic models were done on CO_2 methanation reaction dynamics. Flowsheets and process parameters are proposed and the ramifications of coke oven gas utilization in an ammonia-synthesis-methanation complex are outlined. Gas separation membranes are discussed and simulated based on diffusion laws.
Insight on CO_2 methanation reaction characteristics was gained by temperature and conversion curves recorded at low and high pressure. Models for gas separation membranes were drafted and simulated. A full flowsheet simulation model able to convert 1 t/hr of CO_2 to CH_4 at 97% conversion was designed and optimization curves provided. Reactor performance curves are shown in figure 1. The introduction of N_2 alongside CH_4 at the ammonia-plant front end is assessed by simulation. A complete exchange of external natural gas with natural gas from methanation with coke oven gas as hydrogen source has considerable advantages concerning feed requirements, H_2 loss, recycle gas volume and reaction pressure.
Temperature and conversion curves indicate ranges of operational parameters suitable for CO_2 methanation. They can be used to design process models based on thermodynamic equilibrium and kinetics. Three membrane setups able to reduce N_2 content in synthetic natural gas from 10% to grid levels are proposed. A simulation model for the conversion of 1t/hr CO_2 is designed. A set up with two cooled reactors and product recycle is employed and found to be capable. N_2 has negligible impact on CO_2 conversion and is beneficial in ammonia synthesis feedstock. An implementation of coke oven gas as hydrogen source in the methanation-ammonia synthesis complex therefore leads to substantial economic and ecologic gains.

Keywords: CO_2 methanation, Haber-Bosch-process methanation coupling, process model design

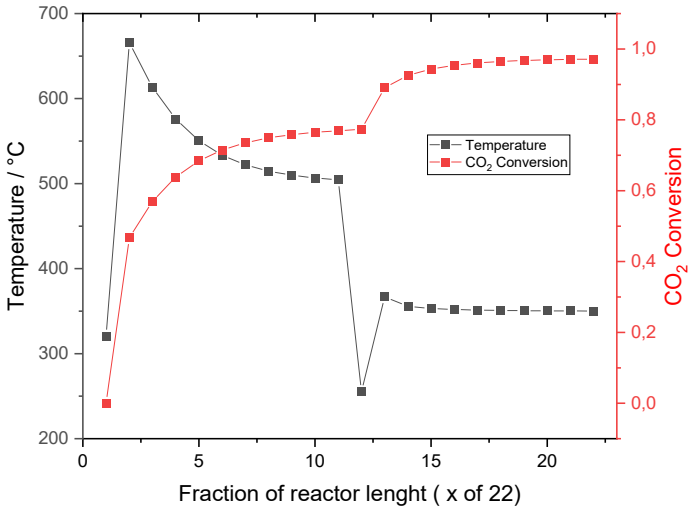

Figure 1: Reactor performance in kinetic 2 reactor model.

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Gas diffusion channels in Li-O_2 batteries: a comparison of wet and flooded electrodes

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Abstract

The projected increase in the market share of renewable energy sources such as wind and solar power will demand a similar increase in the global energy storage capacity. Batteries represent one of the most flexible solutions to cope with this demand because of their easy installation and high energy density when compared to other large-scale energy storage systems. In this context, one of the most promising technologies is Li-O_2, whose energy density can exceed 1000 Wh kg^{-1}. However, many challenges need to be addressed for this battery technology before it can become available to the market. For instance, the O_2 transport inside the battery limits the power density. One of the strategies to improve the supply of O_2 to the battery is the so-called wet electrode approach, in which parts of the O_2 electrode are filled with gas instead of electrolyte, thus serving as a means to deliver O_2 to the interior of the electrode. Bearing all this in mind, this study presents the simulation of two battery models working under different current densities to demonstrate the impact of electrode geometry on the performance of the battery. The models, developed on COMSOL Multiphysics 5.6, consist of two Li-O_2 batteries with either a simple flooded O_2 electrode or a wet O_2 electrode with gas diffusion channels, with both electrodes based on properties of carbon nanotubes. According to the results, although the gas diffusion channels take space inside the battery and decreases the surface area for deposition of discharge product, this electrode design strategy increased the accessibility of O_2 throughout the length of the electrode. The increased transport capacity was fundamental to increase the energy density of the battery. The results also indicate that this design approach was fundamental to enable increased power demand for Li-O_2 batteries without compromising their energy density because of the possibility to deliver O_2 more easily to the whole electrode. Based on this design, it is important to optimize the density of these gas diffusion channels to increase the available surface area of the O_2 electrode without compromising the transport of O_2 to the interior of the electrode. Moreover, the optimization of this design should also consider limitations related to surface properties of electrode materials such as hydrophobicity and hydrophilicity to ensure that the gas diffusion channels stay available for O_2 transport.

Keywords: energy storage, battery, lithium-air, simulation

Acknowledgments

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Techno-economic analysis of flexible AP-X LNG production process under risks and uncertainties

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Abstract

The demand for natural gas is expected to have the fastest growth amongst the fossil fuel mix until 2050, mainly due to its relatively low environmental impact. In the industry, several natural gas-based chemical or physical monetisation techniques are being utilised in the value chain serving international markets. Natural gas liquefaction has been deployed in different countries to produce liquefied natural gas (LNG) for the economic transportation to distant markets wherein LNG is regasified at the receiving terminal and distributed to the local markets. However, when assessing a natural gas monetisation technology, the profitability of the project is evaluated using the economic performance indicator, net present value (NPV), under deterministic conditions. This does not reflect the real-life scenario since the risks associated with exogenous uncertainties arising from emergence of new suppliers and changes in contractual structures are not captured under deterministic analysis. Consequently, risks associated with investing in a mega LNG plant shall be considered in the design stages to decide on an optimal strategy for dealing with possible uncertainties throughout the lifetime of the project.

Industrially mature liquefaction technologies are used for liquefying and subcooling natural gas down to -164 °C. In this work, a techno-economic analysis is conducted for the flexible AP-X LNG production technology licensed by Air Products. The AP-X technology consists of 3 cooling stages: precooling, liquefaction, and subcooling, and produces 7.8 MTPA of LNG. Thus, this work considers a three-steps methodology to assess the AP-X technology: (1) technical assessment; (2) economic evaluation; and (3) techno-economic risk assessment and management. In the technical assessment, an LNG production plant model was developed and simulated using Aspen Plus software, and evaluated under deterministic conditions using the NPV. The process was then evaluated under stochastic conditions using Monte Carlo Simulation to understand the impact of different uncertainties on the profitability of the plant. An active mode of response strategy to deal with risks was tested to increase the responsiveness of the project to exogenous changes through embedding flexibility in production in the early design stages of the project. Results indicate that a flexible system shows a better economic performance than a rigid system. However, the flexibility in the design must be embedded in the early design stages of the project rather than during the project's lifetime.

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Exploring Low Carbon Hydrogen Production and Export in Qatar

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Abstract

Hydrogen has been hailed as a fuel of the future that could help end the world's dependence on fossil fuels and aid the transition to net-zero emissions. However, to harness the full momentum of hydrogen adaptation numerous impediments are to be overcome including a massive amount of energy required. In addition to, the storage and transmission which a sufficient and dedicated infrastructure is yet to be developed. Both aspects need to be understood to fill the missing blocks of the global energy transition roadmaps. Almansoori & Shah (2006) introduced a snapshot model to establish a framework for optimal configuration of future hydrogen networks while identifying a number of decisions related to production, storage, and transportation modes. Hydrogen integration with multi-objective optimization models was studied by Kim & Moon (2008), Guillén-Gosálbez et al. (2010), and N Sabio et al. (2012). Hydrogen time-horizon planning transition through the multi-period optimization model such as the work done by (Moreno-Benito et al., 2017) and Ogumerem et al. (2018). Nevertheless, given that the deployment of reliable hydrogen supply chain network is still challenging, exceptional effort must be made. The scope of H_2 management, especially in the sectors that dominate hydrogen use (e.g., oil refinery), can be an efficient solution to cut down the CO_2 emissions associated with H_2 production. The most common graphical approach in hydrogen management is called Hydrogen Pinch Analysis (HPA) developed by Alves & Towler (2002). In terms of CO_2 management, Lameh et al., (2020), developed a novel and simple graphical technique that identifies an efficient and economic CO_2 Capture, Utilization, and Storage (CCUS) network for known CO_2 sources. This work presents a comprehensive framework for hydrogen infrastructure design as well as CO_2 capture and recovery strategies in an industrial cluster. The framework will identify the optimum decision pertains to production, storage, and transportation technologies.

Various commercially proven technologies to produce H_2 exist, (e.g., Water Electrolysis, Steam Methane Reforming (SMR), Coal gasification etc.…). Each of these technologies produces different types of H_2, namely grey H_2 generated from fossil fuels, blue H_2 produced via fossil fuels with CCUS, and green H_2 through water electrolysis plant powered through renewable energy. The H_2 produced from these plants has to go through the conditioning stage in which the H_2 is liquified and compressed before being transported to a specified terminal. Following the storage stage, H_2 is distributed via pipeline or tube trucks to the local demand within the cluster. The local demand includes the CCUS options for H_2 and CO_2 utilization. For long-distance hydrogen transmission, various options have been investigated. These options are ammonia, Liquid Organic

Hydrogen Carrier (LOHC), and liquid hydrogen. A superstructure optimization-based model is developed to capture the techno-economic performance of the hydrogen network. The mathematical model will capture the optimum hydrogen network design from several possible scenarios.

This case study will resemble Qatar's hydrogen production in an industrial cluster accounting for economic cost and environmental impact. Qatar's abundant reserves of oil and gas resources estimated at 24.9 billion cubic meters (bcm) and could potentially export hydrogen. Qatar currently produces hydrogen domestically, in liquid and compressed form, mostly from natural gas in order to fulfil their oil and gas industries' demand. These industries include refineries, steel and aluminium production, petrochemical production, and fertilizer industries in addition to export demands. A portion of the produced hydrogen can be utilized with CO_2 that is emitted from the cluster in the CCUS options namely, Methanol, Ammonia, Urea to produce added-value products. The Mixed Integer Linear Program (MILP) formulation is solved to achieve the minimum cost of production of hydrogen while meeting the imposed CO_2 threshold. At 75% reduction target of carbon dioxide over the current emission, it was found that exporting liquid hydrogen in pipeline was more economically feasible than trucks locally. Exporting hydrogen in LOCH was the least expensive at the 20% emission target. At higher emission targets, hydrogen export in the form of ammonia was preferred.

Keywords: Hydrogen; Renewable Energy; Carbon dioxide Mitigation; Sustainable hydrogen network; Energy Mix

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Modelling and Parameter Fitting of the Dosage of Hydrogen Peroxide in a Photo-Fenton Process

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Abstract

The most critical operational issue for the photo-Fenton process is the supply of hydrogen peroxide (H_2O_2) that its oversupply leads to unproductive side reactions. Thus, a number of studies have been conducted to improve process performance by limiting the scavenging impact and efficiently using H_2O_2 supply (Yu et al., 2020). Despite recent improvements, solutions fall short to address the dynamic optimization of batch and fed-batch operations of photo Fenton processes using model-based approaches.

This work has adopted the model by Audino et al. (2019), who extended the model by Cabrera Reina et al. (2012), to include the H_2O_2 inlet flow (fed-batch) and describe system dynamics under a flexible reactant dosage. Hence, this work performs computational experiments using Simulink® to examine the behaviour of the model and reduce its complexity, while addressing the computational issues that will arise when fitting the model to experimental data obtained from flexible dosage profiles.

In this regard, the initial set of 12 kinetic and stoichiometric parameters were first estimated through the fitting of H_2O_2, Total Organic Carbon (TOC), and dissolved oxygen (DO) profiles (the experimentally available information). Perfect data was assumed and obtained using the parameter values reported by Cabrera Reina et al. (2012).

Sensitivity analysis was conducted to assess to which extent variations of the model parameters can affect each measured response. Hence the model is discussed in regard to its hypothesis and chances for reducing complexity.

Computational issues, including the definition of the fitting criteria, the sampling method, and setting the operational constraints are discussed to set the procedures and guidelines for designing the experiments to provide data for an efficient fitting of the model.

Computational results show that the fitting process is successful when addressing independently fitting the three measured parameters but the tuned weighting is required for their simultaneous fitting. Convergence and dependence on initial values are also shown and discussed. Hence, these results will provide valuable insight into the planning of the experimental phase of a research aimed at providing model-based optimization for the H_2O_2 dosage profile in the photo-Fenton process.

Keywords: Photo-Fenton Process, Dosage of Hydrogen Peroxide, Parameter Estimation.

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Performance optimisation of condensate stabilization unit in LNG

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Abstract

Nowadays, Liquefied Petroleum Gas (LPG), Natural Gas Liquids Recovery (NGL), and Condensate Stabilization have gained significant interest given their increased selling prices and market demands. Nevertheless, many operational units do not meet the desired profits and lack proper optimization initiatives. In this paper, a case study from Qatar's operating condensate stabilization process has been considered, where sensitivity analysis of key process operating parameters has been applied to investigate process performance. The process has then been optimized to achieve the highest efficient performance, maximum productivity rate, and minimum energy consumption. Based on the available production data and operating conditions, an existing condensate stabilization unit has been simulated using Aspen HYSYS V10 simulator, which is based on the PENG-ROBINSON equation of state. The most significant process variables and constraints that directly affect the performance and production of condensation stabilization unit are highlighted to demonstrate the connection among process operating conditions and the influence on process objectives. The optimal process operating conditions are determined to achieve a stable column operation. The most effective process variables based on the sensitivity analysis are stabilizer column pressure, stabilizer feed temperature, the outlet temperature of process gas from the wellhead, and stabilizer bottom temperature. After collecting process data from the sensitivity analysis, MATLAB has been used to formulate and solve the multi-objective optimization problem. Starting with a natural gas feed flow of 554 MMSCFD, a condensate with 956.9 barrel/day standard liquid volume flow and a reboiler load of 0.86MW have been achieved. After performing the optimization problem in MATLAB, the condensate standard liquid volume flow has increased to 1245 barrels/day and the reboiler load has decreased to 0.8MW

Keywords: Condensate stabilization, optimization, sensitivity Analysis, LNG, simulation

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Data-driven modelling of full batch distillation cycles based on recurrent neuronal networks

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Abstract

In the context of process optimization for the reduction of costs and environmental impact in the chemical industry, prediction of the process behavior under different operating conditions is required. Specifically, online and offline optimization of dynamic operation trajectories applied to real processes remains a challenging task when models are hard to build or evaluate, or when their plant-model-mismatch is unsatisfactory. These issues can be tackled by training data-driven models when sufficient information is available.
Processes with complex dynamics such as discrete changes in the manipulated variables and vanishing phases are no exception, being batch distillation a good example. Here, simplifications such as neglecting the filling, preheating and shutdown batch phases are often made to maintain the validity of first-principles models. The flexibility achieved by machine learning models opened new possibilities to avoid such simplifications. Furthermore, time dependencies in operation trajectories can be exploited by recurrent neuronal networks (RNN), with long short-term memory (LSTM) cells to tackle long-term dependencies (Hochreiter *et al.*, 1997). Successfully applied to fields such as natural language processing and time series forecasting, these models seem promising for predicting operation trajectories of complex chemical processes.
In this contribution, an example batch distillation process consisting of a packed vacuum column separating a binary methanol-water mixture was simulated using a rigorous dynamic pressure-driven model in Aspen Plus dynamics from cold and empty start-up to subsequent shutdown with nitrogen purge. A simulated dataset consisting of batch runs sampled over an operation recipe to enhance the feasibility ratio of the simulations was generated to train and test different data-driven models (Brand-Rihm *et al.*, 2020).
Here, RNNs with simple RNN and LSTM cells with series and series-parallel (teacher forcing) output regressor configurations were trained for their use as surrogate models.
For the presented use case, architectures with LSTM cells outperform simple RNN models. Furthermore, simulated trajectories are outperformed by the predicted ones due to their lack of output regressors. Series-parallel configurations, although faster to evaluate and more accurate than parallel ones, remain constrained to one-step-ahead predictions. Training of the presented RNNs on large simulated datasets provides data-driven models for trajectory optimization in chemical processes with complex dynamics.

Keywords: dynamic data-driven model, recurrent neuronal network, batch distillation

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Stackelberg Game Design and Operation of a Non-Cooperative Bi-Level H_2 Supply Chain Under Cournot Equilibrium

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Abstract

In the pathway toward decarbonization, hydrogen is presented as a great option as it can be produced from a variety of feedstocks, including renewable sources like biomass, wind or solar energy (green hydrogen) and also fossil fuels coupled with processes that capture, utilize and store CO_2 (CCUS) (blue hydrogen). With these multiple production, storage and transportation options for diverse applications, H_2 could provide flexibility and sector-coupling to energy systems. The plethora of sources for hydrogen production, along with the variety of methods for its distribution and storage makes the design and management of the hydrogen supply chain (HSC) a challenging task (Robles et al. (2018)). Until now, most of the HSC designs are treated as problems with single or multiple objectives without any hierarchical conflict. This paper proposes a mixed-integer bi-level programming (MIBLP) approach as a mathematical model of the Stackelberg game. The solution strategy considers the MIBLP as a multi-parametric problem knowing that if the feasible set of the lower level optimization problem (LLP) of a bi-level programming problem (BLPP) is parametric in terms of the optimization variables of the upper level problem (ULP), then it is possible to solve each level with a different approach, as stated Avraamidou and Pistikopoulos (2019). To handle continuous and discrete variables at both levels, we propose a hybrid method involving Differential Evolution (DE) for the ULP and an Integer Linear Programming Solver (ILPS) for the LLP. The developed hybrid evolutionary-deterministic strategy evaluates the performance of two HSC study cases combining Steam Methane Reforming and Electrolysis processes for H_2 production: a classical Stackelberg game design at first and a Stackelberg one leader - multi follower under Cournot competition for the second case. In both scenarios, the ULP objective is to minimize the distribution cost while the LLP objective tries to minimize the production cost of a given producer. Experimental results shows that the solution method is efficient and promising for dealing with multi-objective one-leader multi-follower mono-objective optimization cases.
Keywords: bi-level, hydrogen, optimization, Stackelberg, Cournot, MIBLPP

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Modelling of Heat-Driven Water Treatment Systems: Development and implementation of a Multi-effect distillation (MED) model in Modelica

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Abstract

The simultaneous improvement of water and energy use in the industrial sector is an important concern in the scope to improve the overall techno-economic performance of single plants, at the light of the interdependencies of the use of both these resources encompassed by the water-energy nexus. In the context of single plants, a still emerging approach designated Combined Water and Energy Integration has been proposed for such simultaneous improvement. This work approaches the study of Multi-effect distillation (MED), a heat-driven wastewater treatment technology commonly installed for the purpose of desalination of industrial or sea water (Rahimi and Chua, 2017).

The proposed study is performed through the development, validation and implementation of a complex model using the Modelica language for the simulation of the whole phenomena of fluid flow, heat transfer and salt removal within a MED unit. A simple economic model is developed to assess the economic viability of a MED plant.

The proposed model was validated by comparing simulated temperature profiles with literature data. Having been verified an overall correspondence between simulated and literature temperature profiles, the model is overall considered valid. Furthermore, it was assessed a water production potential of the desalination plant of 843 m^3/day and a payback period of 12.3 years.

This work proved the technical and economic viability associated to the implementation of an industrial MED plant, considering an interval of acceptable payback time of 4 – 16 years for these type of desalination (Baniasad Askari and Ameri, 2021). Furthermore, this work proved the significance of the use of a customized simulation tool developed using the Modelica language for modelling integrated heat recovery – wastewater treatment systems in industry.

Keywords: water and energy integration; Multi-effect distillation; waste heat recovery; water efficiency; Modelica.

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CFD Simulation of Residence Time Distribution in Stirred Tanks

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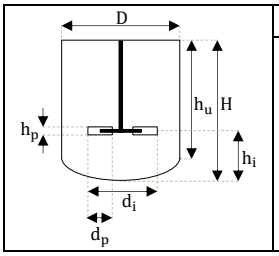
Abstract

Stirred Tanks are operation vessels commonly used in the chemical and biochemical industry. These units are suitable for its mixing capabilities related to turbulent flow induced by an impeller which generates good mass and heat transfer. These phenomena are strongly affected by the kind of impeller, the agitation speed and the geometry, some unsuitable effects are dead zones and high mixing times. Residence Time Distribution (RTD) is a parameter to characterize mixing performance, although, it does not allow a detailed description of mixing. Danckwerts (1953) introduced RTD to understand and quantify mixing behavior; afterwards, a plenty of studies on mixing have been developed. RTD is usually studied experimentally, involving high expenses related to construction, experimentation cost and time. As an alternative, Computational Fluid Dynamics (CFD) has been used widely to simulate the non-ideal hydrodynamic behavior of stirred tanks. Research using CFD are usually done in 0.5 to 1.5 L tanks (Gamba et al., 2012), ignoring the huge impact of scaling on hydrodynamic behavior. In this study, CFD and RTD experiments and simulations were employed to assess mixing in 1, 5 and 100 L continuous single-phase equivalent stirred tanks.

Studied systems consist of cylindrical baffled tanks with equal diameter to liquid level, each tank was equipped with 4 baffles and a 6 blade Rushton turbine operating at 399, 144, and 22 rpm (for 1, 5 and 100 L respectively) to ensure an impeller Reynolds number of 18000, corresponding to a fully developed flow (Bittorf & Kresta, 2000). Other dimensions are shown in Table 1. In each tank, inflow and outflow had the same value and were adjusted using rotary pumps, to obtain a ratio of liquid volume (in L) to flow (in L/min) of 9.8 min. Variation of the impeller speed was measured to be less than 1.6%.

Table 1. Stirred tank general geometry and its values for all the scales used.



Parameter	1 L	5L	100 L
D, H [cm]	18.00	32.30	84.00
h_u [cm]	15.84	28.42	73.92
h_i [cm]	2.16	3.88	10.08
d_i [cm]	5.35	8.92	22.79
d_p [cm]	1.46	2.43	6.21
h_p [cm]	0.86	1.44	3.68

RTD determination was done using 2% of each tank volume of red dye (Wimar®) in a pulse setup 20 seconds after recording started. Dye concentration was measured at the exit through a glass pipe using an Olympus OM-D E-M10 camera with a 50mm lens. RTD was obtained using Tracker 6.8, evaluating luma with a calibration curve. CFD

simulations were done using COMSOL Multiphysics 5.6 and the k-ε turbulence model coupled with a Multiple Reference Frame (MRF) method; each unit was simulated with a $2.8x10^5$ cells mesh. Simulations were done in transient state, coupled to the particle tracing module with a Newtonian approach where mass, collisions, and forces are considered. Flow profiles were determined in the 1 and 5 L tanks using a PIV setup consisting of a Chronos 1.4 high speed camera coupled with a 10mW 532nm laser at 1770 fps. Results were processed using OpenPIV with global and local filtering. Finally, experimental and simulated RTD were compared to assess the mixing behavior.

Results in Fig. 1 show that for employed flow to volume ratio, the time for 90% of dye output was approximately 40 min at all scales. Flow profiles obtained by PIV were close to the obtained by CFD simulation, with a mean deviation of 1.09% on the velocity profiles compared at z/H ≈0.8, where z is the radial coordinate. Sommer (2021) showed there is a peak in radial flow velocity at that position.

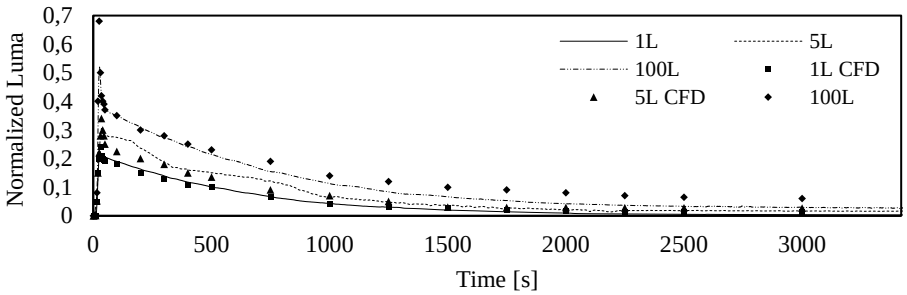


Figure 1. Experimental RTD results for the 1, 5 and 100L stirred tanks. Points are the values from the respective CFD simulation.

This work compares experimental and simulated RTD for three different single phase stirred tanks. As main results, effect of flow/liquid volume ratio on RTD behavior was confirmed. Additionally, RTD from simulation were consistent with experimental ones. As a continuation of this project, assessment of changing agitation speeds, volume to flow rate, impeller position will be considered, that will lend us necessary information to characterize flow in stirred tanks and extend this analysis to gas-liquid systems.

Keywords: Computational Fluid Dynamics, Residence Time Distribution, Particle Image Velocimetry, Stirred Tank

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Continuous operation of a solar photobioreactor with linearizing control – A simulation study

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Abstract

Exploitation of microalgae, microscopic photosynthetic cells present in sea or fresh water, can help to face both economic sustainability and carbon footprint reduction challenges. To this aim, industrial scale photobioreactors operation (systems for microalgal production) must be optimized in order to attain sufficient biomass production amounts. In solar conditions, control strategies for photobioreactor operation should use sunlight energy in the most efficient way, in order to maximize production. In a previous study of the authors Sébile-Meilleroux et al. (2020), an optimal control strategy applied on feeding-harvesting rate, based on Model Predictive Control, has been designed and evaluated in simulation. Using this strategy, the production of *Chlorella vulgaris* strain has been enhanced by 10 or 15 %, depending on the season scenario. However, it induced an absence of harvesting process 48 days a year. Furthermore, the implementation of this strategy requires to know the future sunshine conditions, and therefore the implementation of prediction models with a prediction horizon up to 48 hours.

The main idea of this work is to overcome these issues by adopting a continuous operating strategy, with at first no need of a prediction model. Tebbani et al. (2016) already studied linearizing control on microalgae cultures with constant lights and growth rates but to the best of the author's knowledge, such a strategy was never carried out under solar conditions. Due to inherent low microalgae growth kinetics, tracking an optimal variable setpoint on biomass concentration, related to maximum growth rate, was compromised. Nonetheless, working with an optimal yearly setpoint strategy, harvesting process is off only 5 days a year, with a corresponding total biomass production of 20.7 $t.ha^{-1}$. A suboptimal solution, based this time on a daily optimal setpoint determined by a 1-day weather prediction, improved production by 16 %.

To sum up, linearizing control for microalgae production can be successfully achieved under solar conditions, when seeking for a turbidostat. However, performances in terms of production quantities stay lower when compared to an optimal strategy given by a Model Predictive Control (6 % lower at best).

Keywords: Linearizing control, turbidostat, solar photobioreactor, microalgae, biomass production.

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Dynamic Inherent Safety Analysis of a Distillation Column under Simultaneous Design and Control

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Abstract

Inherently safer design (ISD), which focuses on reducing the inherent hazards of a design before applying any safety controls, is one of the most effective and reliable tools for improving the safety of a process. However, while an intensified process may be inherently less hazardous, if the design restricts the controllability of the process, then the design may have a higher risk and be less safe overall. Therefore, considering both the inherent hazard contained within the process and the ease by which these hazards can be controlled is necessary for a more complete evaluation of the inherent safety of a system. The objective of this research is to implement a strategy to simultaneously design and control an inherently safer distillation column. The PARametric Optimization and Control (PAROC) framework is used as a basis for the simultaneous design and control of a distillation column. An extensive literature review has identified inherent safety indices that can compare the hazard level of different distillation column designs. The Safety WEighted Hazard Index (SWEHI) is incorporated into the PAROC framework, and the distillation column is optimised for cost, while receding control horizon policies are implemented to ensure that the column is capable of controlling disturbances. The dynamic effects of different operating variables on safety are analysed and discussed. The integration of ISD with simultaneous design and control allows for a greater understanding of inherent safety during process design and substantially reduces operability issues that result from an uncontrollable process design and allow for greater tolerance and ease of control.

Keywords: Dynamic Optimization, Distillation Column Design, Inherently Safer Design, Design and Control Integration.

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Modeling of phosphates slurry pipelines through dynamic Non-Newtonian Fluid Model with Modelica

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Abstract

In mining operations, slurry pipelines provide a sustainable and economical way to transport ore, with many advantages than transportation through railways or trucks. The design and the optimal operation of such pipeline system are complex and challenging tasks. Indeed, due to the environment and topography variance along the large transport distance, the geometric characteristics of the pipe are largely varying. In contrast, the only available control for this system are the slurry characteristics and the input pressure imposed at the entrance of the pip. Therefore, flow models are needed to predict the behavior of the system and to avoid issues like ore deposition and pressures drops, and to ensure optimal control. Full 3D flow models with water-particles fluid models are too complex to build and are CPU time consuming to be exploitable in any real process control, optimization or design. Alternatively, one may consider an averaged rheology for the mixture and in this case the slurry can be characterized by a Non-Newtonian rheology. Given the complexity of the non-Newtonian rheological behavior of the phosphates slurry, besides the length of the network, a surrogate model to simulate this flow is requested. Hence, in the present communication, we present a surrogate pressure drop model for non-Newtonian fluids, that we implemented as a new library in Modelica. We use the Modelica FLuid Library included in the Modelica standard library (MSL), and providing components for one-dimensional thermofluid flow in networks. Thereafter, we use the model of Bingham for the rheology of fluid, and we adapt the Medium model containing the fluid properties. The pressure drops due to friction is estimated using generalized empirical formulas of Darby et al. (1992), which combines Swamee and Aggarwal (2011) approximation for solving Buckingham (1921) implicit equation for the laminar regime, with that of Darby et al. (1992) for the turbulent case. Within the Dynamic Pipe model, a new first-order finite volume scheme for the flow of incompressible fluids, with varying density and pipe inclination is implemented. With the simplified library components, we perform a first numerical simulations of the flow in a pipe network of significant length. The computational cost of the performed simulation with MSL components reduced by two orders of magnitude compared to the previous implementation, while the dynamic results are not affected. Finally, we use the implemented model in a predictive control framework using Modelica.

Keywords: Non-Newtonian Fluid, Modelica, Bingham Model

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Feasibility Constraints Implications on Surrogate Models Sampling for Chemical Processes

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Abstract

Due to the increasing amount of data to be treated and, thus, to the need of more computational effective strategies, surrogate modeling has become a topic of major interest during the last decades in the engineering domain. The most critical step during the modeling procedure is related to the data set generation. Either in case of experimental or simulation values, they play a role of critical importance in terms of accuracy of the final solution. Sampling strategies for surrogate design can be mainly distinguished into static (domain-based) and adaptive (model-based) methods (McBride et al., 2019). While the latter approach is mainly used for surrogate based optimization and for machine learning, the former one has the purpose to provide a proper a-priori space-filling design for model aimed at representing the system behaviour over a relatively extended domain. Well-established data sampling strategies are available in literature according to the particular system to be modeled (Bhosekar et al., 2018). However, when dealing with chemical processes, not all the points in the domain of interest can be selected for the model training, since part of them could not lead to conditions that are physically feasible. That is why, the common sampling methodologies need to be integrated with constraints able to describe the feasibility limitations of the system under analysis (Boukouvala et al., 2012). This research work focuses on one-shot sampling and its main purpose is then to assess the impact of two of the most common data sampling strategies when coupled with feasibility constraints. The selected sampling approaches are namely Latin Hypercube (LHS) and Halton since they are able to achieve the best uniform space-filling capability even with a relatively low number of samples (Davis et al., 2018). The selected unit operations concern the separation of a simple Toluene-Biphenyl mixture by means of a single flash unit or a 20 stages distillation column fed at the sixth one. The input variables ranging over suitable intervals for the data sampling and the output variables whose models need to be derived are listed in Table 1. In short, both physical (top and bottom products) and economic (OPEX and CAPEX) output variables are taken into account for variable input streams and operating conditions. In particular, the Murphree efficiency for the distillation column can be used to assess the unit performances for a variable number of theoretical equilibrium stages. Sampling points were generated by means of Matlab® dedicated functions given the input variables domain accounting for physical constraints according to the specific operation, e.g. non-zero products flowrates, inlet pressure higher than flash one etc. The obtained sampling was then exported to Prosim® process simulator and the results to a .csv file. These values were then processed by the ALAMO® software to derive the surrogate models for each output variable. When processing the entire samples at once, the obtained model showed poor accuracy.

	Input	**Output**
Flash & column	Feed toluene	Top toluene
	Feed biphenyl	Top biphenyl
	Feed temperature	Bottom toluene
	Feed pressure	Bottom biphenyl
Column only	Reflux flowrate	OPEX
	Distillate flowrate	CAPEX
	Murphree efficiency	

Table 1 – Model input and output variables

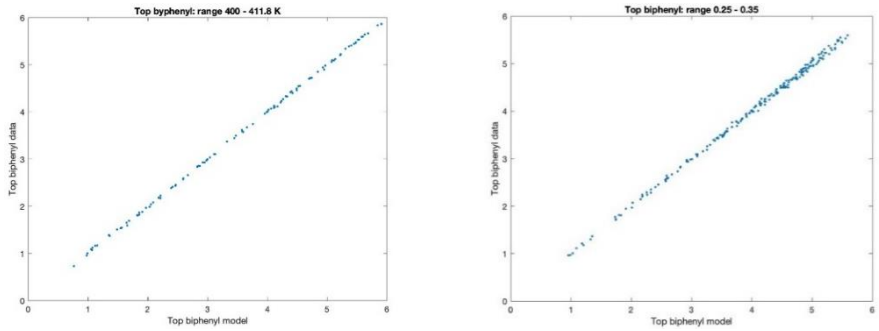

Figure 1 – Top biphenyl trends based on a) feed temperature b) product vapor fraction

That is why the same procedure has been repeated by dividing the samples into subsets both according to input and output variables domain sub-regions. As an example, Figure 1 shows the results for the flash top biphenyl flowrate in case of feed temperature (input) and product vapor fraction (output) sub-region discretization. As it can be noticed, the model accuracy shows a drastic improvement when sampling subsets are employed (MAE 0.93% and 0.707%). In particular, for these two specific case studies, the data sampling partition according to the input variable domain exhibits a higher performance than to the output variable one. Starting from these results, this work set the basis for further developments on more complex chemical processes with highly non-linear behaviour and optimization problems where feasibility plays a key role on the simulation convergence and solution accuracy.

Keywords: black-box modeling, DoE, constrained sampling, unit operation.

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Techno-Economic Analysis of the Conversion of Waste Plastics to Hydrogen Fuel

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Abstract

The need of hydrogen as a clean fuel has grabbed a lot of global attention. Therefore, various processes have been developed for hydrogen production. Conversion of plastic wastes is one of the attractive option to produce H_2 because of its hydrocarbon structure, higher heating value and availability. Polyethylene (PE) and polypropylene (PP) are considered in this study because of their massive worldwide availability in the category of waste plastics. In this study, the simulation of conversion of plastic wastes (PE and PP) to hydrogen fuel via steam gasification process is developed to perform the techno economic analysis. The composition of produced syngas from steam gasification unit was validated with the literature results followed by sensitivity studies to see the impact of various process parameters on the syngas composition. The syngas produced in the steam gasification unit is then treated in the water gas shift units followed by acid gas (H_2S and CO_2) removal to produce pure H_2. To enhance the hydrogen production capacity and overall process efficiency, plastic gasification is further integrated with the steam methane reforming coincided with gasification to utilize the energy from the gasifier to provide heat to the natural gas reformer. It has been seen from results that the new integrated design containing both gasifier and reformer enhances the hydrogen mass production rate per mass feed rate by 5.6%. Furthermore, the process performance analysis showed that the efficiency of the new process is increased up to 1.82%, where the hydrogen production cost showed the reduction of 29% compared to the standalone gasification cases. In terms of carbon dioxide specific emission, the new design showed the reduction in CO_2 emissions by 4.0%. Overall, the technical and economic analysis favored the new design over the standalone plastic gasification case.

Keywords: Gasification: Reforming; Waste Plastic; H_2 production; GHG Emissions.

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Evaluating the flexible operation of vacuum pressure swing adsorption for CO_2 capture from modern gas turbines

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Abstract

To reach net zero targets by 2050, CO_2 post-combustion capture (PCC) technologies need to be capable of transient/flexible operation, in order to combat network imbalances (from intermittent renewables) and maintain security of supply. Several sources have investigated amine absorption for flexible-PCC (Bui, et al., 2018), but for small-scale systems physical adsorption processes are advantageous due to their inherently dynamic nature and low specific energy demand. For PCC vacuum-pressure swing adsorption (VPSA) is attractive as the feed can be at atmospheric or slightly elevated pressures, and vacuum pumps draw the CO_2 from the sorbent material, requiring less energy than thermal regeneration in absorption processes (Jiang, et al., 2020).

This study presents the validation and scaled-up of a dynamic VPSA process model developed in gPROMS Process™, utilising the flowsheeting environment to design the CO_2 adsorption system and using the custom isotherm model to predict the adsorption capacity and CO_2 capture rate. Zeolite 13x chosen as the adsorbent material due to its high CO_2 selectivity and high adsorption capacity at low CO_2 partial pressures. Within each packed column the adsorption amount is calculated through the dual-site Langmuir isotherm model, and validation against pilot-scale data from (Krishnamurthy, et al., 2014) showed the model can accurately predict flow profiles, recovery rate and CO_2 purity. The process model is then used to study cleaning an exhaust flow from a small-scale open-cycle gas turbine (OCGT). The flexible response scenario is based on realistic load changes of an OCGT during a 5-hour period. The OCGT has an output power rating of 10.4 MWe and produces 33.8 kg/s of exhaust with 4.27 vol.% (4.42 mol.%) CO_2 (Wilkes, et al., 2021). To handle the size of flow the system is split into two identical two bed four step VPSA units, enabling the use of smaller columns and allows for better flow control. The results show how the key performance indicators (CO_2 recovery rate, CO_2 purity, and specific energy demand) fluctuate during periods at low-load, assuming load following capture plant operation.

Keywords: CO_2 Adsorption, VPSA, PCC, Flexible Operation, Dynamic Modelling

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Exergoeconomic assessment of the optimized vapour-recompression assisted column for palm-based fatty acid fractionation

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Abstract

Energy utilization has become the major factor in analysing overall distillation column costs. It is of paramount importance to chemical industries to discover alternatives towards energy efficient operation. Many researchers have drawn their attention to the development of external heat integration system; heat pump assisted distillation. In our previous study, vapour recompression (VRC) proved to have a promising energy performance in the case of palm kernel oil (PKO) fatty acid fractionation [1]. Apparently, employment of heat pumps in the process would result in the loss of system energy [2] which was not covered in the study. The measurement of the potential work loss and energy quality can be done through exergy analysis. This paper therefore extends the research on industrial PKO fatty acid fractionation by applying this excellent thermodynamic tool to further enhance the energy utilization by integrating four conventional vacuum fractionation columns with VRC. The simulation of the integrated system is carried out in Aspen Plus V12.0 employing the thermodynamic model of UNIQUAC. Meanwhile, a two-step optimization procedure of response surface methodology is also incorporated to the design with the aid of Design Expert, for the sake of a more sensible outcome. The optimized system is then assessed in terms of its exergetic and economic performance. Capital and operational expenses subsequently compliment the analysis by providing future profit estimation should the exergy performance of the integrated system seems appealing. There are two prerequisite condition that need to be complied during simulation study; exchanger temperature approach of 10 °C and maximum operation temperature of 250 °C to prevent chemical degradation. Despite limited flexibility and familiarity of the PKO fatty acid feed, the successfulness of this research will serve as a benchmark for a more environmental-friendly as well as cost-effective oleochemical separation processes in the future.

Keywords: oleochemical fatty acid, VRC, exergy, process optimization, heat pump.

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A Reduced Population Balance Model for Coupled Hydrodynamics and Mass Transfer in Shallow Bubble Column Reactors

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Abstract

Bubble columns are gas-liquid reactors which are intensively used in chemical industries because of their simple design and efficiency. Shallow bubble column reactors have special design that is characterized by a low height-to-diameter ratio when compared to traditional columns. This can reduce gas pressure drop and make use of the relatively high gas holdup when the distributer is properly designed. The bubble size distribution is an important design parameter that defines the gas–liquid interfacial area which plays an important role in designing and scaling-up shallow bubble column reactors. In this contribution a new mathematical reduced population balance model is developed based on the SQMOM with its base form OPOSPM (Attarakih et al., 2013) to predict the coupled bubble hydrodynamics and mass transfer in shallow bubble column reactors. The model is composed of four partial differential equations where two of which are used to describe the total number and volume bubble concentrations and the other two transport equations are devoted for chemical species balances. Other consecutive equations are used to model the bubble relative velocity, growth, breakage, coalescence, interphase mass transfer, and reconstruction of bubble probability density. The relative simplicity of the model offers the bubble column designers one-, two- and three-dimensional models that can be implemented in complex CFD codes. The model capability to predict the steady state interfacial area concentration in the bubbly flow regime is intensively validated using data in vertical bubble columns. In addition to this, the experimental data for the coupled hydrodynamics and mass transfer in the shallow bubble column reactor of Lau et al. (2012) is successfully reproduced by the present model. The steady state bubble holdup is calculated and compared to the experimental data using different gas velocities with air-water system at 25°C. Moreover, the experimental time evolution of oxygen concentration in the stagnant liquid phase is compared to model prediction successfully. In conclusion, the model is simple and still efficient for modelling bubble column reactors with the essential phenomena captured by the detailed population balance model with considerable reduction in CPU time. The limitation of this model can be relaxed by extending the model using the SQMOM with multiple sections.

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Modeling of the crystallization of gypsum produced in the digestion tank of an industrial phosphoric acid manufacturing process

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Abstract

In the phosphate industry, phosphoric acid is a major component in the manufacture of fertilizers. It is mainly produced by the digestion of phosphate ore by a concentrated sulfuric acid solution. The optimization of the process performances is very challenging and aims (i) to extract the maximum amount of P_2O_5 from the ore, (ii) to crystallize and precipitate a gypsum with optimum filterability and washing characteristics, (iii) and to produce the most concentrated and purest phosphoric acid possible, at a lower cost and with little impact on the environment. In this work, we focus on the crystallization of gypsum which strongly influences the performance of units downstream of the process (e.g. filtration units) as well as the possibility of upgrading gypsum in order to reduce its impact on the environment.

The present communication deals with the development of a crystallization model to enable the prediction of the amount of gypsum produced as well as the time-varying crystal size distribution during phosphoric acid production. A population balance model (Randolph, 2012) is thus developed as well as a Pitzer thermodynamic model (Pitzer, 2018) to predict primary and secondary nucleation and crystal growth rates. Both models involve unknown parameters to be identified from experimental measurements. For this purpose, two databases are used, (i) a first one contains equilibrium measurements such as water activity and solubility data, and is used to identify the unknown parameters of the Pitzer model, (ii) then a second database which contains temporal profiles of supersaturation ratio, is used to determine the nucleation and growth unknown parameters.

The estimability analysis approach that we have recently developed (Bouchkira et al., 2021) is used to determine the most estimable parameters of the models which are then identified using a global optimization solver. The resulting system of equations is finally solved using the method of the moments. The simulation results are in good agreement with the experimental data thus showing the good accuracy of the developed crystallization model. The latter can now be used in the optimization of the performance of the phosphoric acid process.

Keywords: Gypsum crystallization, Population balance model, Pitzer model, Estimability analysis, Method of moments

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Development of a whole-body physiologically-based pharmacokinetic model for high-dose methotrexate

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Abstract

Physiologically-based pharmacokinetic (PBPK) models are a class of compartmental pharmacokinetic models whose compartments are based on the anatomical structure of the organism. Whole-body PBPK models generally consist of a large number of compartments, representing the fluid volumes within several organs and tissues, and emulate the actual human anatomy and physiology. Each compartment is usually described by a differential equation representing the drug material balance, and the overall system of equations features a large number of parameters. Part of such parameters can be estimated and assigned a priori, e.g., from experimental measurements. However, the parameters that cannot be assigned a priori require a fitting procedure, leading to numerical and identifiability issues. In this context, minimal PBPK models lump similar compartments, thus reducing the complexity of the model and the identification procedure.

We present the development of a whole-body PBPK model for high-dose methotrexate (HDMTX, an intravenously administered antitumor drug), that expands a previously developed minimal PBPK model (Pesenti et al., 2021a) by increasing the number of described body compartments. The additional parameters introduced to expand the previous model are obtained by combining a detailed physiological characterization of fluid volumes and blood flows in each tissue (Pesenti et al., 2021b). These parameters are thus assigned a priori, allowing the development of a whole-body PBPK model with few adaptive parameters that do not increase the complexity of the identification procedure. The model features 64 body compartments and is successfully identified and validated with an experimental dataset of 657 plasma concentrations. Plasma predictions show a satisfactory agreement with experimental data. Furthermore, the detailed simulation of concentration trends in each modeled compartment provides greater insight thanks to their physiological interpretation. Finally, this modeling approach can serve as a reference for the development of other whole-body PBPK models.

Keywords: Pharmacokinetics, PBPK, Whole-body, Methotrexate, HDMTX.

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Analysis of an industrial adsorption process based on ammonia chemisorption: model validation

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Abstract

In chemical hazards, ammonia is a component that deserves careful study to protect the health of exposed people. Indeed, when used in large quantities, for example, in agro-chemistry, building and civil engineering, waste treatment and recycling, ammonia can be dangerous to the respiratory tract. Its concentration in the air should therefore be minimized and controlled. One of the most used processes to reduce the ammonia concentration in the air is adsorption. In this work, an industrial ammonia adsorption process used in air purification, where ammonia is adsorbed on a doped activated carbon, is considered. The latter is stacked in a parallelepipedic bed and placed in the centre of a box equipped with a feed and an outlet. The box is designed so that air highly concentrated in ammonia is sucked through the fixed bed of activated carbon, and the purified air is recovered at the outlet. The fixed bed is replaced once the ammonia starts to breakthrough, and naturally, the idea is to reduce the frequency of the renewal of activated carbon. To this end, different adsorption models are developed ranging from a simple single-scale LDF model to a complex multi-scale model (Cardenas, 2021; Cardenas et al., 2021). All these models are identified and then tested with additional breakthrough front measurements performed at three gas flow rates and two concentrations, different from those used for parameter identification. The objective is to statistically validate these models and use them in order to optimize the design and operation of air purification boxes. Many validation tests are used to statistically validate the predictions of the models. They include the Student t-test, the Fisher-Snedecor F-test, and the chi-square test. However, the use of these parametric statistical tests requires normal distributions
of the model predictions and measurements which are very often not respected. To overcome this problem, the Kolmogorov-Smirnov non-parametric test is used. In addition, the performance of the models is evaluated using different criteria such as the Pearson correlation coefficient, the root mean-squares error, the (modified) index of agreement, and the chi-square error. The results show that the multiscale model passed all statistical tests and has the best evaluation criteria. In addition, it best fits the experimental measurements and can now be used to study the effect of different operating conditions in air purification boxes in order to increase their lifetime.

Keywords: Air purification boxes, Ammonia adsorption, Doped activated carbon, Experimental measurements, Model validation

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CFD modeling and simulation of an ammonia adsorption process

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Abstract

The increase in air pollution produced by gases such as ammonia has been demonstrated to be a global concern. Controlling pollutant emissions at the source is the most effective way to reduce total air pollution and protect human health. However, if this is not possible, pollutant concentrations should be targeted with preventative and abatement measures used to help reducing exposure to the remaining air pollution. Due to increased ammonia emissions, there has been a growing interest in developing ammonia removal technologies. One of the most used process to reduce the ammonia concentration in the air is the adsorption process. This study aims to use CFD based modeling to investigate ammonia adsorption on a doped activated carbon. The purification box used for this study is the Filagric K100 from Honeywell SP Défence. It has a parallelepidic shape and consists of four main parts: an inlet channel, a doped activated carbon fixed bed, an air extractor and an exhaust duct. Ammonia adsorption on a doped activated carbon is studied experimentally, followed by detailed modeling of the processes that occur in the box. The hydrodynamic and adsorption models are implemented and solved using COMSOL Multiphysics software in the 5.6 version. The Brinkman equation module was used to simulate the fluid dynamics since it allows us to account for both the turbulent character of the fluid flow and the transport of species in the porous domain at the same time. The steady-state solution of the hydrodynamic model was first computed, then different adsorption models were added and solved under transient conditions using the velocity profile obtained by the simulation of the hydrodynamics. Adsorption was investigated by means of three different models: LDF, single-scale Fickian and multi-scale Fickian. The results of the simulations were then compared to the experimental data under various feed rate operating conditions. After that, the COMSOL optimization tool is used to determine the optimal values of the estimable parameters and their confidence intervals for each model. The fluid dynamic of the purification box was simulated in 3D, whereas ammonia adsorption was modeled in 1D as only one component of velocity is significant in the fixed bed domain. The performance of the predictions of the models was examined using several statistical criteria such as the RMSE and the Pearson correlation coefficient. The Fickian multi-scale model has proved to be the best fit with experimental breakthrough profiles for various inlet airflow rates through the comparison of its predictions with experimental measurements. Although there is still room for improvements by modeling adsorption in 3D, the model may now be used in the design and optimization of air purification boxes in order to extend their lifetime.

Keywords: Air purification boxes, Ammonia adsorption, Doped activated carbon, Experimental measurements, Modeling and simulation

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ElectrolyteMedia: A Modelica package for the modeling of aqueous electrolyte systems

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Abstract

Aqueous electrolyte solutions often are complex systems containing numerous dissolved species that may dissociate and interact with potential gas and solid phases. Modeling these systems is increasingly gaining attention for the design and optimization of processes, where species concentrations become relevant. With our Modelica package *ElectrolyteMedia*, we cope with the challenge of modeling such complex systems while ensuring dissociation and phase equilibria combined with the rigorous representation of species interaction by using detailed thermodynamic models.

For this purpose, we implement multiple Media packages for the representation of gas, liquid and solid phases, as well as combinations thereof. The packages are extended from the Media package provided in the Modelica Standard Library (MSL) (Modelica Association, 2021). To use the underlying functions in the Media package for the calculation of thermodynamic properties of a considered system, the *BaseProperties* model given in the Media package is instantiated in a user-specific dynamic model. Generally, the degrees of freedom of the *BaseProperties* model within a Media package are the independent mass fractions and two further intensive thermodynamic properties to fully specify the thermodynamic conditions. The main feature of the *ElectrolyteMedia* library is the simultaneous incorporation of the law of mass action and isopotential conditions in the *BaseProperties* model to represent dissociation and phase equilibrium. The number of considered dissociation and phase equilibria reduces the number of independent mass fractions, as they become dependent on each other. As a result, the number of degrees of freedom is reduced, and, hence, the independent mass fractions may not be set arbitrarily. Instead, we project the mass fraction vector to the reaction invariants that remain constant at a predefined overall composition (Moe et al., 1995; Kakhu and Pantelides, 2003). The reaction invariants and two further intensive thermodynamic properties are then the degrees of freedom of the *BaseProperties* model. Mathematically, reaction invariants may be interpreted as a linear combination of the mass-based atom balance.

In general, the representation of dissociation and phase equilibria requires special attention as this entails the global minimization of the Gibbs free energy (Smith and Missen, 1982). The first-order Karush-Kuhn-Tucker (KKT) conditions of the Gibbs free energy minimization problem lead to the relaxed law of mass action and isopotential conditions that include a slack variable for the consideration of vanishing species and phases (Biegler, 2010; Ploch et al., 2019). In electrolyte thermodynamics, the Gibbs free energy curves of each phase are generally convex, as otherwise a phase split is possible. Due to this convexity, the KKT conditions are both necessary and sufficient

for the global minimization of Gibbs free energy. Hence, the description of chemical equilibrium with the law of mass action and the isopotential conditions is a suitable approach.

The species concentrations in electrolyte systems may vary by different orders of magnitude and the underlying thermodynamic equations are nonlinear. Hence, the initialization of an electrolyte system in chemical equilibrium is challenging. As a remedy, we include an initialization procedure based on a Newton algorithm that provides mass fractions at dissociation and phase equilibrium (Smith and Missen, 1982). Similar to the *BaseProperties* model, the inputs to the algorithm are the vector of reaction invariants and two further intensive thermodynamic properties, namely temperature and pressure. The procedure iteratively performs Newton steps with updated residuals and Jacobian of the underlying algebraic system of equations to approach the equilibrium composition, while limiting the Newton step size such that species concentrations are always non-negative.

To model a dynamic aqueous electrolyte system, we instatiate the *BaseProperties* model that incorporates the initialization procedure and write mass balances in terms of reaction invariants. We can then integrate the initialized model with solvers provided by a simulation environment, e.g., Dymola (Dassault Systèmes AB, 2020). We show simulation results of multiple case studies ranging from the simulation of titration experiments to industrial unit operations. To illustrate the capabilities of dealing with numerous dissociating species with concentrations changing by different orders of magnitude, we provide exemplary simulation results for the titration of phosphoric acid in Fig. 1.

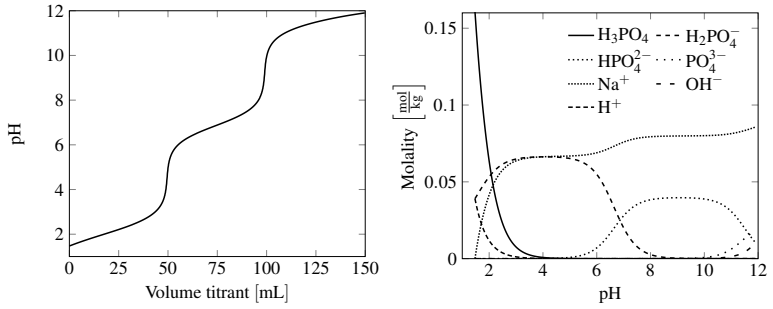

Figure 1: Titration of a 25 mL solution with 0.2 $\frac{\text{mol}}{\text{kg}}$ phosphoric acid with a titrant with 0.1 $\frac{\text{mol}}{\text{kg}}$ NaOH.

Keywords: Modelica, electrolyte thermodynamics, dynamic modeling, chemical equilibrium

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Polygeneration from sugarcane industries enhanced by functionalizing novel cultivars and excess thermal energy

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Abstract

In the context of sustainable developments, polygeneration of crop-derived production processes will have a significant role. For many crops, agricultural operations are followed by industrial processing, and the residues may be used as fuel for operations. However, many crops need to be adapted to local environmental changes, and as new cultivars such as high-yielding cultivars, are introduced, the balance between product and residue yields will change dynamically. Therefore, factories that are considering expanding their functions hereafter need to plan their facilities replacements carefully, considering the balance between maintaining production yield and efficient production of by-products. This study focuses on polygeneration in the sugarcane industry and aims to support the planning of equipment replacement to functionalize new high-yielding cultivars and excess thermal energy using computer-aided process engineering.

A process flow model was developed to simulate the mass and heat balance around a bagasse boiler in a sugar mill, and was incorporated into the already developed integrated modeling of agricultural and industrial processes for sugarcane-derived products (Ouchida et al., 2018). The constitution of cultivars over the next decade were estimated, and the expected sugar production and corresponding required steam, and bagasse production were input into the simulation. The mass and heat balance of the plant for each year was calculated with two cases; a) a boiler was designed based on the current process by fixing the UA value, and b) a boiler was designed to maximize the amount of electricity sold at 10 years later.

As a result, if the boiler is designed to supply the steam required for the current processes, a large amount of heat and bagasse will be left over when the high-yielding cultivar is applied 10 years later. On the other hand, if a boiler with a large heat transfer area designed to maximize energy utilization 10 years from now is replaced at the present time, the sugar mill will not be able to operate because the temperature of the final flue gas will be below the acid dew point due to too large heat exchanger compared to the heating value of bagasse combustion.

Keywords: Sugarcane bagasse, Bagasse boiler, Process modeling, Integrated modeling.

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Sustainable Analysis of Recent Acid Gas Removal Configurations in LNG Production Process

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Abstract

The growing global demand for natural gas increases the pressure on the depletion of natural resources, consequently the significance of natural gas treatment. The variety of wellhead and gas processing conditions and required product specifications place huge challenges and burdens on selecting optimum schemes to meet economic and technical targets of the different project circumstances. Given the huge investment associated with gas processing plants, selecting optimum and fit-for-purpose treatment methods undergoes a rigorous selection process to allocate the most cost-effective and environmentally friendly treatment scheme to remove contaminants. This study analyzes the sustainability dimension of recent Acid Gas treatment schemes associated with Liquefied Natural Gas (LNG) production using Aspen simulation techniques and sustainability metrics. The acid gas treatment process is crucial in LNG production to reduce CO_2 and H_2S from the sour feed gases for safety and environmental concerns. Evaluating the improvement in the acid gas treatment schemes depends mainly on the initial conditions of the sour feed gas, specifications of treated sweet gas, and environmental limitations. The most effective treatment scheme must demonstrate economic effectiveness, accept different feedstock compositions, and achieve sulfur specifications in addition to the highest measures of reliability and quality performance. The recent advancement in acid gases removal units (AGRU) demonstrates the addition of an enrichment step using a low-pressure pre-flash column of Amine solvent along with a tail gas treatment (TGT) unit. The full-integrated scheme includes low BTX AGRU, Acid Gas Enrichment (AGE), Sulfur Recovery Unit (SRU), TGT unit, and common regeneration. The techno-economic evaluation shows the excellence of this technology advancement in providing more flexibility in terms of feed gas quality and efficient adjustment in plant operations. Moreover, the slight increase in the equipment cost is associated with huge environmental improvement and a more integrated system with lower operating expenses and higher efficiency. Performing a case-by-case optimization study is essential to achieve the optimum capital and operating costs and the largest operating parameter window concerning sour feed gas quality.

Keywords: Acid gases removal units, Amine solvent, sour gas quality, Acid gas enrichment, LNG production

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Economic optimization of a reactive distillation column with multiple reactive sections for silane production.

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Abstract

Solar cell manufacturing is based on solar grade silicon which can be obtained using silane as precursor. Silane is produced by redistribution reactions of trichlorosilane. The redistribution reactions of trichlorosilane to silane are carried out in three consecutive stages with rather unfavorable reaction kinetics and a thermodynamic conversion close to zero. These reactions have been studied in intensified equipment such as reactive distillation columns, where the redistribution reactions and the separation of silane are carried out simultaneously. The conventional reactive distillation column scheme for silane production involves a single reactive section where all three reaction stages are carried out. However, Zang et al. (2017) have proposed a scheme with multiple reactive sections to enhance the internal mass integration and/or energy interaction between the reaction operations and the separation operations involved, leading to a great improvement of the performance compared to the single-section system. By adopting multiple reactive sections within the column, more degrees of freedom are allowed for synthesis, design, and process optimization. Thus, this work aims to optimize the multisection reactive distillation column for silane production. The number and location of the reactive sections are part of the optimization variables. The optimization results show significant advantages in reducing the process's total annual cost because the coordination of the three reaction stages is achieved. The additional degrees of freedom result in an optimal integration of the internal mass and internal energy interaction between the reaction and separation operations involved, representing a reduction in economic terms. It can be concluded that a reduction in the economics of the multi-section reactive distillation process was achieved with respect to the single-section process for silane production. It should be considered of general importance to implement and optimize reactive distillation columns that separate complicated reactive mixtures involving multiple reversible reactions in multi-section schemes in order to try to make the processes less expensive.

Keywords: Silane, Multi-section, Global optimization, Reactive Distillation

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A multiscale model of proliferating and quiescent cell populations coupled with cell cycle dynamics

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Abstract

The cells which are subject to division can be categorized into two compartments of proliferating and quiescent cell populations. The proliferating phase represents the cells in all cell cycle phases (G1-S-G2-M) committed to division at the end of cycle. The quiescent cells neither grow nor divide due to insufficient growth conditions, however they transit to proliferating phase upon receiving sufficient growth signals. The balance between proliferating and quiescent cell populations thus play a crucial role in maintaining homeostasis in cell population.

There exist various mathematical models which study the interaction of the two compartments at cell population level. However, the impact of cell cycle proteins on population dynamics, which play an essential role in the cell division mechanism at microscale, has not been studied thus far. Therefore, the focus of this paper is to analyse how deregulation in the balance between proliferative and quiescent compartments, resulting from variations in cell cycle dynamics, can lead to an unlimited tumor growth.

This paper proposes a nonlinear multiscale mathematical model for age-structured proliferating and quiescent cell populations (PDEs) coupled with cell cycle protein dynamics (ODEs). The model further assumes a bidirectional transition between the proliferating and quiescent subpopulations. The coupling between the two scales is introduced on the basis of biological findings inherited from the literature. Thereby, the transition rates between the two subpopulations are defined based on the cell cycle protein concentrations (microscale model), whereas the growth factors derived from total cell population of proliferating and quiescent cells (macroscale model) trigger the cell cycle dynamics. Numerical solution is derived using finite volume method, wherein fluxes are computed by central upwind scheme.

Most of the parameters used in this study are chosen from the literature and the impact of perturbation in the parameters (which theoretically demonstrate a tumor scenario) has been examined via numerical simulations. The coupling of the model and feedback regulation mostly ensures the
robustness and stability of the model, however there are some situations under which model predicts an unstable behavior. Thus, it has been found out that the complex formed by Cyclin D with its inhibitor CDK 4-6 plays a dominant role in the bi-directional transition and some shortcomings in this transition can result in tumor growth.

The proposed model assumes the homogeneous behavior of the cell cycle proteins in the whole proliferating cell population, which is a strong assumption. However, it is intended for the future study to extend the current cell cycle model to stochastic settings which can incorporate the noises and cell to cell heterogeneity lying at the microscale level.

Keywords: Multiscale model, Tumor growth, Population dynamics

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Multi-objective optimization of the food chain as a support for the development of agricultural sector

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Abstract

Motivation: The food supply chain is a complex system that includes the production of agricultural crops and animals, their processing into food products, distribution and consumption of food, and the collection and processing of waste. The agricultural sector is one of the main sources of environmental impacts and is accompanied by a number of uncertainties (Zirngast et al., 2019). There is a need to optimize this system (Põldaru et al., 2018) to determine the optimal distribution of cultivated land that would ensure greater self-sufficiency in locally grown food. This needs to take into account objectives such as the reduction of greenhouse gas emissions, the use of artificial fertilizers, nitrogen inputs, preservation of biodiversity etc. (European Commission, 2019).
Methods: This paper presents a mathematical model formulated as a Linear Programming problem (LP) that determines the optimal distribution of arable land for human consumption and animal feed. The amount of food produced, greenhouse gas (GHG) emissions, nitrogen intake, amount of food waste, etc. are calculated. Production technologies are conventional, organic or conservation agriculture, food production in greenhouses, etc. Several objectives are considered, such as overall self-sufficiency, self-sufficiency for human consumption, GHG emissions, nitrogen input to soil, amount of food waste, economic efficiency, etc.
Results: The paper shows the results of the optimizations of each objective and the normalized weight average of all objectives. The results are useful in guiding national agricultural policy as they indicate the need to promote a shift from intensive meat production, especially cattle, to grass-based production and to change people's dietary habits from meat and meat products to a greater proportion of vegetables. The promotion of organic farming and other unconventional forms of agriculture is another driving force for reducing the environmental impact of agricultural production.

Keywords: food chain, locally produced food, optimization, MILP, multi-objective.

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Efficient design space identification for superstructure optimization subjected to parameter uncertainty

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Abstract

In superstructure optimization of processes and energy systems, the design space is defined as the combination of unit considerations, process conditions and model parameters. Many of the parameters are subjected to uncertainty, such as resource and product prices or impact factors. Investment decisions on industrial energy systems for example are normally based on short-term profitability criteria and assumptions on current and future investment, operating and resource costs (Turton et al., 2008). However, those assumptions are often proven to be wrong retro-perceptively (Moret, 2017). When designing systems and providing assistance to informed decision-making on investments, it is crucial to ensure the robustness of the configurations against this uncertainty, thus to make sure a selected design is attractive despite variations in design space parameters. This might be challenging, since modeling complex systems under uncertainty can be computationally expensive (Beland and Nair, 2016).

The aim of this research is to support the efficient generation of a set of meaningful solutions for a decision-maker by applying a Bayesian methodology to predict Pareto-optimal solutions that are robust under parameter uncertainty. Firstly, an initial dataset is generated by running the original optimization model for a set of design space configurations. Design space configurations in this regard contain sets of parameters subjected to uncertainty. The concept of robustness is addressed and quantified by recalculating -a posteriori to optimization- the 95% of the desired objectives for each solution under the assumed parameter distribution. These newly calculated objectives are used to define the robust Pareto-front. A set of design space parameters and the corresponding solution obtained from optimization is evaluated on their performance of the robust objectives regarding Pareto-optimality. For this, the ε-Pal algorithm for Pareto-front identification by means of machine learning presented by Zuluaga et al., 2016 and implemented by Jablonka et al., 2021 is applied. The algorithm is based on an adaptive learning concept which systematically identifies the next best function evaluation to improve the confidence of the Pareto-frontier identification. For making predictions, Gaussian Process Regression models are applied. The algorithm identifies design points with a high probability of being Pareto-optimal regarding the defined objectives, and evaluates them by calling the original model. The confidence of the Pareto-front prediction is increasing, while simultaneously, the relevant design space is reduced, as in each iteration points are either identified as Pareto-optimal or discarded.

The described methodology is applied to the efficient design of an integrated industrial biorefinery, where a Kraft pulp mill is enriched with biomass-based process units that

convert excess electricity and biogenic residual streams such as bark and black liquor to storable energy in the form of fuel. Optimizer decisions in this regard include system configurations which contain the installation of units as well as the obtained unit sizes. The robust Pareto-front is derived for the 95% of operational expenditure (OPEX) and capital expenditure (CAPEX) given the assumed parameter distribution. Design space parameters subjected to uncertainty include price assumptions for resources, e.g. natural gas, water, electricity and wood, products provided, e.g. pulp, electricity, water and fuels, equipment cost, equipment lifetime and interest rate. Correlations identified prior to the application of the analysis indicate that the two selected objectives are correlated to different design space parameters, which is intuitive when looking at the definition of OPEX and CAPEX. We apply the ε-Pal algorithm to a design space of 17 parameters subjected to uncertainty, and we generate a set of 1000 samples that are continuously labeled, discarded or identified as Pareto-optimal by the algorithm.

First results indicate that the ε-Pal algorithm is a suitable tool to provide an estimation of the robust Pareto-front at good quality, since the points identified as Pareto-optimal are the same as the ones identified when manually labeling all the points in the design space by calling the original optimization. Furthermore, it is observed that the algorithm always manages to identify the important design points, thus the ones close to the currently identified robust Pareto-front, labels them by calling the original optimization model and therefore achieves to continuously improve the prediction confidence in the relevant domain. For a sample set of 1000 datapoints, the algorithm does currently not yield any time savings as the prediction quality is rather low, which results in the algorithm calling the original model all of the sampled dataset. However, for a larger dataset of 2000 samples, only 36% of the samples are labeled by calling the optimization model, the remaining points can be classified as Pareto-optimal or discarded by the algorithm in five iterations. Compared to labeling all points in the dataset with optimization, time savings of 59% are achieved.

We are convinced that improving the machine learning models integrated in the algorithm will help to increase the overall prediction performance, and we hope that we will be able provide efficient exploitation of the design space even for smaller datasets.

Keywords: energy system optimization, machine learning, uncertainty, design space, active learning

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Conceptual Design of Liquid Hydrogen Receiving Terminal

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Abstract

The liquid hydrogen (LH_2) has become an essential energy carrier in storage and transportation because of its high energy density, which makes inevitable to construct transport infrastructure for liquid hydrogen. However, the critical issue of the liquid hydrogen storage comes from the boil-off gas (BOG) generation due to the cryogenic condition. Several studies have been performed to develop the LNG receiving terminal. Park (2012) suggested the optimum operating conditions for BOG handling in the existed LNG terminal to reduce the operating costs of the compressor. Rao (2018) performed the optimization of the superstructure of the LNG terminal to minimize the total annualized cost. Since the configuration of LH_2 terminal considering BOG re-liquefaction is not yet developed, the LH_2 terminal process is modeled, and then the case studies are performed to investigate the impact of the design variables to the energy consumption.

LH_2 terminal sends liquid hydrogen from the storage tank to vaporizer to produce gaseous hydrogen product. The boil-off gas is pressurized by BOG compressor and sent to the recondenser. The BOG is re-liquefied by contacting the cold LH_2 stream in the recondenser. In this case, the LH_2 stream is called as send-out. When the recondenser does not fully liquefy the BOG, the high-pressure (HP) compressor is operated to send the BOG to the gaseous hydrogen product. Modified Benedict-Webb-Rubin (MBWR) is used to calculate the thermodynamic properties of hydrogen as described in Roder (1975). The heat transfer model of the tank is established based on the references by Kumana (1982) and Majumdar (2008) to estimate the boil-off rate (BOR). The volumes of the tanks are selected as 3,000 m^3 and 10,000 m^3. The geometry of the tank such as insulation thickness or wall thickness is based on the reference by Daigle (2013). Since BOR is proportional to the total heat Q within the tank, heat transfer equation is applied. The overall heat coefficient U for spherical tank is suggested by Bergman (2011). The convective heat transfer equation of the fluids is introduced by Majumdar (2008). The BOR shows the range from 0.01 to 0.92 %/day depending on the tank size and the insulation material.

Since the HP compressor requires a large amount of energy as reported by Park (2012) and Rao (2018), the several case studies are performed to investigate the energy consumption of LH_2 terminal. The design variables are set as the insulation materials, the tank size, the residence time of the tank which is defined as the time required to empty the tank by releasing the send-out, and the operating pressure of the recondenser. The insulation materials selected for this process are perlite, glass bubble, and vacuum insulation, and their thermal conductivities are brought from Fesmire (2004). The

residence time is varied from 5 days to 20 days, and the operating pressure is controlled from 4.5 to 12.5 bar.

The base case of the analysis is selected as 3,000 m^3 of the tank volume, perlite insulation, 5 days of the residence time, and 4.5 bar of operating pressure of the recondenser. The energy consumption of the base case is calculated as 146.0 kJ/kg. If tank volume is increased to 10,000 m^3, the energy consumption decreases from 146.0 kJ/kg to 136.9 kJ/kg due to the increased amount of the send-out which contributes to the re-liquefaction in the recondenser. When the residence time increases to 15 days, the energy consumption becomes 218.8 kJ/kg. This is because the boil-off gas is not fully re-liquefied due to the small amount of the send-out, resulting in the increase of the HP compressor duty. If the insulation material is in vacuum condition, the energy consumption reduces from 146.0 kJ/kg to 130.3 kJ/kg due to the decreased heat transfer to the tank. The effect of the LP pressure depends on whether the HP compressor is operating or not. Since the base case does not operate the HP compressor, when the LP pressure increases to 12.5 bar, the energy consumption becomes 158.1 kJ/kg due to the increased duty of LP pump and BOG compressor. When HP compressor is operating, however, if the residence time is 20 days, the energy consumption changes from 313.0 kJ/kg to 259.8 kJ/kg when changing the LP pressure from 4.5 to 12.5 bar. This is because the higher LP pressure reduces the differential pressure of the HP compressor, resulting in the reduction of the energy consumption.

Overall, the configuration of the terminal decides whether HP compressor is in operation, which induces the higher energy consumption. If the amount of send-out is sufficient to re-liquefy the boil-off gas, using the inexpensive insulation material is enough to operate the terminal. If operating the HP compressor is inevitable due to the small amount of the send-out, however, then increasing the operating pressure of the recondenser helps reducing the energy consumption. The optimization will be performed to find the optimum operating conditions to minimize the energy consumption as a future work.

Keywords: Liquid hydrogen, Receiving terminal, Boil-off gas, Re-liquefaction

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Optimal CO2 allocation and scheduling in enhanced oil recovery (EOR) operations in Qatar

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Abstract

Carbon capture and storage (CCS) is one of the most efficient techniques for reducing carbon dioxide (CO_2) emissions into the atmosphere. Combining CCS with enhanced oil recovery (EOR) processes is a very attractive method for carbon capture and utilisation (CCU). These operations enable CO_2 emissions to be reduced through geological sequestration, whilst generating additional revenue from enhanced oil production due to CO_2 re-injection via EOR. In practice, mass balance and temporal features of a given location are considered when planning EOR operations. When numerous oil reservoirs are involved, it is vital to allocate available CO_2 supplies and schedule EOR operations for these reservoirs at suitable timings. As a result, CO_2 allocation and scheduling are crucial for maximizing the economic benefits of EOR operations. As such, this study introduces a resource trade scheme for CO_2 integration and utilisation within the state Qatar, where a mixed integer linear programming (MILP) model is developed to address CO_2 allocation and scheduling based on environmental and economic objectives. The model considers a single CO_2 source (Qatar Gas) within an multi sink scenario in an industrial park setting which includes (QAFCO, QAFAC, PEARL GTL, ORYX GTL, Dukhan Field Well (EOR)). Different scenarios are considered to allocate CO_2 to different sinks (including EOR) to obtain the optimal solution for each scenario.

Keywords: EOR, CO2 allocation, Sustainability, Carbon Dioxide, Carbon capture and storage (CCS)

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Optimal operation of a batch evaporator for the controlled production of Titania nanoparticles

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Abstract

Titania nanoparticles are a useful building block for materials with photocatalytic activity or specific optical properties (Gupta and Tripathi (2011)). The production via the hydrolysis of an alkoxide precursor (Iskandar (2009)) involves a distillation step which is both time consuming and energy-intensive and that is needed to control the final particle size (Vorkapic and Matsoukas (2005)). The concern of this paper is the optimization of the production process by manipulating the trajectory of a batch evaporator, with the goal of maximizing energy efficiency under predefined production constraints, namely the final particle size and the final solids fraction. The problem of developing a suitable model for the process is addressed, with regards to the necessary assumptions. A direct, moment-based model is employed here (Hulburt and Katz (1964)), as it balances descriptive accuracy and implementation effort. The optimization problem is formulated with respect to the process model and the results are presented. It is shown that, compared to the non-optimized operation, it is possible to achieve both energy and processing time savings. Depending on the production constraints, significant reductions in energy consumption are possible, while simultaneously reducing the total processing time. The relevance of the findings is twofold: first, the reduction in energy consumption is beneficial in containing the overall carbon footprint of the process. Secondly, in the situation where electricity from intermittent renewable sources is available, it is possible to tailor the trajectory of the process to exploit this availability efficiently. The project leading to this publication has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 820716.

Keywords: titania, nanoparticle, synthesis, trajectory, optimization

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A model-based approach for predicting banana rust thrips incidence from atmospheric variables

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Abstract

Banana is one of the most important food crops in the world, contributing to the food security of billions of people by providing income and employment to rural populations through exports (Galantini, 2014). In the last ten years, Peru has joined the large community of organic banana exporting countries, with the main production located on its northern coast, reaching around 223,298 tons of organic bananas exported in 2019 (FAO, 2020). Since 2010, red rust thrips have become a serious pest in organic banana plantations, causing yield losses of 30%-40% (Arias de Lopez et al, 2020) if effective measures are not applied.

For this reason, tools that help in the decision-making process of farmers to reduce as much as possible this pest are needed. Precision agriculture offers technologies that can support this development. In this contribution, the development of a mathematical model for the prediction of pest population based on atmospheric variables is introduced. IoT sensors located in an organic banana plot (1 ha area) are used to gather these data. These models are based on population development concepts described by first order differential equations. It improves on existing models, such as the Campbell model (Donatelli et al., 2017) by considering ambient humidity, rainfall and wind speed.

The new additions improve the model predictions significantly and allow farmers to make better decisions to prevent pest infestation and reduce production losses as much as possible.

Keywords: Mathematical model, IoT sensors, Precision agriculture, Organic banana, Red rust thrips.

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Comparison between 3D numerical simulations and experimental results of a lab-scale liquid-solid fluidized bed

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Abstract

The high consumption of fossil fuels is running out the petroleum sources, therefore it is extremely important to improve the efficiency or diversify the industry's main route. To deal with those new processes, the liquid-solid fluidized bed is one of the available technologies. Mastering this complex industrial device requires a better understanding of the intrinsic multi-scale hydrodynamics couplings that play an important role between solid and liquid phases. For that reason, the numerical simulation of multi-phase flow has become an useful tool for examining the particle behavior in fluidized beds. The fluidized bed simulation may be addressed using the Discrete Element Method (DEM-CFD) approach, which is a model that requires a lot of computational effort, because of the large scale of the equipment and the huge number of particles. So for industrial purpose, this approach becomes infeasible, and simulations are carried out in the frame of Euler-Euler model such as implemented in the NEPTUNE CFD code (Neau et al., 2020). But such approach was originally developed for gas-solid flows and specific model developments and validation studies are needed for liquid-solid fluidized bed (Gevrin et al., 2010). This is one of the main objectives of the MUSCATS project (N°ANR-19-CE05-0010-02) which is carrying out an innovative multi-scale modelling program for liquid-solid fluidized beds, based on complementary numerical approaches and carefully designed experiments. In a first stage, 3D numerical simulations were performed using the NEPTUNE CFD code on a laboratory configuration in order to asses the model assumption and to compare the mean and fluctuating fluid and particle velocity predictions with available experiment data from Aguilar-Corona (2008). Thus, some discrepancies on fluid and particle kinetic fluctuating energy and areas of improvement are identified and proposed in order to capture accurately the particle–fluid and inter-particle interactions in the liquid-solid fluidized bed.
Keywords: CFD, Euler-Euler, Fluidized bed, Liquid-solid bed

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Heat Transfer Identification in a Continuous Millireactor via CFD

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Abstract

Millireactors are steadily gaining importance in the chemical industry. While the production of high-volume chemicals has relied on continuous flow processes for quite some time, specialty chemicals and lab-scale processes still typically utilize batch processing. Batch reactors are well established and valued for their flexibility, but cannot offer the same level of energy efficiency, yield, and control over process conditions (Calabrese and Pissavini, 2011). This is particularly true for temperature control, where the large surface to volume ratio of continuous reactors enables fast heat transfer and homogeneous temperature distributions (Roberge et al., 2014). This ratio can even be maintained during scaleup (Biessey and Grünewald, 2015), reducing the need for pilot stages and facilitating the move from lab to production scale.

Millireactors are often characterized experimentally. Since they are small yet complex devices, especially when featuring internal mixing structures, this may pose problems as many of their properties are not readily available (Grünewald and Heck, 2015). An example are large temperature gradients, which cannot be accurately captured due to measurements only being possible at certain points. This may lead to an incomplete or even incorrect understanding of the conditions inside these reactors. Numerical simulations of the fluid dynamics and heat transfer simulations are well suited to fill in the gaps and offer additional insights, as demonstrated in our previous work (Begall et al., 2018).

In this contribution, we examine a special testbed for the Miprowa millireactor (Ehrfeld, 2021) by Ehrfeld Mikrotechnik, shown in Figure 1, with CFD. It consists of a rectangular channel with a cross sectional area of 12x1.5mm and a length of 50mm, containing three layers of exchangeable inserts with variable geometry to ensure thorough mixing of the process fluid. This channel is contained in a solid body of copper, which is enveloped by a service fluid for temperature control in a countercurrent flow configuration. The main aim of the testbed is to determine the heat transfer coefficients of the reactor. To this end, the testbed allows the experimental measurement of inlet and exit temperatures of the process fluid, as well as temperatures at two points in the copper body, for different mass flow rates and service fluid temperatures. Due to physical limitations, such as the measurement points being not close enough to channel walls, this however results in only approximate determination of heat transfer coefficients from the measured data.

To overcome these limitations, we setup a CFD model of the reactor using the finite element analysis software COMSOL Multiphysics (COMSOL, 2021). The model incorporates physics interfaces for both fluid flow and heat transfer, and enables simulations with either bidirectional coupling between these, or one-directional coupling using a segregated approach, where only the influence of the fluid flow on the heat transfer is considered. Both approaches yield similar results that closely match the experimental data, which validates the model and suggests that the influence

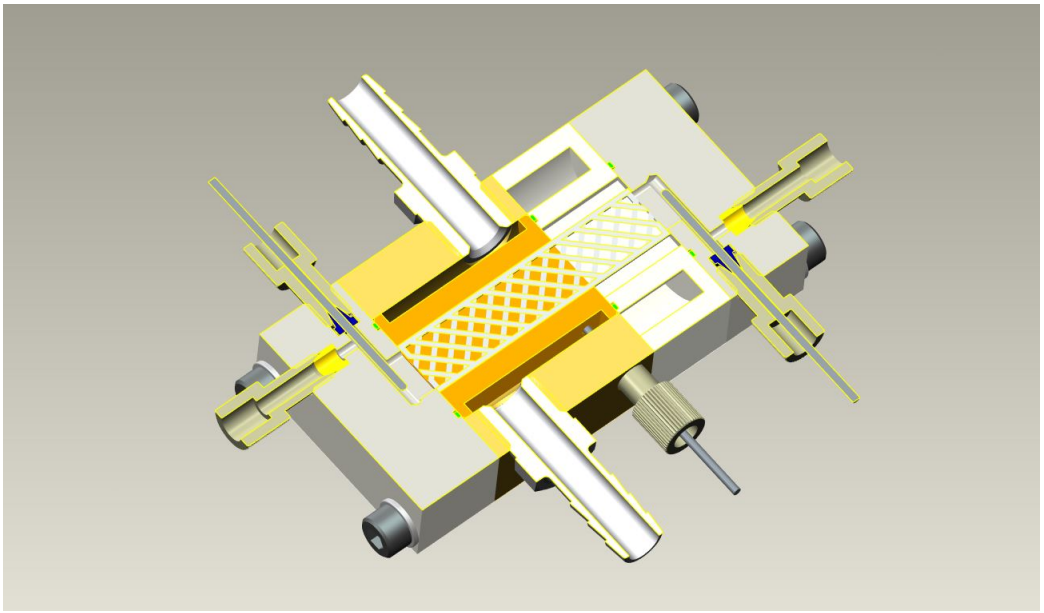

Figure 1: Cut through the Miprowa reactor testbed.

of the temperature on the flow field is indeed negligible.

A major benefit of the model over the physical testbed is the ability to calculate process values not only at specific measurement points, but also at arbitrary points in the domain, thus giving detailed and locally resolved information on fluid flow, temperature distribution and heat transfer, and providing a “look into the reactor”. Further, it is utilized to reconstruct the wall temperatures of the reactor channel, allowing the exact calculation of the heat transfer coefficients of the reactor, for a wide range of process conditions. This includes extrapolations for very low flow rates, which are not experimentally measurable at all.

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Keywords: Millireactor, CFD, Heat transfer, Modeling

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Bio-inspired wave-breakers to reduce swell erosion in the Bay of Biscay, using CFD

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Abstract

With the potential rise in sea level, linked to climate change, coastal management is one of the main concerns of coastal countries (Lacroix *et al*., 2019). Climatic deregulation, associated with the rise in sea level, can accentuate coastal erosion. In France, for example, 270 km of coastline are eroded by more than 50 cm a year. One of the main causes, in France, is swell. This swell generates bi-directional seafloor currents and their speeds are directly linked to erosion.

Several solutions exist to fight against the erosive effects of swells, including wave breakers. Their main problems are that they protect a limited area and that they can increase the erosion upstream and downstream of protected structures (Boulet *et al*., 2018). Therefore, existing wave-breakers can't be a long-term solution to the problem of coastal setback.

This work focus on a part of the France coastline, the Bay of Biscay. It is facing the Atlantic Ocean, it is in a mesotidal area and it is exposed to energic and moderate-to-long period swells (Dodet *et al.*, 2019). Working on the Bay of Biscay allows to quantify the efficiency of the solutions to coastal erosion in an energetic swell context.

The biomimicry and the bio-inspiration are a way to find solutions to our problems and this, for a long time. It is important to understand that biomimicry isn't a goal but a way to find innovative solutions to modern problems. In the wilderness, there are several examples of natural or biological structures that reduce sea currents impacts. There are for example the *Torquigener albomaculosus*' nest and the mangroves' root system. Both inspirations are shapes that are known for slowing the current (Kawase *et al*., 2017; Thom, 1967). Both shapes have inspired two new types of immerged wave-breakers. They have been modelized with CAO on CatiaR2021X®.

The interaction between the wave-breakers and the swell in the Bay of Biscay has been simulated with the software Xflow®2020, using Computational Fluid Dynamics and especially Wall-Modeled Large Edgy Simulations techniques. The results have been treated by a Python algorithm. The analysis of the seafloor current speed allows quantifying the efficiency of the wave-breaker and to see if the model increases the erosion in the non-protected zones.

The experimental data needed to validate the simulations were provided by the scientific literature. Because the results of the control simulations and of the simulation with existing wave-breaker shapes coincided, the results of the other simulations should be relevant too, even if test bench experiments will be performed later in order to deepen these results.

This paper is a proof of concept on the idea of creating bio-inspired wave-breakers that are not increasing the erosion upstream and downstream. The simulations' results show that the nest-inspired shapes are increasing the erosion in the non-protected areas. On the contrary, the mangrove-inspired wave-breakers could divide by two the seafloor current speed (From 0.82 to 0.49 $m.s^{-1}$) without increasing erosion in the non-protected zones. It could be a possible improvement to slow the coastal setback in the Bay of Biscay. A test bench simulation will be

performed in order to deepen these results soon. This study is in a mesotidal area. Results could be different in a macro or microtidal site.

Keywords: wave-breaker; bio-inspired; Computational Fluid Dynamics (CFD); Lattice-Boltzmann Method (LBM); Wall-Modeled Large Eddy Simulation (WMLES)

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Non-process elements in kraft bleach plants: adsorption equilibrium aiming at reducing water consumption

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Abstract

Over the last decades, the pulp and paper production industry has made an effort to reduce freshwater consumption in the process. Currently, water consumption in modern plants is about 25 m^3/tAD (Huber et al., 2014), but further reductions have been explored to make pulp and paper production more sustainable. This point is particularly important when the mill is located in water-scarce areas or if groundwater is used.

The bleaching is responsible for ca. 50% of the water used in a pulp mill (Huber et al., 2014), contributing to 65% of the effluent generated (Gavrilescu and Puitel, 2007). As a consequence of reducing water consumption, an accumulation of inorganic compounds in pulp streams is observed, namely calcium, magnesium, potassium, and chlorine (non-process elements – NPE). NPE accumulation increases the risk of precipitation, creating scaling problems in equipment units and pipes, and a rise of sorbed elements on the fiber's surface that degrade the pulp quality.

WinGEMS is a simulator specialized in pulp production processes. However, some limitations have been identified in terms of its ability to predict the adsorption and scaling phenomena, generating results with large deviations from the industrial data. This work presents a simulation tool in MATLAB integrated with WinGEMS to improve the prediction of the adsorption processes of NPE on the fibers. The Donnan model was chosen to simulate the adsorption equilibrium and was parameterized for the relevant NPE through laboratory experiments (Donnan and Harris, 1911). Hence, partition constants of NPE in the fiber and suspension phases are described as a function of pH and the streams composition and consistency. The model also considers the fiber characterization, the material balances of the NPE, and the conservation of electroneutrality in the pulp fiber and suspension (Towers and Scalllan, 1996).

The simulation results obtained for streams from an industrial pulp bleaching unit show a clear improvement of the predictive quality of NPE adsorption on the fibers, allowing future retrofitting studies to reduce the water consumption in the process.

Keywords: pulp bleaching, Non-process elements, adsorption, Donnan equilibrium.

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Re-design and scheduling of dairy thermal treatment processes for continuous operation

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Abstract

Heat treatment processes of liquid dairy products (pasteurisation, sterilization) are energy, water and wastes intensive. They are normally conducted in an energy integrated system of 3 plate heat exchangers, PHEs, in batch mode, in heating-cleaning cycles. During cleaning, the whole process is interrupted, causing loss of production.
A new pasteurization process is proposed here using some additional equipment (an additional plate heat exchanger and holding tube) coupled with suitable phase switching logic and scheduling. All design changes and operational strategies are studied using a detailed distributed dynamic model of the process (Sharma and Macchietto, 2021, Zhu et al, 2020). The simulation results for four high-temperature-short-time (HTST) case studies at different flowrate settings highlight an interesting interplay between the flow direction of the fluids in the PHEs (which changes as the schedule changes), as well as the trade-off between fouling mitigation and thermal efficiency. The new switching logic causes each PHE stage to switch from heating to cleaning earlier than in the traditional batch configuration; however, appropriate scheduling of the four PHEs and tubes results overall in a semi-continuous operation where milk production can be maintained indefinitely.
The improved productivity (+23% throughput), energy and cleaning used, and total cost (-47%) of this new design and semicontinuous operation are quantified. Finally, the opportunities arising from the interaction of design and scheduling are briefly discussed.

Keywords: interaction between design and scheduling; dynamic modelling; food processes; heat treatment; fouling and cleaning

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Charactérization of buried artificial reefs using simulation CFD with particule based tracking

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Abstract

Artificial reefs are presented as a possible response to the shrinking biological resource in coastal strip. They are intended to protect, regenerate, concentrate and enhance populations of marine organisms. These structures are used primarily in areas where fisheries resources have been over-exploited or are recovering (Becker *et coll*., 2018, Lima *et Coll*., 2019. The introduction of an object into the seabed generates changes in the flow regime around it, resulting in the formation of basins around the reefs by vortices upstream of the structure (Sumer *et al*., 2001). These processes promote local sedimentary capacity and subsequently lead to burial of the structure. The objective of this study is to minimize the landfill of artificial reefs and optimize their lifetime. We assumed that the burial of artificial reefs is due to their shapes and sediment displacements. Our study was applied to the artificial reefs emerged by the Atlantique lands récifs association on the Atlantic coast in France. Two types of artificial reefs were used in this study; the typi reef that is submerged in 2010 and the babel reef in 2015 make concrete with a depth of 20 m, implant in France in the Atlantic coast in three different places (capbreton, soustons/vieux-boucau, and messanges/azur/moliets and maa). In the first step, we designed the artificial reefs as well as the basins on a CATIA V6® design software and then imported them on an XFlow®2021 simulation software. This software uses Computational Fluid Dynamics. It uses a Large Eddy Simulation approach by solving the Boltzmann and the Navier-Stokes equations. With these fluid simulations, we were able to simulate the turbulence. With multiphase simulation, we carried out the modelling of the landfill in order to see the impact of the currents on the artificial reefs. We also observe the phenomena of turbulence and the motion of the sand which create these basins. Our results obtained by simulation validate our hypotheses, indeed, these eddies near the zone of the reefs, we also observe losses of load that occur downstream of the reef which produces to the creation of these basins. To minimize the burial of artificial reefs, ideally, it will be necessary to review the shape of the reefs while considering all the factors related to this landfill. Subsequently, our simulation results were experimentally validated by different devices. We designed a test bed to get as close as possible to the real environment, and taking measurements and with a 3D FDM printer, we were able to produce miniature PETG models of artificial reefs that we used in the latter. The aim of these experiments was to validate the results of the simulations carried out so that they could be extrapolated by change of scale.

Keywords: artificial reef's, burial, Xflow®2021, Computational Fluid Dynamics, multiphase simulation.

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Metamodeling of chemical engineering unit operations using Kriging and prediction error estimation

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Abstract

Metamodeling, or surrogate modeling, refers to the production of a simplified model of an actual model. Such techniques are widely used when the actual model is judged inapplicable or with difficulty in a given context (computing efficiency, informatic complexity etc.). In chemical engineering, actual process models are in general phenomenological ones from molecular scale to plant scale. Challenges arising are thefore to be able to mimic the 'local' behaviors such as stiff non-linearity and discontinuities (activation processes, reactions, thermodynamics, transfer, phase change etc.), while being appropriate in the whole physical domain. The goal here is to evaluate
how Kriging is a suitable method to catch such behaviors, and how to use the ability of Kriging to estimate the prediction error in the whole domain to sequentially build a metamodel.
Three emblematic categories of unit operations are chosen as toy-problems: a molecular separation (binary separation by membrane gas permeation), a heat exchanger (with supercritical CO_2 fluid) and an exothermic catalytic reactor (water-gas shift reaction). The Kriging implementation of OpenTURNS (https://openturns.github.io/www/) is used here, which is an open-source software for data analysis, metamodeling, and treatment of uncertainties (Baudin et al., 2016). Kriging, also called gaussian process regression, is an interpolation method between observations points, i.e. simulation results with the actual model, which provides analytically both the metamodel (mean of gaussian processes) and an estimation of the prediction error in the whole domain (using the variance of the gaussian processes). In this work, starting from a small design of experiments, an iterative algorithm is used to sequentially complete experiments in regions with highest prediction errors, until a given satisfaction criterion is reached.
The procedure using Kriging and sequential addition of new points proved its ability to catch particular behaviors observed in chemical engineering unit operations, and allows to efficiently explore the search space by refining optimally the design of experiments. Notably, nonlinearities near the thermodynamic critical point and stiff reaction fronts are well metamodeled, as these regions are detected with the local prediction error. In addition, less simulation points are required than for other methods. For instance, the metamodeling of gas permeation required 2200 points with a neural network, where 600 are sufficient here to reach a similar accuracy. It is therefore recommended to use metamodeling techniques with a local estimation of the prediction error, rather than an overall estimator (R2, Q2 etc.) providing only a general fit and potentially
missing specific, yet crucial, behaviors of the actual model.
Keywords: Metamodeling, Kriging, separation, heat exchanger, reactor

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On the integration of process engineering with metabolomics for the production of muconic acid: the case for *Saccharomyces Cerevisiae*

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Abstract

Muconic acid is a high value product which has gathered interest in applications in the manufacture of new resins, bio plastics, food additives, agrochemicals and pharmaceuticals. Lots of efforts have been made for an economically viable biotechnological strategy for muconic acid production but as of yet have been fruitless. Directed evolution and DBTL cycles hold important promises for the development of future catalysts with high efficiency and productivity. However, process engineering is typically disjointed from these cycles and more often than not the mismatch of kinetics presents a major challenge and a bottleneck in the scaling up of novel bioprocesses.

The paper addresses the integration of metabolomics and experimental data using the optimization and risk analysis of complex living entities (ORACLE) platform combined with clustering and advanced analytics. The methodology consists of six steps. In the first step, the stoichiometry of the system is defined through biochemical data and experimental data are integrated into the model to further constrain it. In the second step, steady state fluxes and metabolite concentrations are calculated based on metabolomics analysis. In the third step, kinetic parameters for every reaction are sampled to fit in with the steady state fluxes based on mechanistic kinetics expressions. In the fourth step, consistency checks and pruning consider the stability of the system and the consistency with experimental data. In the fifth step, the flux control coefficients for the desired metabolite flux are calculated based on the well-established metabolic control analysis (MCA) framework.

In this project, large-scale mechanistic kinetic models for a muconic acid producing S.Cerevisiae strain were developed using the aforementioned ORACLE platform. A total of 23500 of potential kinetic models were generated out of which 372(1.58%) passed the pruning step and 70(0.12%) models out of the 372 passed the stability check. Enzymes such as glucose-6-phosphate isomerase (PGI), transketolase (TKT2) and enolase (ENO) had large control coefficients on muconic acid flux.

Keywords: S.Cerevisiae; muconic acid; metabolomics; metabolic engineering ; large-scale kinetics;

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Modelling and simulation of a residual lignocellulosic biomass pyrolysis pilot plant

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Abstract

The present work has been devoted to the study, modelling and simulation of a pilot scale pyrolysis plant feed with residual agricultural residues (peach and olive pits) located in Catania, Sicily. A global model representing the process flowsheet was created with Aspen Plus® software and was fed with actual experimental data obtained in the existing pilot plant. The aim has been to develop a flexible simulation model in which different types of local agricultural residues could be fed to the reactor and stablish the optimal conditions for each case. Raw materials' characterization included ultimate and proximate analysis, and biochemical composition (cellulose, hemicelluloses, lignin, and inorganics contents). All these data were implemented in the simulation for the feedstock definition. The base scenario was established by feeding 30 kg/h of biomass under a pyrolysis temperature between 600 and 800°C. The decomposition of the organic matter was defined as a two-stage process: a first decomposition of the organic fraction into a residual solid fraction (char) and a gaseous mixture, and a subsequent cooling of the mixture to separate the condensable part and to obtain the pyro-oil and the permanent gas stream. This latter stream of gas was used to generate thermal power that could be used to support the energy requirements of the pyrolysis process. To reproduce the degradation of biomass and the resulting evolution of chemical species, a new mathematical model, based on the operative temperature and the reaction kinetics was developed. The simulations were designed in order to maximize the gas fraction and minimize the char one. The obtained results were discussed in terms of compound yields (58% gas, 20% bio-oil, 22% bio-char), and energetic content of the generated pyro-gas (about 30 MJ/kg).

Keywords: residual lignocellulosic biomass, simulation, pyrolysis.

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Techno-Economic-Environmental Analysis of Biodiesel Production by Magnetic nanoparticles Cleas of EVERSA® Transform

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Abstract

The urgency of reducing carbon emissions has been constantly reinforced by the scientific community. At the same time, there has been a constant growth in the global demand for energy. In this sense, techno-economic-environmental studies are essential to assess the feasibility of new technologies, seeking a carbon neutral economy. Biodiesel is a biofuel that has many environmental and social advantages, as it replaces its fossil equivalent. However, the production of biodiesel presents problems related to the primary raw materials and the chemical catalysts used. In this context, enzymes are an alternative to solve these problems. The use of Cross Linked Enzymatic Aggregates (CLEAs) together with magnetic nanoparticles allows the reuse of the enzyme, reducing operating costs. In this scenario, this work studied the production of ethylic biodiesel, by transesterification of soybean oil with bioethanol, catalyzed by the enzyme Eversa® Transform 2.0, immobilized in the form of CLEAs. Two distinct purification processes were assessed, distillation and washing of biodiesel. The study was based on process simulations developed in Aspen Plus and EMSO. Economic feasibility was assessed by the net present value, while environmental performance assessment was based on CML-IA midpoint indicators. Both sensitivity and uncertainty analysis were done in order to identify the main process parameters affecting the process performance. As the main results, the purification method did not significantly influence the technical and economic performance. On the other hand, since the distillation process requires fewer separation steps and material inputs, its environmental footprint was smaller than that of the washing process. The economic performance of the process was more sensitive to the reuse of the enzyme, with five reuses (value based on the literature) being insufficient to reach an economic performance superior to the current industrial process based on alkaline homogeneous catalysis.

Keywords: Biodiesel, LCA, techno-economic analysis, eversa® transform.

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Numerical Analysis of Impellers Hydrodynamics Performance in a Bioreactor CSTR with SPH

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Abstract

The biotechnology industry has become very important in recent years, due to the high demand for products derived from biological systems. The main part of these processes, is the bioreactor design which that must fulfill certain requirements that are needed that will ensure the fermentation process efficiency, such as: the agitation speed, the aeration rate, the heating intensity or cooling rate, and the nutrients feeding rate, acid or base valve. The impellers establishing homogeneity in bioreactor, because is this is an especial attention in the mixing, since it is the one that establishes the homogeneity in the reactor of both dissolved oxygen and substrate concentration. So to avoid oscillations in the homogeneity in the culture media, may lower the system efficiency, increase the plasmid instability and produce undesirable and products. Recently, the Computational Fluid Dynamics (CFD), is important for scaling reactors; it is a very useful tool to analyze in detail the hydrodynamics and mixing in bioreactors of agitated tank, which are commonly, used in microbial fermentation processes. CFD allows the numerical solution of the transport equations by computational means. It can generate a huge amount of information that in practice could not be obtained experimentally, or they are very inaccessible by the experimental route, also is an effective strategy to improve or ensure the performance of a process. For this reason, in this paper we analyzed the flow domain of the fluid was simulated three-dimensionally applying the computational fluid dynamics (CFD). The developed model was validated through experimentally. The performances of the impellers in this work they were compared respect to the mixing time, fluid velocity profiles and mixing efficiency. For the simulation of the culture medium, the properties of the viscous fluid resulting in the production of xylitol were considered, which are: ρ= 1240 kg/m^3 and η = 1.587x10-5 m/s^2. This simulation was realized using the DualSPHysics code, using the Smoothed Particle Hydrodynamics (SPH) method. The results validation obtained, shown that the SPH method is capable of reproducing hydrodynamics in stirred tank bioreactors. We compared the hydrodynamic performance of three impellers: anchor, propeller and Rushton, in which it was possible to predict stagnation zones and speed profiles that guarantee a more homogeneous mixing. The optimal impeller for a stirring speed of 200 rpm is anchor.

Keywords: CFD, hydrodynamics bioreactor, SPH

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On the use of embedded models and advanced analytics to model complex processes in the cement industry.

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Abstract

Data-driven models hold significant promises to improve modelling capabilities. Their ability includes the development of deep learning using input-output relationships, model reduction of complex systems and the development of embedded surrogates to improve lower-accuracy models. Cement production offers notable challenges in the analysis of two-phase heterogeneous mixtures considering flow with distributed solid particles as in the case of ball mills. Since cement plants involve energy intensive processes, the development of good models could assist in reductions of energy consumption, and the better use of design parameters to improve the process operation and to meet quality standards. Modelling challenges include the low accuracy of constructions that rely solely on first principles, the need to customize the models using online measurements, and an ambition to reduce the complex space into a simpler, agile constructions to use for decision support. To that purpose, the paper explains a generic and systematic approach in the development of embedded models that could be further used for model reduction. The systems approach makes a structured and systematic use of data as they are produced at three distinct stages: simulation assignments by means of spatial differential equations, optimization runs that regress parameters for each simulation, and deep learning training that converts parameters into functions of system variables. Simulation models refer to steady-state operations of closed-circuit grinding models formulated as differential equations with parameters treated as degrees of freedom. Simulations use the gPROMS Model Builder with its built-in validation module. Mass balances involve 10 particle size intervals axially distributed for each compartment of a ball mill. For each mass balance, the equations include convective mass transfer, diffusion, and breakage phenomena. Quadratic optimization is subsequently assigned to regress real-life data available from the industrial site. For the dry cement plant, different sets of simulations are repeated for a wide range of operating conditions and product specs. Combined with optimization, simulation runs eventually produce sets of input-output data where inputs are the process input (or specs) with the output assigned as the best set of regressed parameters from the quadratic optimization. The data populations are used to train deep learning models and yield process parameters now as functions of the system input. Rather than conventional models where parameters are regressed to minimize errors, the proposed model is producing model parameters as functions of the system variables. Deep learning methods rely on ANNs and are compared with conventional models available using conventional regression methods. Findings indicate a 17-28% increase on Blaine prediction accuracy over the analytical model this method was applied to.

Keywords: Embedded Model, ANN, Deep Learning, Cement Grinding, Ball Mill

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Aspen Plus® modeling approach of beechwood gasification in a fluidized bed reactor using biochar as bed material

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Abstract

Biomass processing is considered a strategy changer in the development of new pathways for green energy production, being the thermochemical processes as pyrolysis and gasification part of the main methods used to produce renewable fuels (Mohabeer, 2019). The purpose of this work is to perform a simulation of the gasification process of biomass using biochar as bed material under Aspen Plus® software. The simulation is supported by the experimental data obtained in our laboratory and published in several journals (Reyes, 2020). The gasification is preceded by a biomass pretreatment process in which the biomass (beechwood pellets) is defined under Aspen Plus® as a non-conventional solid. The biomass is dried to be processed in the RYield reactor which is supported by a set of correlations that were obtained in function of the different gasification temperatures and were set in the simulation using the calculator of Aspen Plus®. This process allows a good reproduction of the gasifier outlet flows. The simulation and experiments were made using different gasification agents (H_2O and CO_2) and the temperature was varied in the range of 600-900°C (Reyes, 2021).
As shown in Table 1, the gasifier predicts syngas, tar and coal yields with a great similitude to the experimental results. This represents a validation step of the simulation. The latter gives a chance to make further evaluations of the gasification variables.

Table 1. Comparison of the experimental and simulated producer gas streams

	Outlet mass flow using different gasifying agents (g/min)			
	H_2O		***CO_2***	
	Experimental	**Simulation**	**Experimental**	**Simulation**
CH_4	4.976	4.976	1.15	1.143
H_2	0.561	0.563	0.081	0.081
CO	20.297	19.976	9.681	9.651
CO_2	19.619	19.776	53.971	53.635
C_6H_6	0.003	0	0.075	0.073
$C_{10}H_8$	2.225	2.23	0.512	5.11
C_6H_6O	8.206	8.271	1.562	1.551
CHAR	13.28	13.515	13.04	12.93

Keywords: Biomass, Gasification, Biochar, Fluidized bed, Simulation, ASPEN PLUS.

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Chemical-looping system modeling for the analysis of oxygen carriers and CO_2 capture benefits

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Abstract

The chemical looping combustion (CLC) is regarded as an efficient technology for power generation at low environmental loads due to its ability for CO_2 capture. The CLC technology consists in avoiding the direct contact between fuel and air during the combustion process, allowing full oxidation of the fuel while preventing the mixtures of nitrogen and flue gases. This process is carried out by dividing the reforming reaction into two separate reactors (oxidation and reduction), connected through a looping mechanism of oxygen transportation. The development of an oxygen carrier (OC) with appropriate attributes is crucial to take full advantage of the CLC technology in terms of low environmental loads. Therefore, this study aimed to perform a detailed simulation of the CLC process to analyze the relation between OC's physical attributes (Density, porosity, available volume for reaction, etc.) and the profitability of the process. Results of a case study for methane combustion using an Iron-based OC shows the impact of the OC's volume for reaction on the economic benefit of the process, considering a constant power output.

Keywords: Chemical Looping Combustion, Oxygen Carrier Evaluation, CO_2 Capture.

Method

This study performed a steady-state simulation analysis of a CLC system of two moving bed reactors by employing open-source rigorous models from the Institute for the Design of Advanced Energy Systems (IDAES) process engineering framework (2021). The method comprised four main stages, a flowsheet design, an initialization procedure, a flow-sheet optimization, and a sensitivity analysis. The mathematical model for the reactors consists of a one-dimension discretization set of differential equations obtained through the application of mass, energy, and momentum balances proposed by Ostace et al. (2018). Equation 1 presents the governing functions for mass and energy balances, respectively. As can be observed here, the gradient of conversion of any component with respect to its axial location, $\frac{\partial C_i}{\partial z}$, is given by the superficial velocities of the solids and gas, $u_{g,s}$, the reactor bed voidage, ε, and the general rate of reaction for the gas and solid phases, r_{gen}. As for the energy balance, the gradient of temperature, $\frac{\partial T_i}{\partial z}$, is given additionally by the specific heat capacity, $C_{\mathrm{p_{g,s}}}$, heat transfer coefficient, h, and enthalpy of reaction ΔH_{rxn}.

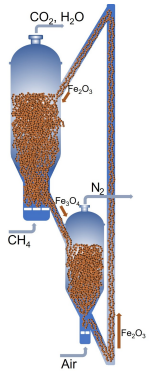

Figure 1: Moving Bed CLC

$$\frac{\partial C_i}{\partial z} = f(u_{g,s}, \varepsilon, r_{gen}), \qquad \frac{\partial T_i}{\partial z} = f(u_{g,s}, \varepsilon, C_{\mathrm{p_{g,s}}}, h, \Delta H_{rxn}, r_{gen}) \tag{1}$$

$$TAC = Min = \phi * f * TEC + TOC, \qquad MSP_{CO_2} = TAC * F_{CO_2}^{-1} \tag{2}$$

The flowsheet was then built by coupling the reactors through a loop of an oxygen carrier, as shown in Fig. 1. To initialize the flowsheet variables at feasible values, this study used the adap-

tive Wegstein procedure proposed by Iumanova and Solodushkin (2016). Later, the optimization mechanism was performed using the Pyomo open-source algebraic modeling language (Bynum et al., 2021). The objective function and the expression to evaluate the profitability of the process are shown in Equation 2. Here, TAC stands for the total annualized cost of the CLC system, ϕ represents the annualization factor for the interest rate, f is the installation factor cost, TEC is the total equipment cost, and TOC is the total operating cost. The indicator used to evaluate the profitability was the minimum selling price for pure CO_2 (MSP_{CO_2}) when the rate of return is equal to zero, defined as the division of TAC into the annual production of CO_2 (F_{CO_2}). Lastly, the sensitivity analysis was performed by evaluating the variations on the OC's physical properties with respect to the variations on the MSP. The case analyzed was a combustion looping of methane, CH_4, using moving bed reactors connected through a flow of an iron-based oxygen carrier, FeO_x. The inlet flows considered for CH_4, air, and FeO_x at 273.15 [K] and 153 [kPa] were 128 [mol/s], 1587 [mol/s], and 591 kg/s, respectively. The optimization of the process was conducted aiming to obtain MSP_{CO_2} by the variation of a_{vol} and market price of the OC, subjected to conversions of CH_4 and OC higher than 99.0%.

Results

Results show a MSP_{CO_2} value of 151 [\$ / ton-CO_2], which represents a benefit of \$110.5 in contrast with the current CO_2 market price in Japan. (OC price= 1200 [\$/ton-OC], and $a_{vol} = 0.28[-]$). Besides this, we were able to determine the relations of the OC's attributes and the economic benefit of the process. For the current case study, we determined the variations of the minimum selling price with the increment of OC's volume rate available for reaction. Figure 2 shows the results of the sensitivity analysis performed for the variations of the market price of the oxygen carrier in contrast to its available volume rate and minimum selling price. It is important to note the significant reduction of the MSP when a_{vol} is greater than 30%, implying that the process remains profitable even when the market prices of the OC increase. This analysis suggests that the efforts in the development of Iron-based OCs with a large capacity of oxygen transportation will be paid off through costs reductions in OC inventory and reactor equipment.

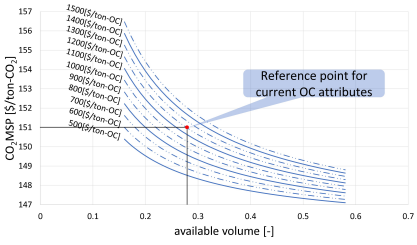

Figure 2: MSP vs a_{vol} (IRR=0)

Conclusions

This study demonstrated the capability of the model developed to generate a robust simulation for the analysis of the chemical looping combustion system, allowing the detailed analysis of techno-economic factors (e.g., price and OC available volume (a_{vol}), which are critical for the scaling and development of this new technology. In addition, this study has contributed with a guide for the investigation of oxygen carriers properties that might improve the profitability of the system.

Acknowledgment

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Mathematical modeling of the diffusion-limited (DLA) aggregation accompanied by particles swarming in reactors

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Abstract

This article is devoted to the development of a new approach to modeling aggregation processes in poly-disperse systems taking into account multi-particle collisions (Brener, 2014), which is of fundamental importance at a high concentration of the dispersed phase in the system.

- Motivation: The aggregation process is accompanied by multiple collisions and swarming of particles, which is due to the complex hydrodynamic situation in industrial devices, and it occurs according to various mechanisms. At the same time, the joint consideration of these phenomena and the creation of a calculation method based on more or less simple models that are convenient in engineering calculations, remains a relevant problem.
- Methods: The presented method is an extension of the method previously developed by the authors (Brener et al., 2017, Musabekova et al., 2019) for the case of a three-dimensional stochastic lattice. This paper presents a new approach based on the discrete-event-simulation paradigm (DES) which extends to the case of three-dimensional lattices. This extension increases the practical value and reliability of the simulation results. According to DES (Brener et al., 2017), the region in which the diffusion and aggregation processes occur is covered by a fixed spatial lattice. In this paper, a three-dimensional array is considered to describe aggregation in the case of kinetics limited by the particle diffusion rate (DLA) with allowance to the swarming process.
- Major Results: The novelty of this approach lies in the fact that it allows one to study the distribution of clusters of different orders over the reactor volume at different times, taking into account multi-particle collisions. Computer simulations were carried out for both batch and flow reactors.
- Conclusion: The results of numerical experiments showed that the change in the number of clusters in a volumetric periodic reactor occurs at the initial stage of the aggregation process at a much higher rate than this phenomenon was described by a numerical experiment on a flat lattice. The results obtained can be used as the basis for an engineering technique for calculating industrial reactors for processing poly-disperse systems.

Keywords: DLA aggregation, swarming, many-particle collisions, 3-D stochastic lattice.

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Hybrid modelling of industrial scale fermentation process

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Abstract

The biotechnological industry increasingly applies mechanistic models because it has realized their significance. These models are preferred as they contain relevant scientific knowledge needed to describe the system behavior. Mathematical models are the ideal tool for process optimization and intensification. However, biological systems are notoriously complex, developing such a model can be a massive time and resource investment. To simplify things, first principles models most often utilize an empirical approach to describe growth of the cell culture, while some relations are more frequent than others the list of appropriate equations to choose from is large Muloiwa (2020) and that is only for cell growth, further modeling is needed to account for production of products, substrate uptakes, gas evolution and more.

The production of pharmaceuticals has always had a strong focus on quality. A common method for producing Active Pharmaceutical Ingredients (API) is via biological processes or fermentation of high producing bacteria or fungal strains. These processes have been subject to mechanistic modeling for use in batch optimization, monitoring and control Gernaey (2010). However, the metabolic pathways responsible for the main product can lead to accumulation of related substances in the batch that hamper the final product quality and may be impossible to remove in the downstream process. Mechanistic models rarely take batch quality into account and most model development is focused on main product only.

Due to the complexity of the biological systems a hybrid model approach is used as an alternative. The concept of hybrid modelling in this context is the combination of a first principles mechanistic model and machine learning models into single model. Machine learning and Artificial Intelligence algorithms such as Artificial Neural Networks (ANN), have seen an increase in popularity in various research fields and the use of Hybrid modelling has seen success in chemical engineering such as in particle processes Nielsen (2020).

This study focuses on the application of a hybrid modelling framework on the fermentation of a filamentous fungi that produces Fusidic Acid. A first principles biochemical model is built influenced by existing literature based on penicillin fermentation models Birol (2002). Sophisticated ANN models are subsequently trained to predict the kinetic expressions for the evolution of products and consumption of substrate. The fully integrated hybrid model is subsequentially used for predicting productivity and quality of industrial scale batches currently in production to facilitate further process optimization to maximize the yield of the batch process without compromising the quality of the final product.

Data is collected by regularly sampling tanks located at the LEO Pharma production site in Ballerup, Denmark. The samples are analyzed by measuring the dry weight for biomass concentration. Main product and related substances are measured using an HPLC on the collected samples. PAT package records all other relevant critical process parameters such as pH, dissolved oxygen, temperature and more. A hybrid model is set up to simulate a production batch using a first principles approach. A shallow neural network is set up to predict the specific rate of change of all batch components based on the current batch state and any external inputs to the batch. The output of the neural networks is then fed to a set of ordinary differential equations that describe the overall change in the batch state. The entire setup is built in MATLAB R2021b and solved using the ode15s solver.

While the model is trained on a few selected batches, the model really only needs information about external inputs and initial conditions when simulating a new batch. This information is recorded on all production and lab batches; thus, the model can be validated by running it on an entire year's worth of production data. The performance indicator of interest is how well the models can predict yield of main product and concentration of related substances during the harvest. When predicting the main product, the mean absolute percentage error (MAPE) of all batches was 9.2% with an R^2 value of 0.94, a good performance indication for biological processes. Predicting related substances turned out a bit more difficult as expected but the hybrid model still achieved a respectable performance with an R^2 of 0.89 and a MAPE value of 11.3%. For both main product and related substance concentrations the model follows the overall trend over the entire fermentation process.

Over the course of this work, we've successfully developed a hybrid model to work as a digital twin of an established industrial pharmaceutical process. This work was started because a mathematical model was needed to facilitate process optimization and intensification. However, traditional modeling methods failed to explain the growth of related substances and thus could not predict the quality of the batches. With no biological information on the production strain the collected data was used to train a Neural Network to predict the relevant biochemical kinetics which was then coupled to a first principles model. The established model predicts the quality of the batches extremely well while also able to be competitive to traditional model when predicting the main product. Hybrid models have major potential in the bioprocess industry as they can facilitate key engineering decisions when relevant scientific information is still lacking.

Keywords: Hybrid-modelling, Pharmaceuticals, Bioprocess, Industry, Neural Networks

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Heat-integrated water network synthesis with improved trade-offs in targeting step

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1. Problem statement

For a given number of process water-using units heat-integrated water network (HIWN) targets (freshwater, hot and cold utility consumption) should be obtained before designing an overall HIWN with minimal TAC. Process constraints include operating temperatures, maximum inlet and outlet contaminant concentrations, and mass load of contaminants transferred to water within process water-using units. Environmental constraints include the temperature of the wastewater stream discharged to the environment.

2. Methodology

The HIWN superstructure (Ahmetović and Kravanja 2012) considered in this work consists of freshwater preheating stages with splitting of water after each heating stage as well as wastewater cooling stages with gradual mixing and cooling (Figure 1a).

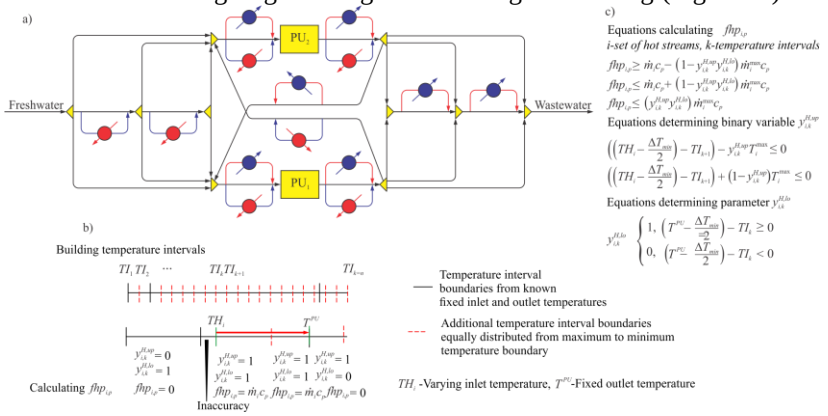

Figure 1: Superstructure, building temperature intervals, and determining heat capacity flowrates in the targeting step of the TransHEN model.

Streams entering and leaving water-using units and streams between water-using units serve as streams for heat integration in this superstructure. Streams entering/leaving process water-using units can be hot or cold. Steams between process units ($p \rightarrow p'$) are identified as hot if operating temperature of unit p is greater than the operating temperature of unit p'. Otherwise, the stream is cold. Based on the proposed superstructure, an overall MINLP model can be formulated and solved in two steps, namely the targeting and the design steps. In the first targeting step the WN (Ahmetović

and Kravanja 2013) is combined with the TransHEN model (Nemet et al, 2019). In this modified TransHEN model inlet and outlet temperatures are considered to be variables for the vast majority of the streams. The fixed (constant) temperatures apply only to the freshwater, process units, wastewater discharged from the HIWN into the environment, and hot and cold utilities. The temperature intervals are constructed to account for the previously listed fixed temperatures in a shifted scale considering the minimum temperature difference. Additional temperature boundaries/intervals are added uniformly across the temperature scale, i.e. between the highest and the lowest temperature resulting from the fixed temperatures (Figure 1b). The higher is the number of temperature intervals, the more accurate is the area cost estimation. The temperature intervals are created as input data for the optimization. During optimization, binary variables are used to select the streams included in particular temperature interval (Figure 1b). The heat capacity flowrate is calculated separately for each temperature interval, based on the binary variables (Figure 1c). The targeting step is used to make all the important decisions about the flowrates, streams selection and type (hot or cold).

3. Case study

A case study presented in Ahmetović and Kravanja (2012) was tested for the proposed methodology. Table 1 presents key performance indicators of two solutions. The TAC with the proposed new approach was 2,201,013 $/y (locally optimal solution), which is about 4.5 % worse than the one presented as the globally optimal solution (Ahmetović and Kravanja 2012). It is worth mentioning that in both cases the freshwater and utility consumption is the same.

Table 2. Key performance indicators of HIWNs and comparison of the results.

Parameter	Ahmetović and Kravanja (2012)	This paper
Freshwater consumption (kg/s)	70	70
Hot utility consumption (kW)	2940	2940
Cold utility consumption (kW)	0	0
Operating cost ($/y)	1,864,380	1,864,380
HEN investment ($/y)	248,189	336,633
TAC ($/y)	2,112,569	2,201,013

4. Conclusions

This paper addresses the synthesis of heat-integrated water networks with focus on the targeting step enabling precise enough decision making about the flows, type of streams (hot/cold), estimated heat transfer and estimated required area, and the selection of promising matches for the design step. The obtained results for a simple case study are in a good agreement with those reported in the literature.

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Surrogate Model for Slurry Pipe Flow Pressure Drop Prediction Using CFD

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Abstract

Pipelines are used to carry liquid-solid slurries in a variety of technical sectors, including mining and chemical processing. They are more efficient and ecologically friendlier than train transportation. However, the flow within the pipeline is typically turbulent and complicated, resulting in issues such as pipe blockage and particulate settling Lahiri and Ghanta (2010). Different factors should be controlled to provide a steady and optimum flow. The efficiency of transport is adequately defined by the specific energy consumption (SEC), which is a measure of the energy needed to deliver a particular amount over a specified distance. It is proportional to the hydraulic gradient immediately, which is a dimensionless quantity that indicates the decrease in static pressure caused by friction in the slurry flow along the pipe's unit length. The lower the SEC, the more energy-efficient pipeline transportation is (Hashemi et al. (2014)).

The primary objective of the present study is to provide the groundwork for intelligent pressure drop management in these types of transport processes using computational fluid dynamics (CFD) simulation models. Indeed, contemporary modeling solutions for industrial processes typically use three-dimensional simulation approaches based on CFD and/or discrete element methods (DEM). These three-dimensional models are then integrated, using surrogate models, for use in operations simulation and monitoring tools (Decision Support Systems) (El Hamra et al. (2022)). Traditionally, response surface methods (RSM) have been used to construct polynomial surrogate models (Rabhi et al. (2018)), but more recently, machine learning approaches such as artificial neural networks (ANN) have been also utilized (Seong et al. (2020)).

The present modeling technique consists in developing a three-dimensional CFD model for a slurry pipe and then using it to create a surrogate that models the pressure drop within this latter. For the CFD modeling, a two-fluid model based on the Eulerian-Eulerian approach along with the $k-\omega$ SST turbulence model is used. To account for particle-particle and particle-wall interactions, the solid phase's motion was described using the kinetic theory of granular flow (KTGF). On the basis of numerical simulations of horizontal pipes with 525 data points, a novel two-phase pressure drop correlation for slurry flows is developed. The suggested model is based on the empirical formula for pressure losses due to friction in horizontal pipes, which is shown in equation (1) :

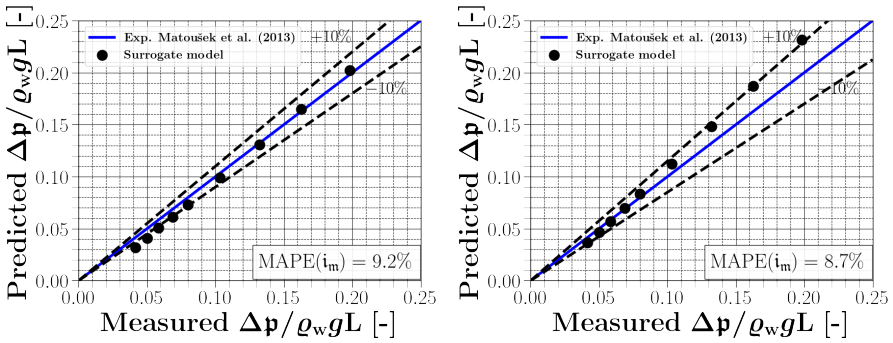
$$\Delta \mathfrak{p}_{\mathfrak{f}} = \mathfrak{f}_{\mathfrak{m}} \frac{\rho_{\mathrm{m}} \mathrm{L}}{\mathfrak{D}} \frac{{\mathfrak{u}_{\mathfrak{m}}}^2}{2} \quad with \quad \mathfrak{f}_{\mathfrak{m}} = \mathfrak{f}_{\mathfrak{w}} + \mathfrak{f}_{\mathfrak{s}}, \tag{1}$$

where the density ρ_{m} and velocity $\mathfrak{u}_{\mathfrak{m}}$ are those of the solid-liquid mixture. The surrogate model is created for the purpose of estimating the mixture's friction coefficient $\mathfrak{f}_{\mathfrak{m}}$. The properties of the phosphate slurry material, at different transport operating circumstances, such as particle size distribution, solid concentration, and velocity fluctuations, are taken into account in the simulations.

The dry solid particle density is of $\rho_s = 2450$ kg/m^3. The particles range in size from $d_p = 44$ μm to $d_p = 250$ μm and the solid mass concentration in the slurry goes from $\phi_s = 20\%$ to $\phi_s = 40\%$. The slurry is transported via a pipe with a diameter of D = 100 mm, with a velocity ranging from 2 to 10 m/s.

Through a minimization approach, the surogate model has been calibrated to identify the friction factor of the slurry mixture f_m, which matches well with the multiphase CFD results. The Levenberg–Marquardt algorithm (LMA) [Marquardt (1963)] is utilized to carry out this optimization process.

After fitting and identifying the optimal f_m, a graphical surrogate model is generated as a function of the particle diameter d_p and the concentration of solids ϕ_s. To assess the model's accuracy, the surrogate model predictions are compared to experimental data published in the literature, using the same physical and geometrical parameters as this study. Parity plots, in Fig. 1, show the good agreement between the predicted and measured hydraulic gradient values. To conclude,



(a) ϕ_s = 20% (b) ϕ_s = 30%

Figure 1: Hydraulic gradient parity graphs between predicted and measured values for different solid concentrations.

the concept of constructing a surrogate model through first principle multiphase CFD simulation has been successful. The advantage of this technique is that it permits the creation of a surrogate model even in the absence of sufficiently big experimental datasets needed for a robust pressure drop correlation for the slurry. Additionally, the constructed model properly estimates the pressure loss for a real slurry running under the input operating circumstances for which it was constructed, with an accuracy of at least 85%.

Keywords: Slurry flows, CFD, Two fluid model, Surrogate models, Horizontal pipelines.

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The Value of Integrated Modeling in support of Determining Optimal Energy and Infrastructure Transition Pathways

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Abstract
The Dutch government requires each industrial cluster in the Netherlands to come forward with plans to lower CO_2 emissions by 50% in 2030 and 100% in 2050 as part of the Dutch Cluster Energy-transition Strategies (CES). This calls for a methodology in which both infrastructure and industry choices need to be aligned in terms of sizing, timing and locations/trajectories. To support this decision process, a QuoMare propriety tool called TEACOS (Techno-Economic Analysis of Complex Options Spaces) is used.

CES Challenges The development of Cluster Energy transition Strategies has a number of key characteristics, like a large set of public and private stakeholders, quite often awaiting each other's key decisions. Stakeholders may miss the ability to oversee the impact of proposed transition projects with respect to timing and effect on the various networks. Furthermore, assurance is lacking that the combined set of proposed projects is sufficiently complete to meet the overall CO_2 reduction goals. At best, it can be shown that implementation of this combined set of projects will meet 2030 or 2050 goals, without ensuring that project investments and delivery over time are accomplished at lowest possible costs at no-regret. Another important challenge in the energy transition space for the clusters is how to best develop, enumerate and evaluate incentive schemes to be proposed by governments such that network owners and industry both move jointly towards most effective and efficient investment proposals. Alternatively, how can industry partners define drivers and boundary conditions for infrastructure owners to identify plans for the best joint financial outcome. Typically, each party trust its own evaluation practices and tools, lacking a high level overall model that brings all elements together to jointly develop a set of coherent energy transition investment proposals.
Scope and Study Design The CES scope for the Rotterdam Port Area includes power producers, refineries, bio-refineries, industrial gas producers, and base chemical facilities. This scope is complemented by an infrastructure network, consisting of the electricity grid, CO_2 evacuation systems, an hydrogen network and the Dutch natural gas network. Decarbonization strategies for the energy-vector of the industrial cluster (energy savings, CCS, hydrogen use, electrification) are incorporated in the model. The model encompasses 35 industrial companies and 14 power producers (coal, gas and waste based), emitting 29 Mton CO_2 per year. The purpose of the TEACOS model is to support policy makers in the development of a cost-effective and robust strategy to arrive at a 50% (or even higher) CO_2 emission reduction in 2030 and 100% in 2050.
Methodology TEACOS is designed to support joint project definition efforts such that all of the above decision elements and project assurance aspects can be addressed in a very structured manner at full transparency to all stakeholders. The large option space requires for a structured methodology to ensure appropriate timing of investments in order

to meet the decarbonization goals. The TEACOS system is data-driven, i.e. all data are stored in an easy accessible database[1]. This allows for efficient sensitivity analysis and robustness analysis (e.g. Monte Carlo Optimization). The model is based on a Mixed-Integer Multi-Period Linear Programming[2] algorithm. TEACOS evaluates the impact of integer decisions (decarbonization strategies) on the objective simultaneously with continuous variables (flows, processing levels) subject to various constraints (like CO_2 targets, infrastructure capacities). The objective is to maximize the Net Present Value of the accumulated Margin, consisting of revenues and costs (for supply, processing, transport, fixed costs and capital expenditures), accumulated over a 30 year horizon.

Main Results TEACOS proposes optimal decarbonization investments for the industrial companies and power producers and corresponding infrastructure investments (for network operators). The model ensures alignment between the choices of industry and network operators. The optimal pathways can depend heavily on the following drivers (but not limiting to): hydrogen price, electricity price, ETS pricing outlook and timing of CO_2 targets.The ETS pricing outlook has a high impact on the decisions of industry and power producers, with consequential impact on the infrastructure. To explain this impact, two scenarios have been evaluated (for illustration purposes): Scenario 1 with a CO_2 ETS price of 30 EUR/t in 2050 and Scenario 2 with a CO_2 ETS price of 160 EUR/t in 2050.

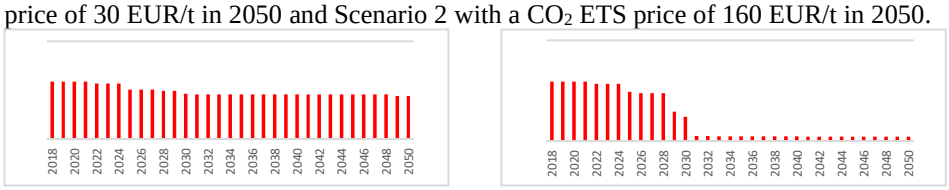

Figure 1: CO_2 Emissions for scenario 1 (left) and scenario 2 (right)

In scenario 1 the CO_2 emission reduction in 2050 is limited, due to the low CO_2 ETS price, indicating that a constraint has to be imposed or that the CO_2 pricing policy needs to be revisited. Scenario 2 shows that a CO_2 ETS price of 160 EUR/ton on 2050, results in a CO_2 emission reduction of more than 90%.

Conclusions The model is considered to provide a structured method that allows for determining no-regret transition pathways, together with the validity window of the basic assumptions, i.e. determining tipping points. In addition to this, the model may illustrate constraints that inhibit optimum pathways to become reality. The TEACOS model can be used in structured discussions with industry, network operators, policy makers, evaluating their role in both an isolated and integrated manner. In this way, the value of industrial/infrastructure symbioses can be significantly enhanced. One limitation of the current model set-up is its implicit modeling of uncertainty. Furthermore, limited attention is given to the social acceptance of possible pathways.

Further Research With respect to scope, effort is geared towards adding decarbonization of the scope 3 emissions, i.e. decarbonization of feedstock/product vector through the use of renewable feedstocks, carbon recycling and re-use of CO_2 with hydrogen. With respect to the methodology, explicit modeling of uncertainty and incorporation of social acceptance criteria are currently part of two separate PhD trajectories.

Keywords: Mixed-Integer Multi-Period Linear Programming, Decision Support, Energy Transition, Optimal Transition Pathways, No-Regret Investments, Policy Making.

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Multiphysics modeling of a continuous flow microwave system

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Abstract

The continuous flow thermal processing of liquid foods aims for the inactivation of undesired enzymes and microorganisms with minimal quality degradation (Tajchakavit, 1998). Microwave-assisted processing is of interest for the food industry due to its rapid volumetric heating. The microwave radiation penetrates directly into the food resulting in high rates of heat transfer and high energy efficiency (Zhu, 2007). The objective of this work was to simulate a continuous flow microwave cavity using COMSOL Multiphysics (v. 6.0) software and validate the model using experimental data from a microwave-assisted pasteurization unit. The Multiphysics model couples the electromagnetic energy propagation to the physics of laminar flow and heat transfer, allowing the prediction of the fluid temperature distribution (Fig. 1b). For accurate temperature prediction, adequate meshing is important. A study of mesh independence was carried out to reduce computational time. The normalized power absorption (NPA), which is a ratio of the power absorbed by the liquid food to the total power fed into the system, was used as a convergence criterion (Zhu, 2018). The number of finite elements chosen for this model was 130,833 quadratic tetrahedral elements, resulting in a total of 906,810 equations (Fig. 1c). The COMSOL model was built in five main steps: geometry definition, physics boundary conditions and initial values setup, meshing, calculation, results and post-processing. For model validation, coconut water was processed at four flow rates (0.5, 0.7, 0.9 and 1.1 L/min) and four target temperatures (80, 90, 100 and 110 °C). Experimental tests were carried out with a MicroThermics (Raleigh, NC, USA) microwave-assisted unit (2.45 GHz and 6 kW) (Fig. 1a) and the experimental process temperatures were measured and compared with the values predicted by the model. Numerical results showed the correlation between the intensity of the electric field and the temperature at the outlet of the tube, and it was possible to observe that the electric field was not homogeneous in the microwave applicator (Fig. 2). Comparison between numerical and experimental results showed that the model is reliable for predicting outlet temperature for thermal treatment of coconut water, with absolute errors under 11.2%. Results showed that the model can be used to improve the process performance and product quality. Prediction of temperature distribution can be useful for determining possible overprocessing zones and consequent product quality losses. This computational model can be used to simulate microwave-assisted processing in continuous flow of green coconut water, evaluate the process variables, the energy efficiency and select the most appropriate process condition for obtaining innocuous and high-quality liquid food.

Keywords: COMSOL, microwave heating, food, pasteurization.

Acknowledgements

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Fig.1. a) Picture of the microwave cavity, b) Schematic representation and c) Numerical mesh for the model solution.

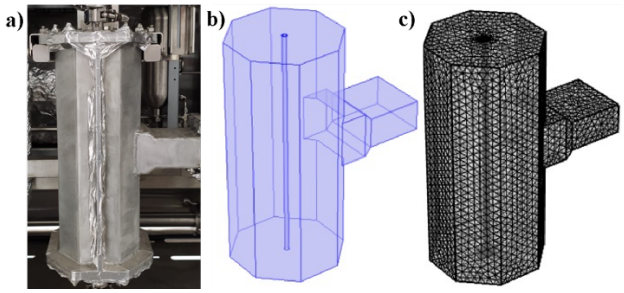
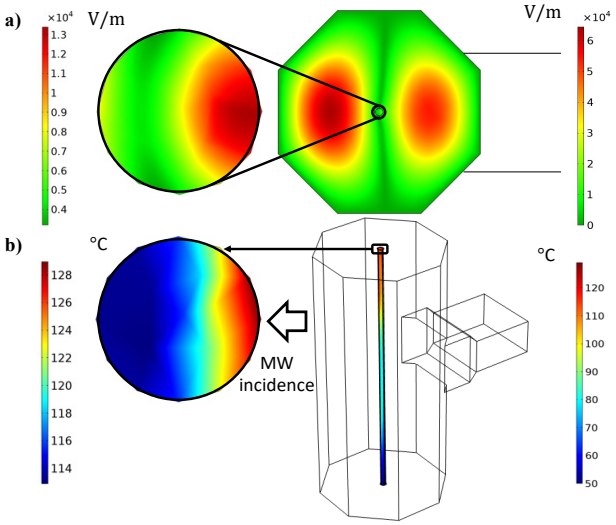


Fig. 2. a) Electric field within the microwave cavity at a 2-kW inlet power and b) Surface temperature distribution within the pipe and the outlet cross-section.



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Simulation-based cost analysis for capturing CO_2 using chemical absorption and membrane separation in power and industrial sectors

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Abstract

Carbon capture, utilization, and storage (CCUS) is expected to mitigate CO_2 emissions significantly since CO_2 is directly captured from the flue gas emitted by large CO_2 sources in power and industrial sectors. However, the high energy consumption for CO_2 capture is the bottleneck in the economic feasibility of CCUS. Choosing a suitable technology with a configuration tailored to the combustion process will assist in the swift deployment of CCUS projects. This study focused on quantifying the effect of membrane properties, including the CO_2/N_2 selectivity and membrane thickness, on the economic competitiveness for capturing CO_2 compared to the amine-based chemical absorption. The process simulations of post-combustion CO_2 capture were performed under the criteria of CO_2 capture rate (90%) at 150 bar and purity (>95%) using Aspen HYSYS V10 and Promax 5.0. Accordingly, the CO_2 capture costs were quantified based on the simulation results, which were retrofitted to existing power and industrial processes. For amine-based absorption, the basic process configuration, consisting of absorber, stripper, intermediate heat exchanger, and compressor train, was adopted. On the other hand, in the case of the membrane separation, three configurations with recycling streams were considered, and one configuration was selected to minimize the energy consumption using heuristic optimization. Monoethanolamine (MEA) was used as the amine solvent, and it was assumed that the relation between CO_2/N_2 selectivity and permeance followed the Robeson upper bound (Robeson (2008), Comesaña-Gándara (2019)). According to the simulation-aided cost analysis, the CO_2 capture cost using amine-based absorption ranged from \$47.2 to \$89.2 per CO_2 captured, depending on the types of combustion processes. Meanwhile, the CO_2 capture costs using membrane were significantly changed at varying membrane properties. In the case of the membrane thickness greater than 5 µm, the CO_2 capture cost increased with higher CO_2/N_2 selectivity, and the amine-based absorption was economically favorable compared to the membrane separation. Contrary, by reducing the membrane thickness less than 1 µm, the CO_2 capture cost was significantly decreased and minimized when the selectivity was between 20 and 40. In addition, the sensitivity analysis was performed to quantify the CO_2 capture cost by changing solvent make-up rate and membrane replenishment since chemical impurities in the flue gas could deteriorate their CO_2-capturing capacities. As a result, the membrane separation could capture CO_2 at a lower cost than chemical absorption, depending on membrane thickness, regeneration cost, and equipment degradation. Consequently, this study evaluated the effect of membrane properties on the CO_2 capture cost and the economic trade-off relationship between energy consumption and membrane area, which

can assist in optimizing the membrane properties for capturing CO_2 in existing power and industrial processes.

Keywords: process simulation, techno-economic assessment, CCUS, amine scrubbing, membrane separation

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Adversarial Reinforcement Learning for the Tennessee Eastman process under Cyberattack

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Abstract

Motivation

The issue of cyberattacks affecting chemical plant and, more generally, Industrial Control Systems (ICS) has received increasing attention following the Stuxnet and TRISIS malware campaigns. When faced with a cyberattack, operators (blue team) must decide the corrective action to take, in a safety-critical environment and with incomplete knowledge.

Reinforcement learning has been used as a means of control for video games (Mnih, V., Kavukcuoglu, K., Silver, D. et al. (2015)), robot arms (Nair et al. (2017)) and tokamak reactors (Degrave et al. (2022)). In this paper, we have implemented a well-understood process control problem as an adversarial reinforcement learning task, simulating the intents and capabilities of a plant operator and threat actor.

Method

We have reimplemented the well-understood Tennessee Eastmann process (Downs and Vogel (1993)) as an OpenAI gym (Brockman et al. (2016)) environment.

The process transforms feedstock chemicals A, C, D and E into products G and H, and has twelve manipulated variables, each assumed to be managed by an independent PLC. The environment will terminate if certain operational parameters are exceeded, as described by Downs and Vogel.

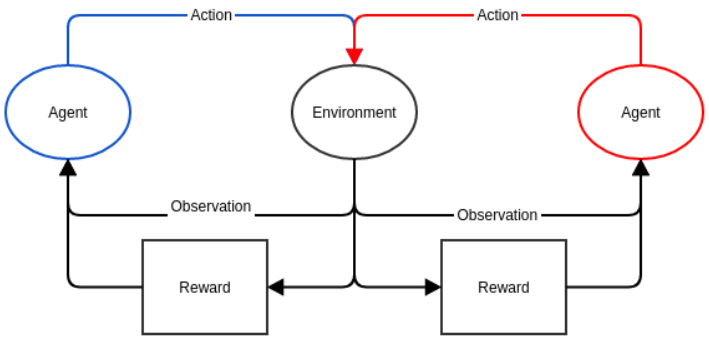

Figure 1: Agent-Agent-Environment loop

Unlike a traditional OpenAI environment, there are two agents and two (separate) rewards; blue team and red team. The blue team's reward is the monetary value of production. The red team agent is similar, but with adversarial goals (e.g to halt production), that can be changed at startup.

Three different versions were created;

- Under the Discrete version, red team can, for each timestep, set a single measured variable, setpoint, or manipulated variable to a predetermined extreme values, or take no action; the blue team can override a single control loop (defaulting to open loop control for one hour), restart the entire plant (halting production for 24 hours), or take no action.
- Under the Single-Action Continuous version, red team's capability extends to spoofing a single measured variable (the reactor pressure readout), and blue team can adjust a single manipulated variable (A and C feed).
- Under the Full-Control Continuous version, red teams' capability extends to perturbing all 41 measured variables and all nine setpoints, and blue team can adjust all 12 manipulated variables.

The Single-Action Continuous and Full-Control Continuous versions were implemented with Deterministic Policy Gradient methods and the Discrete version with Q learning.

Results

Table 1 details the win rate with the red team attempting to terminate the environment, under Discrete, Single Continuous, and Continuous versions:

Version	Blue team win rate (0 - 10 episodes)	Blue team win rate (90 - 100 episodes)	Modal failure and time
Discrete	0.9	0.9	Reactor pressure low, 151 ± 30 s
Single Continuous	1.0	0.0	Reactor pressure low, 27 ± 1 s
Continuous	0.7	0.0	Separator level low , 356 ± 1 s

Table 1: Evolution of blue team win rate in different variants

Conclusions

- Initial results show that adversarial control of a single measured variable, the reactor pressure readout, was sufficient to destabilise the reactor. Limiting the adversary to a smaller range of pre-generated attacks, however, resulted in a blue team that could recover.
- Further work includes giving blue team a prior model ("digital twin") to generate the value function, and longer learning periods.

Keywords: Agent-based modelling; Reinforcement Learning

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Dynamic simulation of distillation columns for flexible operation of Air Separation Units.

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Abstract

Today, the power consumption of an Air Separation Unit (ASU) is highly correlated to its production. However, the natural fluctuations in energy supply induced by the integration of intermittent renewables into the electricity grid mean that the ASU must be able to provide a constant supply of air gases to customers regardless of the dynamics of energy availability.
ASUs are generally not designed to respond to large and fast fluctuations in air supply, as they are intended to operate around a nominal operating point that is often the optimum. Therefore, the design and operation of ASUs must be reinvented and be flexible enough to adapt to energy supply variations. Although effective control strategies have been developed in the past, the effects of rapid air load changes induced by this new flexible operation must be understood to ensure reliability and robustness of oxygen, nitrogen and argon production. This is especially critical for argon distillation columns, which are very sensitive to changes in column concentration profiles during operation. Several days of re-startup may be required when an argon separation column is no longer working properly, which means a risk of the customer supply interruption due to argon unavailability.
Although steady-state models for distillation columns are state-of-the-art in academia and industry, there are numerous situations where such steady-state models fall short, such as column startup and shutdown or transition between operation points [Hoffmann, et al. (2020)].
In order to evaluate the effect of fast load changes on ASU stability, we developed a dynamic model of the distillation system including the high and low-pressure columns, the condenser-reboiler between them, as well as the argon mixture column. This model was developed using AspenTech Aspen Custom Modeler (ACM) software. The simulation environment was used to finely define the geometry of the internals of the distillation columns, as well as to specify the control strategies.
In a normal scenario, without an effective control strategy, by reducing the air load of an ASU by 25%, dynamic simulations showed that the oxygen content at the feed of the argon column would drop sharply and the nitrogen content at the top of the argon column would increase to 14% (compared to less than 1% in steady state operation). This would mean that the condenser at the top of the column would stop working. By evaluating the dynamic responses of the distillation columns, an effective control strategy based on controlling liquid flow and holdup in the columns was implemented. As a result, the nitrogen content at the top of the crude argon column could be kept below 1%, ensuring continuous operation of the argon column. Dynamic simulations are a valuable tool, still insufficiently used today, that opens the way to the optimization of ASU control in order

to enhance their reliability and flexibility when faced with load changes driven by energy availability constraints.

Keywords: Dynamic simulation, Air Separation Unit, Aspen Custom Modeler, Process Control

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A Cautionary Tale about Machine Learning: Case Study on Catalyst Deactivation

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Abstract

Machine Learning (ML) is increasingly used to simulate industrial processes and many ready-to use ML tools, such as scikit-learn, have been made freely available to the modelling community. Applying ML models to problems where deriving models based on first principles is not feasible but sufficiently large datasets are available has become an exceedingly simple and tempting option.

Estimating hydrotreatment catalysts deactivation is one of such problem. The reaction in question is Vacuum Gas Oil (VGO) Hydro de-Sulfurization (HDS). Reactor temperature is increased, up to the maximum operating temperature of the unit, along the cycle to compensate for deactivation. Deactivation is principally due to coke formation, blocking the catalyst surface. The precise mechanisms involved are poorly understood and model development is recognized as challenging due to:

1) Impossibility to derive first-principle model because of feedstock complexity, with 1000000s of complex hydrocarbon species, impossible to analyze completely.
2) Impossibility to perform dedicated experiments because pilot plants are not representative of industrial units with respect to catalyst deactivation.

The availability of large historic dataset with around 18,000 points from 42 cycles (i.e. individual time series) makes this problem well suited for ML approaches. A maximum of 17 descriptors were used. Different ML approaches, including linear and mixed-linear regressions, Ridge Regression, Elastic Net, Random Forest, kriging (Gaussian Process), ARIMA, Support Vector Regression (SVR), as well as aggregations of the different models, were tested on the dataset. A selection of the best performing models is shown in Table 1. An aggregation of Mixed Linear and ARIMA with Covariate model was proposed. Mean average errors were calculated by cross-validation for each cycle.

Table 1 Mean Average Error (in °C) for Selected ML Models

Multivariate Linear	Ridge	Mixed Linear	SVR	Elastic Net	Aggregated Model
7.0	6.6	5.9	7.7	6.5	6.3

Performance of the ML models was found to be within the acceptable range of ±6°C. However, a sensitivity study revealed systematic flaws in all the ML models: the expected trends were not respected, rendering the models highly unreliable for practical applications. Issues with identifiability of the model descriptors in the dataset were identified as the principal reasons for this problem. For example, increasing the hydrogen partial pressure in the reactor is known, from experience, to decrease deactivation

(because H2 prevent from coking) and to increase HDS. , For this reason, higher pressures are systematically used when processing heavier feeds (high feed density). This is illustrated in Figure 1. When considering the dataset, without injecting a-priori knowledge, it seems that increasing ppH2 leads to a decrease of deactivation (as expected). But as Feed_d154 is correlated to ppH2, it seems then that increasing Feed density and then increasing ppH2 leads to a decrease of the deactivation, but some of the higher pressure points have much faster deactivation because heavier feeds are processed. This counterintuitive and clearly erroneous observation will be reflected by any ML algorithm calibrated only on the dataset.

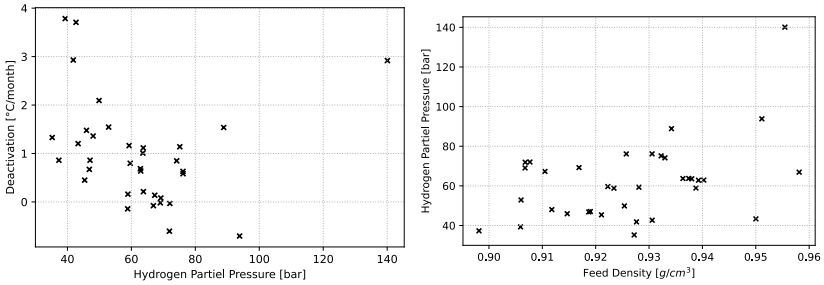

Figure 1 Relationship of deactivation slopes, ppH_2, and feed density

A semi-physical model, with as structure imposed based on expert knowledge was then developed. The model combines a classical kinetic model for the HDS reaction with a deactivation model which principally depends on temperature, ppH2, and various feedstock descriptors. It is important to note that the model structure was not derived from first principles, but rather by reformulating well-known "rules-of-thumb" as mathematical equations. Parameters of the model were calibrated on the same database as for the ML models. The model performance was found to be at least as good, if not better than the ML models, with a mean RMSE of 3.7°C. By construction the expected trends are respected by this model.

The conclusion of this exercise is that not all datasets, even if sufficient large, are well suited for the use with ML models, even if the resulting model(s) may seem precise. Real-world datasets often are inherently biased, which may lead to erroneous conclusions without a-priori knowledge of the physical nature and expected behavior of the system. In the case study presented here a relatively simple model derived from well-known reaction kinetics combined with the expected behavior of the system (expert knowledge) proved to be more robust than the pure ML models.

Future work in this area aims to combine the two approaches. An expert model is used to impose the underlying structure, while ML approaches are used to determine more complex corrective factors to the model.

Keywords: Machine Learning, Catalyst, Deactivation, Modelling

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Energy Management in a Modern Integrated Natural Gas and Electricity Network: A Techno-Economic Approach

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Abstract

Optimal operation of natural gas and electricity networks in the integrated manner cause to reach a more economical and technical results. In this paper, the supplied and demanded natural gas and electricity are managed simultaneously to reach more benefits from both technical and economic. The studied integrated network includes power plants, gas supplier, gas storage, water electrolyzer, fuel cell units, wind energy and hydrogen vehicles. Both natural gas and electricity demands are supplied optimally using the proposed optimization algorithm. The models and proposed methodology are simulated over GAMS programming software and the extracted results are discussed.

Keywords: Natural Gas, Electricity Network, Energy Management, Energy Storage.

1. Objective Function

In equation (1) the objective function is presented for operation cost minimization that includes two parts: the emission cost is presented in part one, while part two presents the operation costs of different components (i.e. GFU, gas supplier, and hydrogen system)

$$min \sum_s \omega_s (\sum_t (\underbrace{COE_{s,t}}_{1} + \underbrace{\sum_g OC_{g,s,t}^{GFU} + \sum_n OC_{n,s,t}^{GS} + \sum_h C_{h,s,t}^{HY}}_{2})) \quad (1)$$

$$\mathrm{COE}_{s,t} = \sum_{et} \sum_g COE_g EF_{g,e}^{GFU} P_{g,s,t}^{GFU} \quad (2)$$

2. Simulation results

In order to evaluate the capability of the proposed methodology, the integrated networks which is shown in figure 1 is simulated over GAMS programming software.
In figure 2, the performance of hydrogen system is shown. The amount of fuel cell unit production, the amount of power used by water electrolyzer for hydrogen production, and the stored hydrogen are shown. The extra power during a day is utilized by water electrolyzer to produce hydrogen and it is stored in hydrogen systems or is utilized by fuel cell units. The stored hydrogen is used for hydrogen vehicles demand. In figure 3, the amount of gas demands are presented. As can be seen the consumed gas by the power plants are in maximum levels at the peak hours because at this period the power plants have the maximum generation. In table 1, different parts of the operation cost of the integrated networks in presented. As can be seen the gas cost has the most portion in the total cost.

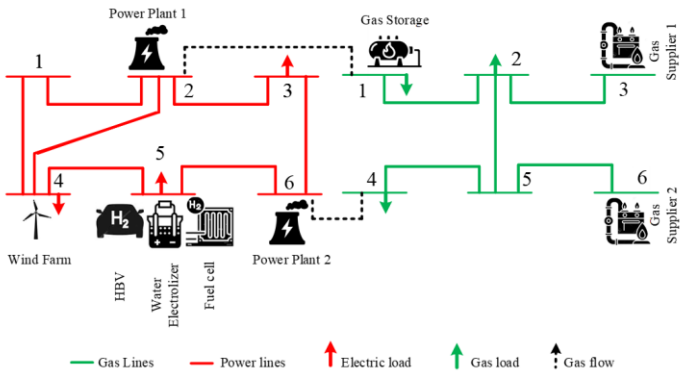

Figure 1. The understudy integrated natural gas and electricity network.

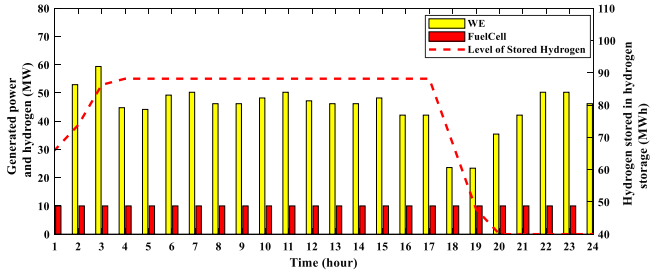

Figure 2. Hydrogen system results including water electrolyzer's power consumption, fuel cell unit's power production, and level of stored hydrogen in storage

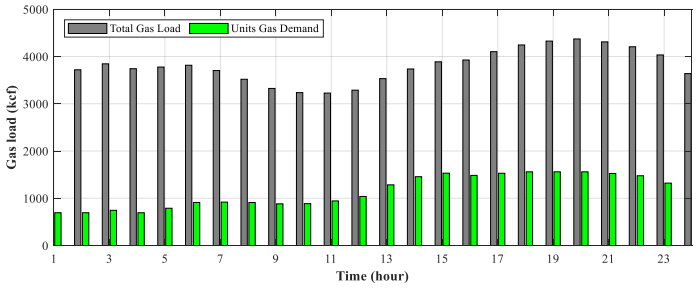

Figure 3. Gas consumption of power plants and total gas demand

Table 1: Different parts of operation costs of the studied network

Parts	Value of Cost ($)
GFU units cost	52502
Gas cost	242867
Hydrogen system cost (WE and fuel cell costs)	8534
Emission cost	6532
Total cost	310435

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Study of the interactions between microwaves and composite materials with views on waste recycling

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Abstract

This paper is part of a project which aims to better understand how the microwave field interacts with a solid heterogeneous medium consisting of a discrete phase dispersed in a continuous phase. The application target is the industrial recycling of waste with such characteristics, but also the manufacture of products to be recycled by microwave heating at the end of their life. The approach used to solve this problem consists of going back and forth between a fully instrumented microwave system in which real materials can be tested and the numerical equivalent of this same system. The aim of this paper is to present the real and virtual configurations used to carry out this research work, as well as some preliminary results.

Experimental microwave set-ups and simulation

In the first step, this study requires the design of an instrumented single-mode microwave heating system. For real or simulated microwave heating experiments, the size and dimensions of the cavity, the shape and position of the sample inside the cavity and the geometry of the waveguide all affect the interactions between the electromagnetic field and the sample, and thus the overall sample heating process.
For the experimental work, the LSPC laboratory has several WR340 single-mode microwave systems with a wide range of input powers. This work uses two of these systems, with a maximum input power of 300 W and 2000 W respectively and a frequency of 2.45 GHz (Figure I). They are equipped with accurate forward and reflected power and temperature measurement devices. An integrated system using LabVIEW® is used to record the data and control the input power.

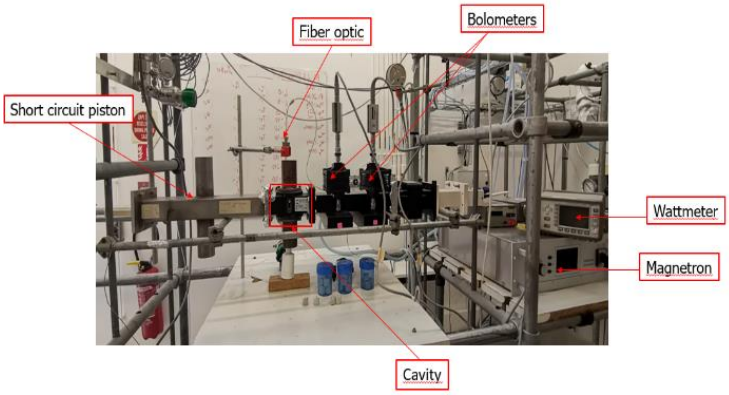
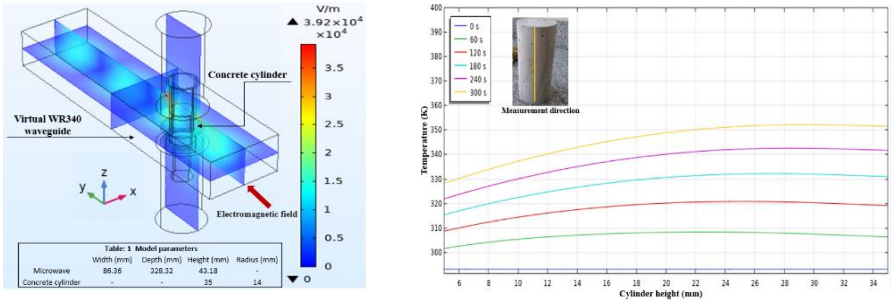


Figure I. Experimental WR340 single mode microwave system

This research also uses a vector network analyzer (Agilent Technology N5230A PNA-L) and coaxial probes to measure the dielectric properties (permittivity) of the materials of interest. These measurements are imperative because these properties vary with frequency, temperature and composition.
Figure II, the method is illustrated with a simulation of the heating of a concrete cylinder in a waveguide, which opens up a wide range of possibilities for exploring the recycling of concrete using microwaves. Indeed, the simulation allows to easily change the frequency, power, application mode and more.



(a) **(b)**

Figure II. (a) Simulation of WR340 system with cylindrical concrete sample; (b) Predicted time evolution of the temperature distribution inside the concrete cylinder along the z-axis for a 100 W power input.

To obtain the figure II (a), several steps are needed, first the geometry and a meshing are defined. Then the simulation of the effect of the electromagnetic field is solved using the electromagnetic module of COMSOL®, similarly to simulate the heating of the material, the heat transfer module in solids and the conduction heat transfer equation in COMSOL® are used. The boundary conditions are also specified. The solution of this coupled system of equations allows to study the propagation of the electric field as well as the maximum temperature reached and the power absorbed in the concrete cylinder (Figure II (b)). The concrete cylinder heats up due to the continuous conversion of electromagnetic energy into thermal energy. The temperature distribution follows the variation of the electromagnetic field inside the cylinder. The temperature is highest where the electric field is mostly absorbed, i.e. on the part of the cylinder that faces the direction of propagation of the electromagnetic field, which comes from the right of the picture.

Conclusion and Perspectives

However, before the simulation results can be used to guide practical developments, several challenges need to be overcome, including:

- Proposing a realistic model of concrete heterogeneities.
- Comparing the predictions of the simulation to controlled experiments, one of the issues being the fate of water in heated concrete.
- Converting the predicted thermal gradients within the material into a stress field to relate to concrete recycling.

Keywords: Microwave heating, Multiphysics simulation, Waste recycling, Concrete.

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Computer Program for Economic Evaluation of Chemical Processes

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Abstract

The implementation of an industrial chemical plant passes previously by the discussion of its economic viability. Aiming to realize this evaluation the software developed used profitability indexes that facilitate the decision making of the investment in a given enterprise, being: profitability index; payback period; net present value; internal rate of return; breakeven point. The reach of these parameters is based on the investments associated with the plant. In this case, correlations were implemented capable of predicting equipment costs based on their specifications and thus carrying out the economic evaluation of the process from the user's data. The platform used was VBA and the model validation was carried out through case studies compared to other known software. The software also proved to be efficient when working in conjunction with ASPEN's standard economic reports.

Keywords: economic evaluation, profitability indexes, software, VBA.

1. Introduction

The simulation of a chemical process is of paramount importance for the development of an industrial plant both for the understanding of the associated phenomena as well as the choice of utilities and equipment. However, even well-defined and optimized product routes may not prove to be attractive for investment, since the cost of implementation and operation may exceed the financial return within a stipulated period. In addition, there are numerous factors that influence this aspect, and the preliminary analysis of equipment costs, raw materials, product value, among others, becomes fundamental for project decision making. As a result, it is necessary to be aware of the behavior of financial parameters such as present value, internal rate of return, and pay-back period, all based on the total investment and cash flow of a plant. (Timmerhaus, 2003)
Therefore, the profitability indexes of the chemical process under study are obtained from the development of software with a database of equipment for calculating profitability indexes for economic analysis.

2. Methodology

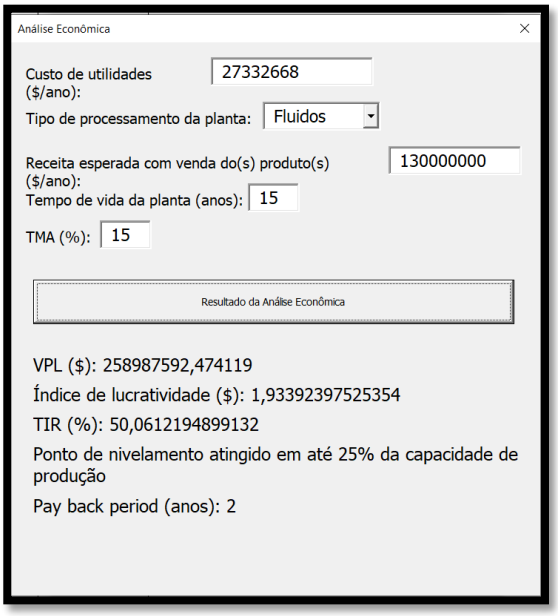
The methodology used for the development of the computer program began with the organization of all data considered valid for implementation. This validity, in turn, is based on the concept of the correlation used to meet a good range of equipment estimation, simplicity of choosing the specification needed for the calculation, author's credibility, and annualization of the index used. All these parameters could be evaluated in the document of the Ministry of Mines and Energy, 2018, which includes correlations of more than 80 pieces of equipment from different authors such as Corripio (1995),

Icarus (2002), CAPCOST (2009), Timmerhaus (2003) and Guthrie (1974). In addition, to confirm the correct use of the parameters, the equipment selected for implementation was also searched in the sources available from the mentioned authors, also own correlations were developed for the software.

3. Results

The validation itself was made by two studies of cases and the software was used in the article "A Sustainable Urea Plant from Maize Ethanol in France: A Brazilian approach" to make the economic evaluation of the process along with some equipment calculated by ASPEN PLUS V.11, the software developed and SuperPro Designer.
With all the features properly programmed and tested, the result of the program's interface in its version 1.0 is as follows:

Figure 1: Software Economic Analysis of Chemical Processes (case study Results)



4. Conclusion

From the data and considerations exposed in this report, it was possible to observe the functionality of the methodology applied to the selected equipment and for the economic analysis of processes. During the use of the software, updates of new equipment and indexes may appear so that the software remains representative. Version 1.0, based on the studies carried out, proved to be efficient both as the only software for evaluation and as an auxiliary software.

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Promising future for biodiesel: Superstructure optimization from feed to fuel

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Abstract

Biodiesel, derived from renewable biobased feedstock, is an attractive alternative to fossil fuels in reducing greenhouse gas (GHG) emission in transportation. Its share reached 80.6% of total biofuel consumption in the European Union (EU) transport sector in 2019. However, the public perception of bioeconomy is changing, i.e., the growth of biofuel has been slowing down recently with an increase of only 6.8% from 2018 to 2019 because of its high production cost and the change for non-food feedstocks.

Most of published researches focused mainly on only one aspect between finding inexpensive feedstocks and developing optimal processes for biodiesel production. However, a combined strategy of economic feedstock and innovative processes for biodiesel production has not been addressed adequately. This work fills the gap by connecting appropriate feedstock selection and process synthesis with superstructure optimization.

Superstructure optimization is a model-based computer-aided method of process systems engineering for optimal process synthesis. A superstructure is a collection of numerous alternative feedstock and equipment options that can combine to form various possible process flowsheets. The superstructure can be formulated as a mathematical model by using variables, equations and constraints to describe its options and flowsheets. The best flowsheet for predefined criteria and constraints can be identified by solving the model with optimization software tools.

A superstructure model for maximizing the profit of biodiesel production is presented in this work. The superstructure encompasses a wide range of feedstocks (e.g., waste cooking oil, rapeseed oil and algae), conventional reaction and separation equipment (e.g., continuous stirred tank reactor, decanter and vacuum distillation) and intensified operation units such as membrane reactor and reactive distillation column. The model has in total 60 equipment options, 4119 variables and 8967 constraints. The superstructure model is implemented in Advanced Interactive Multidimensional Modeling (AIMMS). The results present an optimal design of a biodiesel production process from waste cooking oil with a heterogeneous acid catalyst, a reactive distillation column and additional purification steps for producing pure glycerol which is 40% higher in price than technical glycerol. The reactive distillation column reduces the total capital investment by 16% by combining the reaction and methanol separation into one unit operation. For the net profit after tax, the optimized flowsheet is 20% more profitable than conventional processes.

Keywords: Superstructure, Optimization, Biodiesel, AIMMS, Design.

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Model-based solvent selection for the integrated synthesis, crystallization and isolation of pharmaceutical compounds

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Abstract

Solvents are extensively used in the pharmaceutical industry for a variety of processing tasks, such as promoting chemical reactions, facilitating separations and formulating pharmaceutical products. The use of solvents has been identified as a main source of waste and carbon emissions in the pharmaceutical industry, contributing to the poor environmental performance of the sector relative to other chemical industries, and highlighting the need for systematic solvent selection tools to develop resource-efficient processes (Papadakis et al., 2018). Furthermore, given the profound interactions between solvent and process efficiency, solvents represent a major green chemistry theme, with much room for improvement. In this work, we present a systematic process-wide solvent selection tool based on computer-aided mixture/blend design (CAM^{b}D) (Gani, 2004) for the integrated synthesis, crystallisation and isolation of pharmaceutical compounds. The proposed method simultaneously identifies the optimal solvents, mixture composition and process temperatures that minimise the solvent E-factor while achieving high crystal yield, process yield and mass purity of the target molecule. Additionally, the method entails comprehensive design specifications for the integrated process, such as the miscibility of the synthesis, crystallisation and wash solvents, and includes criteria related to the environmental, health and safety impacts of the process. The design approach is illustrated by identifying optimal solvent mixtures for the synthesis, crystallisation and isolation of mefenamic acid. The use of the proposed CAM^{b}D for solvent selection and process design can guide experimental efforts during early-stage pharmaceutical process development.

Keywords: Synthesis, crystallisation, isolation, CAM^{b}D, mefenamic acid.

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Computer-aided solvent design for suppressing HCN generation in amino acid activation

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Abstract

A highly toxic compound, hydrogen cyanide (HCN), was discovered to result from the reaction between Ethyl cyano(hydroxyimino)acetate (Oxyma) and diisopropylcarbodiimide (DIC), a popular reagent combination for amino acid activation (McFarland et al., 2019). The reaction solvent has been found to influence the amount of HCN produced so that judicious solvent choice offers a route to suppressing HCN formation. Given the safety implications and the time-demanding nature of experimental solvent selection, we employ a methodology of quantum mechanical computer-aided molecular design (QM-CAMD) (Struebing et al., 2013) to design a new reaction solvent in order to minimize the amount of HCN formed. In this work, we improve on the original QM-CAMD approach with an enhanced surrogate model to predict the reaction rate constant from several solvent properties. Density functional theory (DFT) in conjunction with the thermodynamic cycle (TC) method is used to calculate activation free energies which are then converted into rate constants via application of the transition state theory (TST). A set of solvents is selected for model regression using model-based design of experiments (MBDoE), where the determinant of the information matrix of the design, known as D-criterion, is maximized. The use of a model-based approach is especially beneficial here as it links the large discrete space of solvent molecules to the reduced space of solvent properties. The resulting surrogate model demonstrates an improved adjusted coefficient of determination and predicts more accurate rate constants than the model generated without using MBDoE. The QM-CAMD algorithm reaches convergence within only two iterations; a list of promising reaction solvents is generated. In the future, the main reaction of amino acid activation will be considered to design a solvent that maintains the rate of the main reaction while minimizing the generation of HCN.
Keywords: computer-aided molecular design, design of experiments, solvent effects

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Improving sustainable CHOSYN´s targets through process intensification

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Abstract

The Carbon-Hydrogen-Oxygen symbiosis networks (CHOSYN's) are integrated multi-plants that pursue a proper use of mass and energy resources among a set of hydrocarbon processing plants, this concept moves towards more sustainable designs for facing the ongoing problem of environmental and climate change by meeting performance targets as environmental concerns and profitability enhancement. This work addresses CHOSYN's synthesis using process intensification, which has been widely used for enhancing the performance of industrial processes in terms of economy, environment, and safety. The purpose is to show the impact that can be produced through the implementation of processes intensification in CHOSYN's performance targets. This work is focused on the intensification of distillation sequences due to the intensive energy use of this separation process, and since thermodynamic efficiency ranges for conventional distillation is 5-20%, using thermally coupled configuration this work seeks important improvements in energy efficiency. A case study is proposed, the methodology is presented in three stages: intensification of selected flowsheets of the case study, integration of the plants into the CHOSYN, and analysis of results. Thermally coupled equivalent configurations for selected distillation sequences are determined and optimized through the dynamic method known as the moving section method proposed by Hernandez & Jimenez (1996). Once obtained these sequences, the different configurations for the CHOSYN are built through a sequential integration method. The performance analysis of the different obtained CHOSYN configurations are addressed by the metric known as Sustainability Weighted Return on Investment Metric (SWROIM), which integrates the conventional ROI and sustainability indicators, in this case, the performance targets used for the term of sustainability in the metric are thermal energy savings, water footprint reductions, and CO_2 emissions. The resulting gap between SWROIM values for the conventional network and the intensified alternative measures the total positive impact by intensification over the cost and sustainability indicators of the CHOSYN in general.

Keywords: process intensification, process integration, resources management

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A novel process design for automated quality analysis in an integrated biopharmaceutical platform

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Abstract

We are currently seeing a great need for global accessibility and lower prices of a wide range of vital biopharmaceuticals, e.g. mAbs for cancer treatment. With upstream processing having seen recent productivity improvements by switching from batch to continuous mode, the on-going paradigm shift towards continuous, integrated and – eventually – autonomous downstream processes is therefore critical in order to make new, life-saving pharmaceuticals more readily available at a global scale. A concrete example of this paradigm shift is the process design for automated lab-scale production of a recombinant protein presented by Gomis-Fons et al. (2019). However, in order to achieve autonomous production of biopharmaceuticals, there is a further need to implement advanced analysis capabilities. The purpose of the current work is to satisfy this need by presenting a custom process design, where an HPLC with a diode-array detector was integrated with the aforementioned process and its control software, allowing for automated quality analysis of specific pools and/or entire system flows. The work was carried out by connecting the flow-paths of an AKTA pure 25 and an Agilent 1260 HPLC by utilizing the loop and injection valves, as well as a flow splitter. In order to integrate the HPLC system and the A¨ KTA system, the Agilent API known as Instrument Control Framework was used to develop a C# based software called Satellite, in turn used to link the HPLC hardware with the previously developed control software, Orbit (Andersson et al., 2017). The major results are presented as the full wavelength spectrum generated by the HPLC diode-array detector analyzing the continuous process flow. This spectrum highlights the expected purification, and contains a factor of roughly 100 times more data than a standard chromatogram, which can be utilized for further analysis, data-driven modeling, and subsequent autonomous control. In conclusion, the study shows that the setup works as intended, capable of providing large amounts of data, which is a necessary step towards autonomous biopharmaceutical production, and the use of the diode-array detector was shown to have great potential in generating data that can also be used for e.g. identifying different species. However, challenges pertaining to determining the next step towards autonomous control remain as an important future challenge. Finally, the concept carries promise as a generalizable Orbit-controlled analysis platform.

Keywords: novel process design, chromatographic purification, automated analysis, integrated downstream processing

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A multiscale approach towards the use of Urban waste within the energy transition strategy

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Abstract

Waste is a major issue of our society due to the amount generated annually as well as the challenge its management represents. It is estimated that by 2021, 6.1 Mt/d of municipal solid waste (MSW) will be generated in urban areas (World bank, 2012). In addition to MSW, sludge that reaches a production of 13 Mt in 2020 (EU, 2008), can also be used as a resource. Both show a high potential to contribute to the energy transition.

The use of municipal solid waste and sludge within the waste to power initiative is evaluated following a multiscale approach. At process level, a technoeconomic analysis based on systematic process design is developed to determine the optimal operating conditions and to estimate the yield and investment cost of the facilities as a function of the processing capacity. The facility consists of the boiler, the flue gas treatment chain, the steam turbine, and the cooling tower that are modelled using an equation-based approach. Experimental data and first principles are used to model the boiler and the pollutant abatement techniques, while detailed thermodynamics and transport phenomena are used to model the turbine and the cooling tower (Guerras and Martín, 2020). Next, at country level, an extended facility location problem is formulated to select the location of facilities for a given budget, aiming at an electricity production cost and water consumption, considering the economies of scale and social indexes to promote the development jobs in regions suffering from depopulation (Heras and Martín, 2021)

To produce power at a competitive price, below 0.06€/kWh, a facility has to process the waste generated at cities above 250k habitants. For this critical size, the investment cost is beyond 25 M€. At country level, for the major cities in Spain (over 65 across the mainland) it would be possible to produce up to 235 MW from the waste generated with a production cost of 0.05€/kWh. While the average costs are competitive, some regions would produce at a high cost and only the national strategy would justify the use of waste at smaller cities. The facility location problem allows performing a sensitivity study for different objective functions, economic and social, and maximum budgets to select a set of locations for a given electricity cost.

Keywords: Waste to energy, pollutants abatement, process design, multiscale

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Don't compress the compressor (model): Integrated design of refrigerants and heat pumps

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Abstract

Vapor-compression heat pumps are a key technology for decarbonizing our energy systems. Due to more stringent regulations and new applications, vapor-compression heat pumps require novel efficient and environmentally friendly refrigerants. Current systematic refrigerant-selection methods screen large databases (McLinden et al., 2017) or employ computer-aided molecular design (CAMD) (Schilling et al., 2017). The performance of the selected refrigerant is evaluated in a process model. This process model should capture all interactions between the refrigerant and the heat pump that significantly influence system performance while still being computationally tractable. Current refrigerant-selection methods often model the compressor as fluid-independent, assuming one constant compressor efficiency for all refrigerants.

In this work, we first investigate if the widely used assumption of constant, fluid-independent compressor efficiencies is justified for reciprocating compressors. For this purpose, we develop a loss-based compressor model that tailors the compressor design to the refrigerant by scaling the compressor geometry and by reducing prevalent losses for each refrigerant. The model assumes constant operating conditions. We compare the resulting compressor efficiencies before and after the tailoring for ten common refrigerants. The results show that the compressor efficiencies depend strongly on the refrigerant. In contrast, tailoring the compressor design has less impact on the refrigerant performance.

Based on these findings, we propose integrating a refrigerant-dependent compressor model into refrigerant-selection methods to capture the impact of the compressor on refrigerant selection. For this purpose, an integrated design method of molecules and processes (Schilling et al., 2017) is combined with a detailed reciprocating compressor model (Roskosch et al., 2017) that accounts for refrigerant and operating-point-dependent compressor efficiencies.

For the integrated design, the 1-stage CoMT-CAMD method (Schilling et al., 2017) is applied to the design of heat pumps and refrigerants. 1-stage CoMT-CAMD combines a process model with a CAMD formulation and a thermodynamic model of the refrigerant, the perturbed-chain statistical associating theory (PC-SAFT) equation of state (Gross and Sadowski, 2001). PC-SAFT is linked to the CAMD formulation by the homosegmented group-contribution method (Sauer et al., 2014). The resulting mixed-integer nonlinear optimization problem is implemented in Python and solved using Knitro (Byrd et al., 2006).

For the compressor, we couple the refrigerant-dependent reciprocating compressor model (Roskosch et al., 2017) with PC-SAFT. The compressor model discretizes the compression cycle and solves time-dependent mass and energy balances to obtain compressor

efficiency, refrigerant mass flow, and outlet temperature for a given inlet state and outlet pressure. We implement the compressor model using the computationally efficient programming language Rust compiled as a Python package to ensure a computationally efficient integrated design.

We perform the integrated design for a residential heat pump with fixed heating power and determine the best-performing refrigerants. The objective is to maximize the coefficient of performance (COP). As a benchmark, we assume a constant compressor efficiency of 70 % (Roskosch and Atakan, 2015). The top refrigerant designed is dimethyl ether (RE170) which is currently discussed as potential green refrigerant (Semmel et al., 2021). Comparing the resulting rankings of refrigerants shows that neglecting the compressor's fluid-dependency leads to suboptimal choices (Figure 1). In particular, the best refrigerants differ strongly in performance for a fluid-dependent compressor efficiency. In contrast, all refrigerants are predicted to perform very similarly when assuming a constant compressor efficiency. Switching from constant to fluid-dependent compressor efficiency changes the observed trade-offs between the refrigerants not only quantitatively, but also qualitatively.

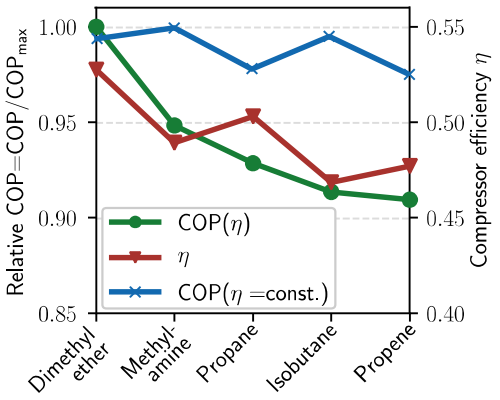

Figure 1. Coefficient of performance (COP) and compressor efficiency η of five best-performing refrigerants for the fluid-dependent compressor (COP_{max} = 6.97) compared to the corresponding COP with constant compressor efficiency of 70 % (COP_{max} = 8.80).

The work shows that detailed compressor modeling is crucial in systematic refrigerant selection to identify an optimal combination of refrigerants and heat pump processes. The integration of detailed compressor models into systematic refrigerant selection is possible by using computationally efficient model implementations.

Keywords

Vapor-compression heat pump, computer-aided refrigerant design, PC-SAFT equation of state, compressor modeling

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Integration of thermo-chemical energy storage for flexible operation of decarbonized power plants

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Abstract

The energy sector is facing fundamental challenges in transition to a low carbon economy as well as in relation to the higher penetration of renewable energy sources. Most of renewable energy sources (e.g., solar, wind) are highly time-intermittent which put an additional operational burden to the back-up capacities most of them based on conventional fossil fuels. This work evaluates the integration of an innovative thermo-chemical energy storage system based on calcium sorbents for flexible operation of decarbonized coal-based super-critical power plant. The reactive gas-solid cycle is used for both power plant decarbonization as well as a time-flexible thermo-chemical energy storage system in conjunction to a 500 MW net power output plant with 90% carbon capture rate. Flexible operation of the calcium looping thermo-chemical energy storage system is based on sorbent storage facilities in both regenerated and carbonated forms (Astolfi et al., 2019). Overall techno-economic and environmental implications of flexible decarbonized power plant with calcium-based thermo-chemical energy storage system were evaluated using process flow modeling and thermal integration analysis. For economic evaluation, estimation of capital investment, operational costs, electricity production costs as well as CO_2 capture costs were done using relevant methodology in the field. For comparison reason, similar decarbonized power plant operated in base-load conditions as well as a non-capture power plant were also considered to assess the overall performance indicators (Cormos and Dinca, 2021). As the results show, the utilization of calcium looping cycle for time-flexible thermo-chemical energy storage system in conjunction to a decarbonized fossil-based power plant bring significant benefits in term of reducing specific capital cost (down to about 10%), electricity production cost (down to about 5%), CO_2 capture costs (down to about 10%), all compared to the base-load operation of similar decarbonized power plant. Although very promising in delivering better techno-economic performance indicators than other decarbonization systems (e.g., gas-liquid absorption), the calcium looping technology still requires significant scale-up efforts from the current development level (up to 10 MW) to full industrial sizes.

Keywords: Thermo-chemical energy storage; Calcium looping cycle; Decarbonized power plants; Flexible operation; Techno-economic and environmental assessment.

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Superstructure optimization for sustainable design of an algae biorefinery

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Abstract

Microalgae are a promising replacement for fossil based feedstock. Microalgae can be used to produce biofuels, but more importantly they are the source for a plethora of added-value products such as omega-3, carotenoids and glycerol. They do not compete with food production and do not require arable land for growing. Over the last years it has become evident that biomass will not be the main source of renewable energy, the costs are too high and the efficiency is too low. However, by extracting valuable biocomponents from the biomass, the process can become economically viable.

The objective of this work is to identify the most promising pathways for the combined production of added-value products (omega-3, glycerol, carotenoids) and biodiesel from microalgae.

The approach followed exists of setting up a comprehensive superstructure with all available technologies of each stage of the biorefinery. The superstructure represents a mapping of all microalgae feedstock via different technological options into all final products. Each node in the superstructure represent a technology that is modeled via mass- and energy balances. The associated costs are described by economies of scale equations. In addition, logical constraints are needed that ensure logical connections between the nodes. The result is a mixed-integer nonlinear programming model. The Advanced Interactive Multidimensional Modeling (AIMMS) software is used to solve the model, with 4779 constraints and 5307 variables. The outer approximation algorithm by using CONOPT and CPLEX solvers are utilized for nonlinear and mixed integer parts, respectively. The model is solved less than second on 5-core processor @ 1.8 GHz with 8 GB RAM.

The proposed superstructure allows for quickly and efficiently identifying cost effective routes from many alternatives. It turns out that the open pond, sedimentation, flotation, flocculation, hydrothermal liquefaction, organic solvent-based extraction, n-butanol based lipid extraction are selected as the suitable method. With this production route, about 6 million tone wastewater as feedstock is treated and 1.5 million US$ income is generated annually.

The next step will be an extension of the superstructure with using a life cycle analysis to map eco-environmental pathways for producing added-value products and biodiesel from microalgae.

Keywords: Algae biorefinery, added-value products, superstructure, MINLP.

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Economic and Environmental Optimization and Feedstock Plannig for the Renewable Jet Fuel Production Using an Intensified Process

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Abstract

Global warming is becoming an overwhelming issue that strongly relates to the increasing amount of global carbon emissions. The aviation community has set targets for reducing greenhouse gas emissions by improving the fleet fuel efficiency by up to 1.5% per annum and promoting alternative fuel use for reducing the net aviation carbon emissions by 50% in 2025. Biojet fuel made from sustainable raw materials can be an option. A path capable of achieving a green process is the ATJ (alcohol to Jet) process which offers more advantages over the widely known oilseed paths. Considering the use of lignocellulosic material, proper planning to meet the demand for biojet is necessary, in conjunction with an adequate process in an attempt to compete with fossil fuels. This work design and optimize a biojet fuel process from lignocellulosic residues with bioethanol as an intermediate modeling biomass-to-ethanol (BTE) and ethanol-to-biojet (ETB) subprocesses. An annual feedstock planning was designed considering sugarcane bagasse and corn stover as feedstocks trying to cover a considerable percentage of the mexican demand. BTE process modeling covered pretreatment, hydrolysis, fermentation, and ethanol purification. ETB process modeling included ethanol dehydration, oligomerization, hydrogenation, and biojet purification. To meet sustainability goals, the process was intensified in the zone of purification of ethanol with schemes of vapor side stream column (VSSC) and dividing-wall column (DWC). All processes and the planning were optimized by minimizing total annual cost (TAC) and ecoindicator-99 (EI99) as economic and environmental objective functions, respectively. The stochastic optimization method of differential evolution with tabu list was employed through a hybrid platform incorporating Aspen Plus. As results, the method selected sugarcane bagasse as the optimal feedstock. Besides, the conventional BTE process achieved minimum TAC and EI99 of 1.295 USD/kg EtOH and 0.4716 ecopts/kg EtOH, respectively. In intensified option, TAC savings of 5.56% and 5.02% for VSSC and DWC schemes, respectively, were achieved. Also, EI99 reductions of 1.72% and 2.92% were recorded for VSSC and DWC schemes. In summary, ETB intensified process achieved minimum TAC and EI99 of 0.275 USD/kg biojet and 70.18 ecopts/kg biojet, respectively and the minimum fuel selling price is closed to conventional jet fuel. This study shows that with proper planning and through process intensification techniques, it is possible to reduce costs and environmental impact by using agro-industrial wastes to replace a percentage of fossil fuels in the medium and long term in a circular economy framework.

Keywords: stochastic optimization, process intensification, biojet fuel, lignocellulosic biomass, bioethanol.

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Heat exchanger networks with different shell and tube configurations

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Abstract

In a growing energy consumption world, energy efficiency has become mandatory. In this context the design of heat exchanger networks (HEN) is of crucial importance. Consequently, there are many methods available for HENs design Klemeš et al. (2018). Most of those approaches consider that the net is formed by shell and tubes heat exchangers (S&T) with a perfect countercurrent heat transfer while the 1-2 heat exchanger, one shell pass, and two tubes pass, are at least as common or even more.
In this work, we present a two steps sequential algorithm that allows the design of HEN to capture the main details of the heat exchangers (number of tubes passes, number of shells, logarithmic mean correction factors) that influence the cost estimation. The first step is inspired by the transportation model by Nemet et al. (2018). It uses the concept of temperature intervals and considers the possibility of heat transfer between the hot and cold streams inside those intervals. Then, it is possible the a priori calculation of the logarithmic mean temperature difference between matches, the efficiency factor, and the number of shells in series, maintaining the area linear in the model.
The second step uses a superstructure with all the possible alternatives in which the heat exchangers predicted by the first stage model can exchange heat to design the final heat exchanger network.
We have used a set of benchmark problems commonly used to test HEN algorithms. For the case in which we constrain to 1-1 S&T heat exchangers the results are close or are even better than the best-known solution.

Keywords: HEN, Energy Integration, Shell and Tube heat exchangers.

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Considering Environmental and Social Impact in Optimization of a Supply Chain for Bio-Jet Fuel Production

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Abstract

Climate change has a great negative influence on the ecosystem thus becoming one of the most pressing global challenges. The leading causes of climate change are excessive carbon and other green- house gas emissions in human activities. Air transport is a cornerstone in current globalization, supporting the movement of more than 4 billion passengers and nearly 61 Mt of freight and US$3.5 trillion in world economic activity, before the SARS-CoV-2. At Latin American level, Mexico is the second most important aviation market. Only in 2018 was transported in Mexico 98 million passengers, generating 1.4 million jobs and 3.05% of Mexico's GDP. Nonetheless, the economic outlook for the next 20 years anticipates the number of air passengers to double. Simultaneously, aviation fuel consumption will rise accordingly, leading to increased greenhouse gas emissions (12.9 Mt of CO_2 in 2019). As there is a global shortage of energy and resources research efforts are being made to develop innovative and practical technologies to recycle useful mate-rials from waste. There are several ways to produce bioturbosine, however, nowadays the alcohol to jet (ATJ) appears to be a feasible and attractive route to produce bioturbosine. The ATJ process transforms the biomass to alcohol and then to jet fuel through several steps like dehydration, oligomerization, and hydrogenation. However, the ATJ process needs to overcome some important challenges to be implemented at an industrial scale, some of these are biomass seasonality, regional availability, and its lower energy density. These problems can be overcome through a suitable design and implementation of a supply chain (SC). This work proposes a SC to process bioturbosine in a decentralized scheme, in which biomass is densified at pretreatment depots (PD) to an intermediate product like ethanol to reduce transportation costs. Also, the ethanol sale as oxygenating gasoline is considered. The demand for bioturbosine was set at 4 million tons according to data from the Mexican government. The SC model proposed in this work consists of a MILP model optimized in GAMS. To use biomass at an industrial scale and in a sustainable manner, the economic, environmental, and social aspects were considered as metrics to evaluate the SC solution, which is considered as the three pillars of sustainability. The economic aspect consists in the maximization of net profit, the environmental impact is the minimization of eco-indicator 99 and the social objective is the maximization of social welfare. The result shows that is necessary the installation of PD in several points of the country, which provide support to the biorefineries and attend different ethanol markets. In addition, the results indicate that bioturbosine production using the existing agricultural residues has the potential to cover around 450 thousand tons of bioturbosine, which represents about the 10% of Mexico's jet fuel demand. Finally, the PD installation showed its potential in transportation cost reduction, primarily in raw materials transportation.

Keywords: optimization, biojet fuel, lignocellulosic biomass, bioethanol, supply chain.

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Superstructure Optimization of Dimethyl Ether Process

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Abstract

Environmental concerns and economic considerations make it an inevitable task to integrate new fuel alternatives in the energy markets. Dimethyl ether (DME) is a relatively cleaner fuel and can be produced with many pathways. Superstructure optimization-based process synthesis is an important approach for obtaining feasible and competitive process among high number of alternatives in addition to calculation of corresponding operating conditions. Superstructure optimization incorporates a simulation environment for the calculation of the process output and a mixed integer-nonlinear programming problem (MINLP) [1] which include integer variables for the selection of units or streams and continuous variables for the temperature, pressures and many other variables. Such a simultaneous approach exploits the potential of mathematical models and advanced optimization algorithms as superstructure contains a wide range of processing units, which hinders the decision-making through traditional methods.

In the literature, many studies were conducted using commercial simulation environments (e.g [2]). In this study, we used open-source DWSIM and ChemSep for the calculation of optimum DME process architecture and operating conditions using Genetic Algorithm which is a common evolutionary metaheuristic optimization. The evolutionary algorithms and black-box architecture of process simulations environments enables relatively practical solution of non-convex process design tasks without formulating rigorous mathematical programming problems. Despite sub-optimality, the ease of implementation would not only increase the attention on optimization-based design but also provide satisfactory process architecture thanks to relatively simpler process models. The optimization problem is comprehensive as raw materials, reactor dimensions, distillation pathways and associated operating conditions are included. Preliminary calculations show that significant economic impacts can be obtained through the method.

Keywords: Superstructure Optimization; Mixed Integer Nonlinear Programming.

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A comprehensive evaluation on the COSMO-SAC-dsp model for vapor-liquid equilibrium predictions of refrigerants

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Abstract

Accurate predictions on mixture properties are the key of reliable computer-aided molecule design (CAMD) for refrigerant mixtures. Various mixing rules have been developed enabling improved prediction accuracy, where activity coefficient models (ACMs) are embedded (Hasan,1998). COSMO-SAC approaches utilize universal parameters and molecule sigma profiles from quantum mechanical calculations for activity coefficient predictions. They are considered to be more generally applicable than other ACMs based on group contributions, which contain many adjustable parameters.
This work presents the first time a comprehensive evaluation of the performance of COSMO-SAC approaches for mixed-refrigerant properties predictions. In particular, the most recent version of the COSMO-SAC approaches (i.e. COSMO-SAC-dsp (Hsieh,2004)) is adopted to predict the vapor-liquid-equilibria (VLE) of binary refrigerant systems. Valid VLE datasets for 139 refrigerant pairs are collected from NIST and by an exhaustive literature search. The refrigerant types cover hydrocarbons, halogenated hydrocarbons as well as inorganics with high diversity. The COSMO-SAC-dsp is combined with the Peng-Robinson equation of state using the Wong-Sandler mixing rule (i.e. COSMO-PR-WS) for the VLE prediction. The results are compared with that from UNIFAC (i.e. UNIFAC-PR-WS) and also two other well established models (i.e. VTPR (Schmid,2012) and PSRK (Horstmann,2000)).
The fitting performances of the VTPR, the PSRK and the UNIFAC-PR-WS are generally better than the COSMO-PR-WS, however with very limited applicability due to many missing group pure or binary parameters. The COSMO-PR-WS fails to provide accurate predictions in particular on some fluorine containing refrigerants. An optimization on atom dispersion parameters in the COSMO-SAC-dsp model is currently under development for improving the prediction accuracy.

Keywords: Peng-Robinson, COSMO-SAC, VTPR, PSRK, Wong-Sandler.

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Design and Evaluation Strategies for a Novel Hybrid Trigeneration System

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Abstract

Renewable energy sources that involve the use of Concentrated Solar Power systems (CSP), are receiving increased attention due to many of the prominent features that it can provide. Most importantly, the simultaneous production of thermal and electrical energy that can be achieved via CSP systems is of great value, and constitute many cogeneration processes. Moreover, CSPs have been proven to be an effective source of energy for industrial applications that require high amount of clean energy, such as desalination. Hence, combining water production activities together with thermal and electrical energy production options via CSP technologies results in novel hybrid tri-generation systems. The possibility of locating such tri-generation systems on the eastern shore of the Mediterranean Sea will be investigated in this paper. As such, several potential sites that can allow for the integration of CSP with desalination opportunities will be evaluated. Aspects such as the effect of direct normal irradiance (DNI) on the production freshwater via desalination will be investigated. The daily and seasonal intermittency of sunlight, which consists of a major challenge for CSP, necessitates the implementation of hybrid systems to ensure continuous supply of energy for desalination purposes. This paper studies the design of a hybrid trigeneration system under different weather conditions corresponding to the four seasons. The trigeneration system consists of a CSP plant as a main source of energy coupled with conventional fuel, natural gas, to serve as a backup energy source in the absence of solar energy, in addition to a desalination plant comprising thermal and membrane desalination technologies for freshwater generation. The design problem is translated into a Mixed Integer Non-Linear Program (MINLP) mathematical model that can be solved for the optimal network structure based on the appropriately selected technologies for steam, power and freshwater production. The environmental aspect of the system is also studied by quantifying the amount of carbon dioxide emissions, as well as the integration of a carbon capture technology to regulate those emissions subject to an appropriate value for the overall net carbon reduction target of the tri-generation system.

Keywords: Concentrated Solar Power, desalination, design, hybrid, trigeneration system.

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Molecular design of spark-ignition fuels by combining predictive thermodynamics and machine learning

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Abstract

The molecular structure of products, such as renewable fuels, can be tailored in silico by computer-aided product design (CAPD). Tailored CAPD requires a suitable criterion to assess the product's performance as a function of its physicochemical properties. However, to date, CAPD methods for fuels mainly rely on assessing the candidates' thermophysical properties instead of their performance in a given application. For example, renewable fuels are usually designed for physicochemical property targets rather than the expected efficiency of an internal combustion engine (König et al., 2020). Recently, prediction methods for the engine efficiency of spark-ignition (SI) engine fuels were developed. These methods consider interactions of various fuel properties and have been applied to database screenings to identify promising fuels based on a zero-dimensional engine model (Gschwend et al., 2019) or an efficiency merit function (vom Lehn et al., 2021).

Here, we present an optimization-based framework for the computer-aided product design of fuels using predicted engine efficiency as a performance metric for product use. We base our automated CAPD framework on a genetic algorithm for candidate generation (Douguet et al., 2005). The genetic algorithm optimizes molecular structures using 3D-molecular fragments considering constraints on molecular properties, e.g., minimum fuel oxygen content to mitigate in-cylinder soot formation. Each candidate molecule is assessed based on predicted thermodynamic and combustion properties. Thermodynamic properties, i.e. boiling point, melting point and enthalpy of vaporization (H_{vap}), are estimated using the predictive thermodynamic model COSMO-RS (Klamt et al., 2010). Combustion properties that substantially influence engine efficiency are the Research and the Motor Octane Number (RON and MON) as well as the laminar burning velocity (LBV). We predict RON and MON using the graph neural network by Schweidtmann et al. (2020). For LBV prediction, we integrate the group contribution-based artificial neural network by vom Lehn et al. (2021). Based on RON, MON, LBV, and H_{vap}, each candidate fuel is evaluated by the engine efficiency merit function (Szybist et al., 2021). The engine efficiency merit function computes the expected engine efficiency improvement of a

candidate fuel compared to RON95 gasoline reference fuel and serves here as a performance metric of product use. Moreover, viable fuel candidates must fulfil constraints on boiling point and enthalpy of vaporization to ensure proper operation of the engine in cold conditions.

Our framework identifies 14 candidate fuels outperforming the benchmark RON95 gasoline. As the optimal fuel, we identify furan with a predicted increase in engine efficiency of about 10 %, which is in good agreement with results from the literature (vom Lehn et al., 2021). Since the molecular design space for pure SI fuels is strongly limited by the property constraints, we also use the framework to design a two-component fuel blend with ethanol. Blends can satisfy the property constraints by balancing the properties of individual pure components. Besides the molecular structure of the candidate blend component, we optimize its fraction in a blend with ethanol. As a result, 291 suitable blend components are identified that lead to a positive merit function value; 70 blend components yield a higher merit value than pure furan. The presented method thus evaluates fuel performance using quantum-chemistry based predictive thermodynamics and machine learning in a molecular optimization algorithm to identify promising candidate fuels with high efficiency in spark-ignition engines.

Keywords: Product design, computer-aided molecular design, neural networks, COSMO-RS, engine efficiency.

Acknowledgement

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Techno-economic analysis of CO_2 compression and liquefaction processes including distillation column

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Abstract

The concentration of CO_2 in the atmosphere continues to increase due to the use of fossil fuels according to industrial development, economic and population growth. Attention has been paid to carbon capture and storage (CCS) technology for thermal power plants to mitigate CO_2 emission. The CCS technology includes CO_2 capture, compression, and liquefaction to transport it to sequestration or utilization. However, there are few researches in technical and economic aspects of CO_2 compression and liquefaction.
In this study, the techno-economic analysis (TEA) of CO_2 compression and liquefaction processes was presented, which included a distillation column to remove any impurities that may provoke safety and physical problems in geological sequestration.

Keywords: Carbon capture and storage (CCS), CO_2 compression and liquefaction, Distillation column, Techno-economic analysis (TEA), Climate change mitigation.

1. Introduction

The increase of CO_2 concentration in atmosphere may accelerate climate change (Cannone et al., 2021). In 2019, 34.4 Gt of CO_2 emission from fossil fuel use was emitted to the atmosphere (Friedlingstein et al., 2020). Approximately 34% of the CO_2 emission from fossil fuel was generated for power generation (IEA, 2020). It is necessary to capture CO_2 emitted from power plants to meet the growing energy demand and achieve carbon neutrality (Pellegrini et al., 2020). CO_2 capture, utilization, and storage (CCUS) technology has attracted attention worldwide with the CO_2 treatment from power plants (Jackson and Brodal, 2019). The pipeline or ship is used for transport and sequestration of captured CO_2 (Seo et al., 2016). The CO_2 mixture should meet the recommendations for pipeline transportation and sequestration (Abbas et al., 2013; Li et al., 2015). The CO_2 mixture captured from power plants such as coal-fired power plants and natural gas combined cycle power plants contains different components and compositions. Therefore, it is necessary to remove impurities (N_2, O_2, H_2O, H_2, Ar, etc.) to satisfy the recommendations for CO_2 pipeline transportation and sequestration. However, few studies have been conducted on CO_2 compression and liquefaction processes compared to capture processes (Moon et al., 2018).
In this study, a process flow diagram (PFD) including a distillation column for removing impurities after CO_2 compression and liquefaction was presented. Based on the process simulation, economic values such as total capital investment (TCI) and total production cost (TPC) of the CO_2 compression and liquefaction processes were analyzed.

2. CO_2 liquefaction with 7 stage compressors

The 10,000 kg/hr CO_2 mixture (0.92 mol% CO_2, 0.02 mol% N_2, 0.02 mol% O_2, 0.03 mol% H_2, 0.01 mol% Ar, 1500 ppm H_2O) is liquefied to 79 bar using a 7-stage compressor and heat exchanger, temperature swing adsorption (TSA), and distillation column, as shown in Fig. 1.

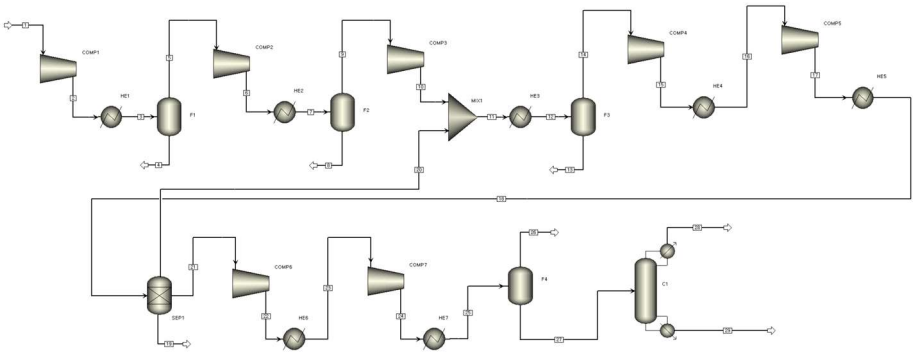

Fig. 1. Process flow diagram (PFD) of CO_2 compression and liquefaction with distillation column.

3. Results

As a result of TEA, 890 kg/hr of CO_2 mixture was liquefied to 0.96 mol% CO_2, 0.01 mol% N_2, 0.01 mol% O_2, 0.01 mol% H_2, 0.01 mol% Ar, and 17 ppm H_2O for pipeline transport and sequestration. The TCI for CO_2 liquefaction and impurity removal was $8.3 million, and the TPC was calculated to be $1.5 million/y.

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Process synthesis for desalination using superstructure optimization of membrane technologies

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Abstract

Desalination processes are important for different industries and for fresh water supply. Desalination technologies have been widely studied to achieve improvements in energy performance (EP). Multiple stage flash (MSF) is the most deployed technology at industrial scale Subramani and Jacangelo (2015). However, Reverse Osmosis has been implemented as an alternative process to improve EP. Nevertheless, there is still opportunity to evaluate and optimize other membrane technologies regarded as an alternative to MSF. Membrane distillation (MD) has not been tested at industrial scale. Pagliero and al (2021) identify a growing interest on these technologies due to the capacity to treat high concentration brines, but there are still technical challenges related to rigorous evaluation of the energy performance. MD technologies cover a wide range of operative modes as vacuum (VMD), sweep gas and direct contact MD. VMD has been tested at pilot scale for desalination. MD research has been focused on new membrane materials and geometries for contactors. Nevertheless, simulation tools to gather the material characteristics, module geometries and operating conditions at industrial scale remains a challenge. This work aims to present a modified method by Zhao and al. (2018), to obtain a membrane process adapted to various brine conditions (feed temperature), to compare membrane technologies. Thus, computer aided process simulation is used to achieve the results; the mathematical model was coded (FORTRAN) and added to a commercial software (PROSIM) as external subroutine to simulate MD and RO units. Geometry and material parameters are set according to the commercial module Dow SW30HR-380 data. Then, a superstructure is defined and optimized within an ant colony algorithm (MIDACO). Operational conditions (pressure and in-process temperature), stages and number of modules parallel are obtained by superstructure optimization. As a major result, a plot of a Pareto-front from a multi objective calculation is obtained. These results can be deployed as a baseline for further calculations with specific electric, heat and membrane cost, then supporting decisions of investment for desalination plants in preliminary studies.

Keywords: Process synthesis, optimization, desalination

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A comparison of process synthesis approaches for multistage separation processes by gas permeation

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Abstract

Various optimization-based process synthesis approaches exist to propose a process structure and associated parameters, which have been applied on many applications. The goal of this work is to provide a comparison of synthesis methods on a common process synthesis problem. Three approaches, developed by the authors (Ramirez-Santos et al., 2018; Zhao et al., 2018; Neveux, 2018), are used on an identical problem. Methods differ in the synthesis approach (based on a superstructure or ab-initio without predefined structures), process modeling (equation- or simulator-based), optimization algorithms (global NLP, MINLP, evolutionary) and implementation (dedicated or commercial softwares). The production of N_2 from air using membrane gas permeation is chosen from a synthesis point of view due to the numerous possible stages, recycling, design variables, nonlinear economic objective and constraints. In terms of solutions, known process structures are found by the three methods , with processes between 1 and 3 stages of membranes and usual recycling strategies, depending on the targeted N^2 purity. The interest of the ab-initio method (no superstructure) is highlighted as better structures are found, which were not included in the superstructure of the other two methods (but with a small reduction of 3% on the levelized production cost). In terms of number of evaluations, superstructure based methods need around 10 times less evaluations than the ab-initio method whose search space is not restricted by a given set of alternatives. In terms of ease of use, implementation within commercial simulators allows process engineering to use familiar tools instead of programming languages. Another highlight is the need for accurate unit operation models, even for the exploration of the process structure (large) search space. Tests performed with a simplified model showed that different structures and associated parameters are obtained, which were not viable once tested with the rigorous model. This comparison can be extended to more constrained separation problems (meaning a smaller feasibility region) and other types of processes.

Keywords: Process Synthesis, NLP, MINLP, separation processes

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Bifurcation analysis of combined agglomeration and layering granulation in fluidized bed processes

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Abstract

Particle growth in fluidized beds is an important unit operation in chemical engineering. It is applied widely in the agricultural, pharmaceutical and food industry, due to the possibility of defining particles with desired properties, particularly the particle size. The basic size-enlargement processes which can be performed in fluidized bed are layering growth, particle clustering (agglomeration) or a combination of both. For continuous layering granulation processes in fluidized beds with sieve mill cycle instability may rise in the form of self sustained oscillations of the particle size distribution (Neugebauer et al., 2019). Avoiding such undesired instabilities is of high importance from a practical point of view. In contrast to this, for the corresponding agglomeration process only damped oscillations were found (B¨uck et al., 2016) and the questions arise whether this is due to the specific choice of process conditions considered in this paper and whether combined layering/agglomeration processes in continuously operated fluidized beds can also be unstable. To answer this question, a bifurcation analysis of a combined layering and agglomeration process is presented in this contribution. To this end a multiple parameter continuation is applied to a population balance process model with external screen mill cycle. The main bifurcation parameters are the milling grade as well as the ratio between agglomeration and layering growth. The analysis reveals stability borders for different process parameter combinations and shows the stabilizing effect of agglomeration when being the dominant growth mechanism. The results of this contribution are relevant for the design and dimensioning of new fluidized bed granulators and appropriate control strategies.

Keywords: fluidized bed, granulation, agglomeration, layering growth, bifurcation analysis

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Enhancement of energy saving of reverse osmosis system via incorporating a photovoltaic system

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Abstract

Undoubtedly, Reverse Osmosis (RO) desalination capacity noticeably increases. However, the necessity of developing an efficient design becomes more vigorous. This study shows the development of a conceptual design of an efficient energy medium-scale RO brackish water desalination plant of the Arab Potash Company located in Jordan. In this regard, a photovoltaic (PV) solar farm has been combined the original RO process to professionally generate electricity in a sustainable way and decrease the overall energy consumption. To obtain an accurate estimation of the process performance, this work shows the utilisation of an efficient process model for the spiral wound RO process. The model prediction is compared against experimental data gathered from the literature and showed a good agreement. Also, an accurate model for the photovoltaic system was gathered from the literature to conduct preliminary calculations of the proposed new configuration. To systematically evaluate the process performance, the influence of the hourly solar irradiation, and the duration of daylight on the specific energy consumption was evaluated. This also guides to understand the efficient control variables of PV that integrate the production of low total dissolved solids (TDS) drinking water at the lowest energy consumption. The simulation results of the proposed RO design are compared to the original ones and showed a considerable energy saving. Thus, it can be said that this research has achieved a satisfactory room of improvements.

Keywords: Brackish water; hybrid system; RO-PV system; Energy saving; Hourly solar irradiation.

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Design and simulation of methanol synthesis using heavy residues with carbon utilization

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Abstract

The continuous rise of global carbon emissions demands the utilization of fossil fuels in a cleaner and sustainable way. Gasification is a potential technology that can convert the dirty fossil fuels to produce clean and environment friendly fuels in an economical manner. In this study, vacuum residue is employed as a feedstock to produce high grade methanol. A vacuum residue to methanol (VRTM) process is simulated using Aspen Plus for a methanol production capacity of 90 t/h with 99.9 wt.% purity as shown in Figure 1. The developed VRTM process is bench-marked with the conventional steam reforming to methanol (SRTM) process through energy, environmental and economic analysis. The performance of vacuum residue gasifier, natural gas reformer and the methanol synthesis reactor are validated against the plant data and the simulation results are found to be in good agreement. The results showed that the VRTM process offers a process energy efficiency of 49.5% which is 1.6 % higher than the SRTM process. The unit cost of methanol product from the VRTM process is \$ 317/tCH_3OH which is 14% lower compared to the SRTM process. In terms of environmental analysis, SRTM process emits less carbon emissions than the VRTM process. However, the VRTM process offers a high purity captured CO_2 stream that can be utilized for another application that can further offset the methanol production cost.

Keywords: Methanol; carbon capture and utilization; vacuum residue gasification; economic analysis; process simulation.

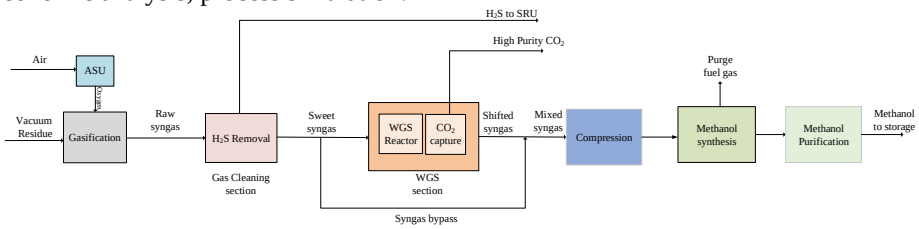

Figure 1: Block diagram of vacuum residue to methanol (VRTM) process – sweet shift

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Integrated process synthesis and design of intensified/hybrid processes

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Abstract

Process intensification is defined as a set of innovative solutions, which aims to improve the whole process performance, such as lower capital/operating costs, minimizing waste, and carbon emissions. Because of environmental concerns and strict government regulations, the process industry moves toward more efficient and sustainable designs. As a potential method for process improvement, identifying and applying process intensification will be critical. A phenomena-based methodology has been proposed to identify and incorporate intensified equipment options into process synthesis. Furthermore, researchers have evaluated different hybrid distillation configurations, and the results show potential 20% energy savings and capacity enhancement. Applying intensification in the early stages of process design could generate sustainable process flowsheets with higher energy efficiency and lower environmental impact.

This work focuses on expanding the thermodynamic insight-based process synthesis method by Tula et al. (2015) to include hybrid/intensified separation techniques, such as distillation-membrane/adsorption, dividing wall column, etc., and solve both retrofitting and new process design problems. A new ranking algorithm based on enthalpy balances and first principle-based models is developed and applied to evaluate all the process alternatives. The expanded method has four steps. In the first step, the raw materials, products, and base case process (retrofitting) are identified. Then, azeotropic/eutectic analysis is performed, and binary ratios of thermodynamic properties are calculated. Based on the data from the analysis step and predefined selection rules, all feasible separation techniques are identified, and multiple process alternatives are generated. Finally, the ranking algorithm evaluates the process alternatives, and the top selected processes are further evaluated using rigorous models. In this way, the method identifies the best process alternatives and their optimized design/operating conditions. This framework was used to solve a range of case studies, both retrofitting problems (cumene production and styrene production) and new process design problems (dimethyl carbonate (DMC) production). A dividing wall column could be applied for the separation of cumene products, which saves 20% utility cost for the downstream separation section. In the DMC production case study, 166 process alternatives were generated, and the top selected alternatives showed 53% energy savings compared to literature configurations.

Keywords: hybrid technologies, process intensification, process synthesis.

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Macroalgae-based integrated biorefinery for hydrocolloids, chemicals and advanced biofuels production

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Abstract

In this work, we propose a mixed-integer nonlinear programming (MINLP) model for the optimization and heat exchanger network synthesis of a macroalgae-based integrated biorefinery. The proposed framework is based on a biorefinery model previously published (Casoni et al. 2020) in which a platform molecule (isosorbide), biogas and fertilizers are produced from the brown macroalgae *Macrocystis pyrifera.* Isosorbide is used to obtain four final products: a flame retardant, a biopolymer, a bio-solvent (dimethyl isosorbide) or a drug for heart disease (isosorbide dinitrate). The model was extended to include the production of alginate, a hydrocolloid with applications in several industries (e.g. pharmaceutical, food, cosmetic, biomedical), and the sequential production of hydrogen and biogas through two-stage anaerobic digestion. The proposed superstructure includes the heat exchanger network synthesis (HENS), by considering three potential heating utilities and two cooling utilities. In this way, the optimal solution of the model looks for a trade-off between utility cost and area targeting, and provides heat exchanger unit matches. Due to the large number of heat and cool streams, the resulting model is challenging, including around 35000 constraints and continuous variables, and around 9000 discrete decisions. The mathematical problem is formulated and implemented in GAMS, and is solved using DICOPT. Numerical results show the economic feasibility of macroalgae biomass valorisation through high value-added products, energy and advanced biofuels production, including heat integration within a circular economy framework for the sustainable use of macroalgae biomass resources of the Argentinean Patagonia. The reduction in energy consumption led to a potential decrease in utility cost up to 75 %, while the increase in investment cost is negligible, compared to a plant that is not heat integrated.

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Design Space Determination of Mesenchymal Stem Cell Cultivation by Dynamic Modeling under Uncertainty

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Abstract

Mesenchymal stem cells (MSCs) are a promising cell source for regenerative therapy due to their multipotency, self-renewability and ethical compliance (Ullah et al., 2015). While various technologies exist for MSC manufacturing at scale, many challenges remain, especially in managing variability, critical for ensuring product quality (Lipsitz et al., 2016). Design Space (DS) is one strategy for ensuring quality in pharmaceutical production where a feasible region of process parameters can be identified (García-Muñoz et al., 2010). However, the DS determination in MSC cultivation is complex due to: time-dependent nature of operations, process variability, lack of experimental data.
This work determined the DS in the MSC cultivation using literature data (Jossen et al., 2020) based on a four-step computer-aided workflow to address these challenges. STEP 1: Relevant Critical Quality Attributes (CQA's) and Critical Process Parameters (CPP's) were identified based on expert know-how. STEP 2: An ODE based mechanistic model was developed to represent system dynamics of MSC cultivation. STEP 3: A probabilistic DS was determined based on dynamic modelling and stochastic simulation. STEP 4: A DS-based operational strategy was established to support decision-making.
Seeding density and medium change ratio were selected as CPPs while the number of cells and the ammonia concentration were CQAs. Monod kinetics based modelling and stochastic simulation were used to determine a probabilistic DS (Figure 1), where shades of grey represent the probability (P) a production run meets all CQAs. The analysis found that donor variability (source of the initial MSCs) and the culture period influenced the DS, illustrating the need to incorporate time and uncertainty into DS determination.
Keywords: Decision support, quality by design, regenerative therapy, stochastic simulation.

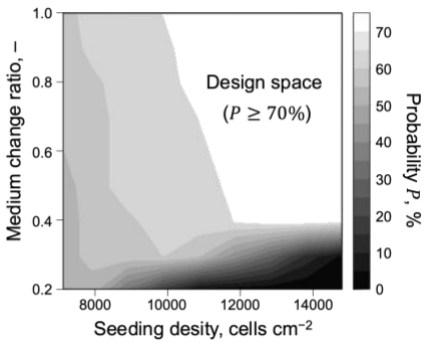

Figure 1: Design space diagram at day 10. 70% of the batches are expected to meet CQA's if the process is operated within the white region.

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Deterministic global optimization of multistage layer melt crystallization using surrogate models and reduced space formulations

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Abstract

Layer melt crystallization is a thermal separation process with very high theoretical selectivity in case of eutectic mixtures, lower required energy for the phase change than e.g. distillation, and the ability to treat heat sensitive substances. Crystal layers that grow on a cooled surface incorporate impurities from the melt if the growth rate is not extremely small, which may necessitate additional crystallization steps in a multistage process to achieve a desired purity. The layer growth process determines the separation efficiency of each stage and can be described by complex dynamic models. However, including differential equations in mathematical process optimization is computationally unfavorable, and using strongly simplified correlations for the separation efficiency could lead to significant prediction errors and suboptimal design decisions. Instead, an artificial neural network that reproduces the separation efficiency accurately is used here as a surrogate for a dynamic model adapted from (Beierling et al., 2014). The surrogate model is trained on simulation data from the dynamic model and combined with mechanistic equations to create a hybrid overall process model that is used for the optimization of multistage crystallizer networks. In order to obtain certified globally optimal designs, the deterministic global solver MAiNGO (Bongartz et al., 2018) is used to solve a reduced space formulation of the optimization problem, i.e. a formulation in which the dimensionality of the problem is not increased by intermediate variables, e.g. those appearing in artificial neural networks. In summary, this work extends the capabilities for deterministic global optimization of multistage layer melt crystallization processes via surrogate modeling and solving the resulting problems with MAiNGO using reduced space formulations.

Keywords: deterministic global optimization, layer melt crystallization, surrogate modeling, reduced space formulation, multistage crystallizer network

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Multi-scale and multi-objective integrated design of a batch food processing plant

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Abstract

A batch mobile unit to limit post-harvest losses in sub-Saharan Africa: an interesting but complex solution

In sub-Saharan Africa, post-harvest losses are estimated at 40% of the food production per capita, of which fruits and vegetables represent the largest share. In order to reduce these losses, AS FOOD International aims to develop and sell a mobile processing unit (MPU) to stabilize produce directly at the point of production, thus reducing transport distance and improving the quality of the final food products. However, designing a MPU is a complex task, as many constraints and objectives must be met: mobility, compactness, cost effectiveness, product quality, etc. It must also be flexible enough to handle different fruits and vegetables, follow their seasonality, and handle multiple final products. Consequently, batch production appears more relevant than continuous production.

Multi-objective optimization and multi-scale

The design of batch food processing units (FPUs) can be achieved using multi-objective optimization (MOO) methods that are able to identify the best compromise between several conflicting objectives, but are hardly used in agribusiness and only partially (Madoumier, 2019). Moreover, the performance of a FPU depends on phenomena occurring at different scales: roughly product, process, unit/factory. Thus the development of the representation models describing these phenomena, and combining different length scales and time scales, is a difficult task and requires methods (Ingram et al. (2004), Panchal et al. (2005), Yang & Marquardt (2009)).

Development of a methodology integrating MOO design and multi-scale modeling

To address these challenges, a methodology for building a design support tool was developed, called "Methodology for the Integrated, Multi-scale and Multi-Objective Design of Systems" (MIMMODS). It consists of seven tasks:

1. Clarification of the design task and problem statement;
2. Development of a multi-scale simulation model of the system to be designed;
3. Modeling preferences and choosing a selection method;
4. Choice of an optimization method;
5. Implementation of the design support tool;
6. Visualization and analysis of the results;
7. Iterative and systematic refinement of the design support tool.

The resulting decision support tool can i) simulate the behavior of the FPU and predict an estimate of its performance, ii) include the preferences of the decision maker, and iii)

identify the design solutions that best satisfy the design objectives and the preferences of the decision maker.

Case study: scenario and objectives to be satisfied
MIMMODS was applied to the design of a fruit and vegetable processing MPU in Côte d'Ivoire. The equipment transported in the container must process okra, pineapple and mango to produce purees, nectars and juices. The design objectives are: economic viability, quality of finished products, ability to operate in remote areas, operator-friendly workflow and space, and efficiency of energy and water consumption. Each objective was translated into a number of indicators to quantify the estimated performance of the PMU.

Decision support tool developed
Following MIMMODS, a design support tool was developed, including i) a multi-scale simulator of the MPU, ii) desirability functions to take into account the preferences of the decision makers, iii) a genetic optimization algorithm using the minimum value of the indicators to identify the Pareto-efficient solutions, and iv) a selection method based on the geometric mean to select the best solutions in the set of Pareto-efficient solutions. The design variables are mainly i) the operating conditions of the thermal stabilization, ii) a reference of equipment for each operation of the unit, and iii) a quantity of said equipment to increase or decrease the productivity of the MPU.

Results
The design support tool has produced an initial solution for the design of the MPU. The solution appears satisfactory with respect to the decision makers' preferences, and also feasible and consistent. Through detailed visualization of the trade-offs in the objectives and comparison with other possible solutions, it was found that the okra puree limited the overall performance of the MPU, raising questions about the appropriateness of processing this product with the MPU.

Conclusions
Thus, although the construction of the decision support tool implementing MIMMODS was challenging due to the complexity of the system to model, the potential of this methodology has been demonstrated. The design support tool allowed for improved understanding of the design problem, iterative refinement of the design solution, and thus reduced trial and error in the physical construction of the upcoming prototype.

Keywords: food plant design, multi-scale modeling, batch, multicriteria decision making.

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Model-Based Design Space for Optimisation

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Abstract

As demand for biopharmaceuticals rises, manufacturers are required to meet multiple competing key performance indicators (KPIs) such as process sustainability, efficiency and product efficacy and quality. At the same time challenges related to measurement unavailability, large amount of waste, and the high manufacturing costs (Nasr et al., 2017) may hinder process innovation. In that respect, advanced process optimisation and control in biopharmaceutical manufacturing is challenged by the lack of online Process Analytical Technologies (PAT). This results into processes relying heavily on statistical-based experimentation which may be costly and inefficient (Narayanan et al., 2020). In this work, we are proposing a novel methodology for evaluating process robustness and process optimisation using model-based design space to accelerate process design and optimisation.

We focus on the capture step, which is the initial separation process in the production of monoclonal antibodies (mAbs) separating the majority of process impurities generated upstream using affinity (protein A) chromatography. The mathematical model of this process presented by Steinebach et al. (2016) is used to computationally explore the multi-dimensional design space. This design space considers design parameters such as resin properties and column dimensions, generated by sampling a high-fidelity model. The methodology is evaluated against three different resins for three different parameter sets; namely switching times, column dimensions, and feed concentration and flowrate. The results indicate that column switching time, column dimensions, resin properties, feed concentration and flowrate are amongst the most impactful parameters. By using a higher protein A density resin, the process step gains greater operational flexibility.

Keywords: computing and systems engineering, process design and development, process optimisation, pharmaceutical manufacturing.

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Optimal Design and Planning of Renewable Energy Systems toward Net-Zero Emissions

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Abstract

Cornell's Climate Action Plan called for reaching climate neutrality at its Ithaca campus by 2050 when it was first proposed. In 2016, the Senior Leaders Climate Action Group calls for analyzing viable energy alternatives for the Ithaca campus to achieve carbon neutrality by 2035 to accelerate its efforts (Andersson and Grönkvist, 2019). Carbon neutrality refers to attaining net zero-direct carbon dioxide emissions by balancing carbon emissions with carbon sequestration. The choices Cornell makes today to enable a carbon-neutral campus of the future will lead to investment, which would insulate Cornell from unknown future volatility in fossil fuel markets and associated carbon fees. This study aims to address the sustainable design and economic optimization of the Cornell campus energy system towards carbon neutrality. The proposed 100% renewable campus energy system involves the combination of renewable energy technologies and options based on local conditions and resources, such as lake source cooling (LSC), earth source heating, and green hydrogen, among others, coupled with advanced energy storage technologies.

This work addresses the economically optimal and environmentally sustainable design of the campus energy systems with earth source heat, LSC, and peak load, as well as long-term energy storage. The proposed hybrid energy system generates power, heat, cooling as products. A novel energy systems superstructure (Gong and You, 2015) is proposed to embrace all the aforementioned generation and energy storage technologies. We will consider monthly demand over the year 2035. Based on the superstructure of the proposed hybrid energy system, we develop a multi-period optimization model to minimize the total annualized costs of the campus energy system. The aim is to determine the optimal configuration of the campus energy systems and corresponding capacities of technology units by minimizing the total annualized cost. The applicability of the proposed modeling framework will use real data from Cornell University's main campus located in Ithaca, New York State.

Keywords: carbon-neutrality, earth source heat, lake source cooling, peak fuel, energy storage.

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Computer-aided molecular design of working fluids for adsorption heat pumps based on density functional theory and PC-SAFT

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Abstract

Adsorption heat pumps are a sustainable alternative to compression heat pumps because waste heat can be exploited to drive the process. To maximize the performance of the adsorption heat pump, not only the solid adsorbent material needs to be carefully chosen but also the corresponding working fluid. The optimal working fluid also has to fit the process and should therefore be identified in an integrated design (Papadopoulos et al., 2018). Such an integrated design of working fluid and adsorption heat pump has to consider the interactions of the candidate fluids and the solid adsorbent material. On the process level, the interactions are typically described by adsorption isotherms. The prediction of adsorption isotherms usually requires computationally intensive molecular simulations methods that currently render design problems challenging.

In this work, we present an efficient method for the computer-aided molecular design of working fluids for adsorption heat pumps. The fluid design method aims to identify fluids with the best performance for the given process conditions and a given adsorbent material. For this purpose, our method builds on the 1-stage Continuous-Molecular Targeting – Computer-aided Molecular Design (CoMT-CAMD) method (Schilling et al., 2017).

We base our method on three building blocks: 1) a CAMD formulation (Schilling et al., 2017) for fluid design, 2) a thermodynamic property model, and 3) a process model. Linking the three building blocks enables the design of the working fluid for a preselected adsorbent material using a process-based objective function. The key of our method is the thermodynamic model to calculate the equilibrium properties of the fluid/adsorbent pairs. To efficiently capture the interactions between the fluid and the adsorbent material, we use classical density functional theory (DFT) (Sauer & Gross, 2019) based on the PC-SAFT equation of state (Gross & Sadowski, 2001). PC-SAFT is related to the CAMD formulation by the homosegmented group-contribution method of PC-SAFT (Sauer et al., 2014). The DFT model enables us to calculate adsorption isotherms. Based on the isotherms, we determine the thermodynamic states of the process model. The process model is given by a simplified equilibrium model of an adsorption heat pump. In the model, the enthalpy of adsorption is approximated by the enthalpy of vaporization. With the predicted isotherms, all heat flows of the adsorption heat pump can be calculated for a specific application. The heat flows allow determining the coefficient of performance (COP)

of the heat pump which is used as process-based objective function within the integrated design problem.

The linked three building blocks result in a mixed-integer nonlinear program (MINLP). Solving the MINLP yields an optimal working fluid with the maximum COP for the considered adsorption heat pump. Here, we use the solver KNITRO (Byrd et al., 2006). The integer constraints are first relaxed, and a hypothetical, optimal fluid, the so-called target, is identified. Afterward, real molecular structures with a COP close to the target are identified. By applying integer-cuts, we obtain a ranking of promising working fluids.

The developed fluid design method is applied to a case study for waste heat utilization for a cooling application. Waste heat at 90°C is used to drive an adsorption chiller that satisfies a cooling demand at 16°C. The ambient temperature is 30°C. A COP of 0.5 is obtained for the hypothetical target (Table 1). The best real fluid is ethanol with a COP of 0.442. The result is in line with Boman et al. (2021), who state that adsorption chillers usually have COPs below 0.5. The top 5 identified real molecules are small alcohol molecules, pointing to the good performance of the molecular family. The results show that the highest loading difference does not indicate the best COP. The heat of evaporation correlates better with COP. However, 2-butanol compensates low heat of adsorption with high loading. Thus, even for the simplified process model employed, only a process-level objective reflects all trade-offs in the selection of a working fluid.

Table 1: Target and top 5 identified working fluids and the corresponding optimal COP, heat of evaporation, and loading difference of the loaded and unloaded state of the adsorber.

Rank	Name	Loading difference Δw in $\frac{\mathrm{kg_{ad}}}{\mathrm{kg_{sor}}}$	Heat of evaporation $\Delta h_{\mathrm{evap}}(T_{\mathrm{Ads}})$ in $\frac{\mathrm{kj}}{\mathrm{kg}}$	COP
-	Target	0.286	977.2	0.500
1	Ethanol	0.250	899.4	0.442
2	1-Propanol	0.259	800.0	0.437
3	2-Butanol	0.292	672.6	0.401
4	2-Propanol	0.253	740.2	0.392
5	1-Butanol	0.265	705.6	0.391

Our presented fluid design method is able to identify the best fluid for the considered adsorption heat pump and adsorbent. The method can be easily applied to other adsorbent materials and case studies with other temperatures. Thereby, the presented method allows to systematically exploit the potential of fluid choice for adsorption heat pumps. Future work will also consider the adsorbent material as a degree of freedom.

Keywords: adsorption heat pump, classical density functional theory, waste heat utilization, computer-aided molecular design

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Isopropanol/ n -Butanol/ ethanol separation from diluted fermentation broth by distillation. Process optimization using Mixed Integer Linear Programming (MILP) techniques

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Abstract
This work has been performed in the framework of the development of the bio-based fermentation process to produce IBE (Isopropanol/ n-Butanol/ Ethanol). The so-called IBE fermentation is indeed an interesting sustainable alternative for the production of fossil-based products (Kujawska (2015)). However, product inhibition in fermentation leads to dilute fermentation broths in water (15-25 g IBE /L) which implies high energy demand for products / water separation. Several solutions can be implemented such as hybrid distillation/ liquid-liquid extraction processes (Kraemer (2011), Zhang (2020)) to separate such a dilute broth or such as In Situ Product Recovery Techniques to overcome product inhibition and produce concentrated broths (Outram (2016)).
In the present study focus has been put on ready-to-industrialize downstream processes for Isopropanol/ n-Butanol/ Ethanol separation from dilute fermentation broth, using conventional distillation and shell-and-tube heat-exchanger technologies. The conventional distillation sequence such as described by Zhang (2020), using 5 distillation columns, was used as a reference case. This reference scheme as well as an IFPEN patented distillation sequence with 3 columns only were indeed optimized using an in-house tool. The latter tool allows to simultaneously optimize the heat exchanger network configuration and the distillation columns' operating pressures for a given material balance, using Mixed Integer Linear Programming (MILP) optimization techniques. For each case, utilities (electricity and steam consumptions) are first calculated; then main equipments (columns, heat-exchangers, pumps…) are designed and corresponding investment costs are estimated which can further be used for total production cost estimation. An optimum heat-exchanger network is proposed by the tool, together with optimum columns' operating pressures.
When comparing to the distillation reference process, the optimized heat exchanger network leads to a 37 % vapor consumption reduction and to a 28 % total separation cost reduction, when both investments and utilities costs are considered. The IFPEN patented scheme even without optimization is found to be more interesting than the reference scheme with a separation cost 19 % lower. It is shown to be even more interesting after optimization: its separation cost is 34 % lower than the one of the reference scheme.
The present work shows that process optimization is very important to allow IBE fermentation deployment with acceptable cost. It is also discussed how optimization tool can be applied to any distillation process leading to meaningful cost savings.
Keywords: Isopropanol/ n-Butanol/ Ethanol fermentation, Distillation, Optimization, Mixed Integer Linear Programming

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Automatic synthesis of hybrid processes using distillation and liquid-liquid extraction for the separation of azeotropic mixtures

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Abstract

With the increasing need for more energy efficient and economical downstream processes, improved separation processes become necessary. Especially for the separation of highly diluted and azeotropic mixtures, which are gaining prominence with the transition to bio-based feedstock, solvent-based separation processes are a promising and well-proven alternative to azeotropic distillation processes. As the choice of solvent is of utmost importance, various methods for solvent screening and computer-aided molecular design have been proposed. However, these methods generally assume a fixed process structure based on a combination of a counter-current extraction cascade and a single distillation column for solvent recovery. Consequently, certain properties have to be met by the desired solvent, especially considering the formation of azeotropes and the boiling point. While such constraints might be reasonable in many cases, an extension of the search space first of all requires the consideration of additional and alternative process configurations. In order to overcome this limitation and enable the selection of a solvent-specific process configuration, the current work introduces a novel approach that enables an algorithmic synthesis of separation processes combining liquid-liquid extraction and simple distillation columns. The approach builds on the algorithmic framework, which was previously introduced for distillation processes (Sasi et al., 2020). For the necessary extension to extraction-distillation hybrid processes, the feasibility test and tree generation algorithms are extended for liquid-liquid extraction as an alternative unit operation and the pinch-based shortcut method of Redepenning et al. (2017) is applied to determine the minimum required solvent flowrate. Using the extended synthesis method, different solvents can be compared based on the minimum required solvent flowrate and the minimum energy required for solvent recovery, without a-priori specification of the process configuration. The method generates hybrid extraction-distillation process alternatives solely based on a thermodynamic model of the chemical system. The application of the extended synthesis method is illustrated for relevant case studies.

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A framework for optimal and flexible scheme design under uncertainty & sustainable aspects

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Abstract

The design of sustainable processes implies multi-criteria and multi-objective decision-making problems associated with multiple uncertainty sources, where the use of statistical indicators can be employed as a tool for the robust design of systems subject to uncertainties (Gargalo & Sin, 2015).

In this study, a computer-aided framework for sustainable, optimal and flexible process design under uncertainty has been developed and implemented, based on the energy, exergy, economy, and environmental analysis (4E analysis); in addition to statistical indicators integration as decision-making design criteria. The framework has been developed using Matlab r2019a ® and Aspen Plus V8.8 ®. Both tools were interconnected through a COM interface®.

The separation of acetone-butanol and ethanol (A-B-E) fermentation broth was employed as case study, the employed flowrate range (kg/h) was for A: 2,276±112, B: 5,931±276, E: 1,593±135, water: 10,479±498 and carbon dioxide: 82±5. The separation and purification scheme (SPS) included one liquid-liquid extraction column, four conventional distillation columns, evaluating four non-toxic extracting agents.

The Latin hypercube sampling was used to propagate the uncertainty on the feed flowrate employing 75 scenarios. Additionally, Gamultiobj, a suite of Matlab based on multi-objective genetic algorithm (MOGA) optimization (50 generations, 200 individuals, and crossover fraction of 0.8) was used to solve each scenario. The decision variables in the optimization were the extracting agent flowrate (EAF), number of stages (NS) and feed stages (NF) for each column. Three statistical indicators were selected as decision-making criteria for the SPS design: mean, mode and the value of 80% of the cumulative distribution function (CDF). The SPS flexible designs were evaluated considering the feed flow values and extracting agents, where the mean and standard deviation for each structural design specifications were NSC101: 45±1, FMAEX: 55,198±23,013, NSD101: 39±3, NFD101: 19±3, NSD102: 41±2, NFD102: 20±1, NSD103: 46±1, NFD103: 19±2, NSD104: 47±2, NFD102:15 ±1. The final designs were tested using minimum, mean, and maximum feed flowrates samples.

The results obtained by the designs of the 80 % of the CFD showed the possibility to synthetize a single design, capable of operating with any proposed extracting agent and with flexible operation subject to variable feeds (mass flow, and concentration); furthermore, the use of this statistical criterion for process design guarantees the total convergence for each scenario as opposed to the other two design indicators.

Keywords: Optimization; Uncertainty; MOGA; Statistical indicators; Sustainability

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Optimization-based assessment framework for CO_2 utilization to fuels strategies

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Abstract

Carbon capture and utilization for fuel production is one of the attractive and effective solutions addressing climate change and energy security. In which, captured CO_2 is considered as raw materials for high-energy-density products (e.g., methanol, dimethyl ether, Fischer-Tropsch fuel, gasoline) via different technologies (catalytic conversion, thermochemical energizing, electrochemical reduction). This study developed an optimization-based framework to analyze and assess CO_2 utilization strategies for fuel products regarding technical, economic, and environmental performance. To achieve this goal, we first generated a superstructure involving a series of technologies (carbon conversion and separation) to produce value-added fuels from captured CO_2 as a feedstock. We then simulated all the involved processes, and estimated the technical and economic parameters (mass and energy flow, and sizing and costing data) that were further adopted into the optimization model. The optimization models were developed to identify the optimal CO_2 utilization strategies with different criteria: energy efficiency, production cost, profit, and CO_2 reduction. As a result, we can determine the best CO_2 utilization strategy over various technological pathways to produce different targeted fuels, which makes CO_2-based fuels economically and/or environmentally viable.

Keywords: Process design; CO_2 utilization superstructure; Optimization.

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A novel approach for continuous extraction of active ingredients from essential oils through combined chromatography

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Abstract

Bioactive ingredients from plant extracts are the basis of many innovative products in the food, cosmetics, or the pharmaceutical industries. However, at present, mainly diluted products are extracted as complex mixtures, as a large amount of by-products accumulates as waste at the end of the process, and can only be recovered with increased effort. Essential oils are complex volatile substances composed of many ingredients with broad spectrum of bioactivity and, therefore, subject to extensive research (Chouhan et al. 2017). Various processes have been used to extract these ingredients: harvesting as plant materials, washing, extraction of phytonutrients, or purification of the components of interest (Belwal et al. 2020). Traditional techniques consist of liquid-liquid extraction, solid-liquid extraction, or solid phase micro-extraction. Modern techniques include ultrasound-assisted extraction, pressurized liquid extraction, supercritical fluid extraction, microwave-assisted extraction, or instant controlled pressure drop extraction (Yahya et al. 2018). Often, for the same plant, extraction conditions may vary in terms of extraction time or amount of solvent used. Conventional methods suffer from some serious disadvantages, such as excessive solvent, time and energy requirements, which demand the development of new techniques that are more efficient, less expensive and least hazardous (Abbas et al. 2021).

This contribution introduces a combined liquid chromatography purification designed for a continuous and resource-efficient process, integrating the rotating columns and the simulated moving bed principles. The approach is demonstrated on the example of bisabolol oxides A and B, effective ingredients with anti-inflammatory and spasmolytic effects, prepared from chamomile essential oil.

Keywords: Essential oil; Preparative chromatography; Simulated moving bed (SMB)

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Digital design and optimization of an integrated reaction-extraction-crystallization-filtration continuous pharmaceutical process

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Abstract

Over the last few years, continuous pharmaceutical manufacturing has become reality and proved to be more flexible and viable compared to the traditional batch processing (Benyahia, 2018; Cole et al., 2017). However, the successful design, development and operation of integrated continuous pharmaceutical plants is still considered as a major challenge in pharma. The emerging digital transformation is urging pharma to adopt more systematic digital tools for optimal process development and operations. This includes the development and implementation of high-fidelity digital twins, soft sensors and advanced quality and process control technologies.

This work investigates the digital design of a continuous pharmaceutical plant comprising a continuous three stage reaction, liquid-liquid extraction, multistage cooling and antisolvent crystallization, and wash-filtration. Firstly, the mathematical models were developed and validated in conjunction with the available experimental data obtained from the literature or/and research partners. The resulting digital twin was used for steady state optimization to deliver optimal options for plant design and operation, including process capacities and number crystallization stages (Liu and Benyahia, 2021), along with the optimal design of the recycle and purge streams. After the identification of the optimal design and optimal steady state operation, the digital twin was used to perform uncertainty propagation and global sensitivity analysis (Fysikopoulos et al., 2019) to identify the Critical Process Parameters (CPP) and Critical Material Attributes (CMA) which are essential in the subsequent implementation of Quality-by-Design. This approach is aimed at demonstrating that the plant can be operated within the robust quality bounds which provide a built-in quality assurance for the final product. The average crystal size, crystal size distribution, coefficient of variation and purity were considered as the Critical Quality Attributes (CQA) and all simulations were performed using gPROMS formulated products 2.0.1 which provides a robust platform for process simulation and optimization.

Keywords: Integrated continuous pharmaceutical plant, Continuous multistage crystallization, Global Sensitivity analysis, Uncertainty Analysis, Digital Twin.

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Multi-objective optimization of natural gas liquefaction process simulation via kriging surrogate model

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Abstract

Multi-objective optimization is a key to success in engineering design when the decision-making task involves multiple, competing objectives. However, optimization techniques require models that, for complex chemical process, are often not available in algebraic form but accessible via numerical methods in black-box process simulators. The main challenge of optimizing simulated models is dealing with the simulator-dependent black-box functions that are usually noisy and simply unavailable in symbolic form to be included into a multi-objective mathematical programming model. The propane-precooled mixed refrigerant (C3MR) natural gas liquefaction process is an example of a complex system mainly for its multi-stream heat exchanger model. The goal in optimal C3MR process design is achieving high energy efficiency, while maintaining the process pieces of equipment as small as possible. The present work tackles the design of C3MR natural gas liquefaction processes using a novel multi-objective optimization framework that is based on embedding the process simulator into a nonlinear programming (NLP) problem via kriging surrogate model. The C3MR process is simulated rigorously in Aspen HYSYS. Kriging models are trained to some simulation data and their algebraic formulation substitutes the black-box objectives and constraints functions. To deal with the conflicting objectives, the ε-constraint methodology is applied. The values of ε are evenly distributed between limiting values determined by single-objective optimization of each objective function. The surrogate NLP subproblems (fixed ε) are solved in GAMS using CONOPT to determine an iterate that is expected to be a non-dominated solution of the original subproblem. The Pareto Front achieved with the present framework is compared to the results of the well-established meta-heuristic algorithm of NSGA-II, considering the same simulation evaluation budget of 200 times the number of decision variables. Every solution in the best Pareto Front determined by NSGA-II is dominated by the results of the present approach endorsing the good performance of kriging-based multi-objective simulation optimization. Although applied to C3MR design, the present framework can be readily employed to different multi-objective simulation optimization problems with around ten decision variables. The success of the multi-objective optimization approach depends mainly on the performance of the kriging surrogate model to fit the black-box functions.

Keywords: Multi-objective optimization, Kriging surrogate model, Natural gas liquefaction, Simulation optimization, C3MR process.

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Integrated synthesis, modeling, and assessment of waste-to-resource alternatives

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Abstract

There is an urgent need to change the world's economic paradigm towards a more circular one as well as to convert waste into resources and reduce environmental impacts. A considerable number of technologies are now being developed to solve such challenges. Thus, decision-makers need to assess these alternatives and select the best ones for each kind of waste attending to all three main objectives: economic, environmental, and social. However, traditional optimization methods are very complex and not efficient enough when the number of alternatives is very large. To address this challenge, we are proposing a way to integrate several models and procedures to generate, assess, and optimize the most promising alternatives for the treatment and revalorization of a generic waste stream, providing a systematic and fully integrated tool to support decision-making towards the circular economy. The resulting framework encompasses interoperable modules, which exchange the necessary information to perform a comprehensive route generation and assessment, as well as the optimization of a waste-to-resource network considering the best options. The first stage corresponds to the knowledge management, where processes are characterized, using an ontological approach (Marquardt et al., 2010). Then, an algorithm uses the information from the ontology to implicitly generate the feasible routes. Once the routes are selected, they are sorted according to a proposed GPI (Pacheco-López et al., 2021). In the third stage, a more extensive process screening is performed, where a superstructure with the most promising alternatives is optimized to find a set of network configurations (Somoza-Tornos et al., 2021). Finally, a rigorous simulation can be performed to obtain the optimal configuration of the processes in the selected route. The obtained parameters are then used to update the ontology with enriched process information. The methodology is tested in a case study for the treatment plastic waste to obtain valuable products and reduce the environmental footprint.

Keywords: circular economy, pyrolysis, plastic waste, integrated modeling, sustainable development.

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MINLP model for work and heat exchange networks synthesis considering unclassified streams

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Abstract

The optimal synthesis of work and heat exchange networks (WHENs) is deeply important to achieve simultaneously high energy efficiency and low costs in chemical processes via work and heat integration of process streams. This can be accomplished with superstructure-derived mixed integer nonlinear programming (MINLP) models. The main challenge of WHENs synthesis is the lack of predefined pressure and temperature change routes of process streams, i.e. stream classification. In other words, differently from heat integration and because of temperature variation in compression and expansion, a stream may change its thermal identity throughout the process from hot to cold or vice-versa, making it difficult to target energy demands. The resulting MINLP models are intrinsically difficult to solve due to nonconvexity and combinatorial complexity that scales up quickly with the size of the problem (number of streams and superstructure stages). The main goal of the present approach is to develop an efficient MINLP model for optimal WHENs synthesis derived from a superstructure that considers unclassified streams. The developed model is then solved using a global optimization solver. The superstructure considers multi-staged heat integration section with isothermal mixing, temperature adjustment section with hot or cold utility, and work exchange section for streams that are not classified a priori. The leading advantage of the present optimization model is the capability of defining the temperature and pressure route, i.e. heat up, cool down, expand or compress, of a process stream entirely during optimization while still being eligible for global optimization. The present approach is tested to small-scale WHEN problems. The results surpassed the ones from the literature with global optimality guarantee.

Keywords: Work and heat exchange networks, Mixed-integer nonlinear programming, Unclassified streams, Process synthesis, Global optimization

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Planetary Boundaries Assessment of Flue Gas Valorization Into Ammonia and Methane

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Abstract

Chemical and energy sectors are currently striving to transition to low-carbon technologies to mitigate climate change. Carbon capture and utilization (CCU) has attracted growing interest to potentially curb CO_2 emissions while generating valuable chemicals. These emerging technologies will coexist with their fossil analogs in the near future, creating opportunities to combine both. Notably, valorizing flue gas from power plants has a double advantage: first, it could reduce CO_2 emissions from carbon-intensive processes while generating useful products; second, it could serve as a testing ground for new, disruptive technologies that could later be deployed also in the absence of fossil fuels. The success of CCU technologies will ultimately depend on its environmental sustainability, which should be evaluated based on global indicators such as the Planetary Boundaries (PBs). This approach defines a set of critical biophysical limits on key Earth-system processes regulating the Earth's resilience. Here we assessed the absolute sustainability level of an integrated facility producing ammonia and synthetic natural gas (SNG) using hydrogen from water electrolysis and nitrogen and CO_2 from flue gas from a combined-cycle natural gas power plant. To this end, the process was simulated by combining Aspen HYSYS®, and Aspen Custom Modeler®. The flue gas was separated using a four-stage membrane process, while alkaline, proton exchange membrane and solid oxide electrolysis were considered as alternative scenarios. Ammonia was produced via the Haber-Bosch (HB) process, while SNG was generated using the Sabatier reaction. Onshore and offshore wind and the German power grid supply the electricity for both present and future scenarios. The cradle-to-gate LCA-PBs assessment showed that the alternative technologies could contribute to operating the Planet safely by significantly reducing the impact on the climate change and ocean acidification indicators, compared with fossil HB and conventional steam reforming processes. Moreover, the process is economically unappealing at its current state, although the economic gap may be reduced as the electrolyzer technology matures and wind electricity becomes significantly cheaper. Overall, the investigated process could smoothen the transition of the chemical and energy industries towards low-carbon technologies but it would require incentives by governments. More broadly, the successful application of the PBs to quantify the environmental performance of the integrated system opens up new avenues for the absolute sustainability assessment of emerging low-carbon technologies, within the chemical sector and beyond.

Keywords: flue gas valorization, planetary boundaries, life cycle assessment, techno-economic analysis.

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A techno-economic assessment of biochar production from date pits in the MENA region

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Abstract

The Middle East and North Africa region (MENA) is the largest producer of dates worldwide, with an annual production of more than 6 million tonnes. The date palm has been an iconic part of this region's culture since 3000 BC and played a key role in its development over the centuries. At the same time, the date pits account for around 10% of the fruit, representing a vital biomass resource due to its high carbon and low ash contents. Several studies investigated the valorization of date pits into biochar via pyrolysis and the product applications as solid fuel, adsorbents, or soil enhancers. However, very little literature works evaluated the economics of pyrolysis using date pits as feedstock. As such, this study presents a techno-economic assessment of biochar production from date pits. Proximate and elemental analyses of date pits samples are conducted in the laboratory, while a 500 tonne/day biorefinery is designed and evaluated using adapted pyrolysis prediction models. In addition, the process is evaluated at two modes: slow pyrolysis at 250°C and fast pyrolysis at 400°C. The obtained results are promising, where slow pyrolysis yielded 50 wt.% of biochar with 62% elemental carbon content. Besides, it achieved a return on investment of 19.8% and a 5-year payback period. Whereas fast pyrolysis yielded 24 wt.% of biochar with 77% elemental carbon content, while the return on investment is 17.7% with a 6-year payback period. Both modes of pyrolysis using date pits proved to be feasible in the MENA region for the production of high-quality biochar.

Keywords: Date pits, Pyrolysis, Biochar, Biocrude, MENA.

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Design of sustainable processes for CO_2 capture

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Abstract

Electricity production from the burning of fossil fuels, is one of the main sources of Carbon Dioxide (CO_2) emissions. Moreover, it is projected the growth of electricity demand. Therefore, it is a non-sustainable process in accordance with the principles of green chemistry and circular economy. With this scenario, it is necessary to develop sustainable alternatives for power generation, as well as alternatives to mitigate CO_2 emissions. Due to global environmental problems, it is imperative to seek industrial processes in accordance with the UNO sustainable development goals. An alternative is the implementation of carbon dioxide capture and storage plants (CCS). To convert the energy production process into sustainable process that matches the principles of green chemistry and circular economy. There are several studies on post-combustion capture technologies focusing mainly on chemical absorption using aqueous mono-ethanolamine (MEA) solution due to its great capacity to capture CO2. Despite its high efficiency, MEA is considered highly toxic so that its implementation entails a high environmental impact. Moreover, there are no studies that report a full design considering environmental impact and the process economies as a sustainable indicator.

In this work is presented the design of a CO_2 capture plant coupled to a power plant considering a stochastic optimization having as objective function the minimization of the environmental implications of capture plants using MEA as solvent (Ecoindication 99), as well maximize the return on investment (ROI) as sustainable indicators. The analysis considered the most used fuels in the power plant: biogas, coal, non- associated gas, and associated gas. All the cases were standardized to recover at least 95% of the CO_2 produced. The results indicate that for a fuel feed flow of 1000 kmol/h it was necessary to vary the air ratio to achieve the CO_2 recovery objective. The design with the best overall performance is when natural gas is burned. For the environmental analysis, the natural gas presents the lower impact with 22618.4 kEcopoints and a return on investment of 295.62%. This as a result of a sustainable process with less environmental impact.

Keywords: CO_2 Capture plant, biogas, coal, non- associated gas, associated gas.

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Water network optimization in chemical complexes: a refinery case study

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Abstract

Large industrial sites such as refineries are known as intensive users of water, which has become a vital resource in our society. Even biorefineries based on wet processes tend to use large quantities of water, that needs to be efficiently managed and recycled, to ensure their sustainability.

Constrained mathematical programming is used to identify the "best" designs, mostly formulated as nonlinear global optimization problems. However, these problems can be large and difficult to solve, as the refineries' sites can have extensive and complicated networks, with a multitude of individual plants and processes, multiple contaminants, different water sources, multiple discharges with different typologies and constraints. Different operating regimes might also correspond to different stream availabilities and / or distinct optimal topologies, which complicates further the problem.

In order to overcome these difficulties, a two-level MINLP model is used for water network optimization of large sites, composed of several independent plants. At the lowest level, the water consumption within a given plant is first minimized, considering feasible connections between the units of this plant, using a predefined set of interplant connections and capacities. During the second step, the water needs and wastewater emissions of each plant are coordinated, to minimize the network costs for the entire complex. The units considered in this case have multiple water inlets and outlets, to account for the fact that they can represent a subset of atomic operations.

Several complementary aspects were implemented in this model: wastewater can have different final discharge destinations, including the possibility of discharges priced according to the effluent contaminants' concentrations, grouped into discrete cost classes. Several initialisation techniques were also experimented and compared, since this was also found to be a critical step for the efficient solution of the optimization problems.

This strategy was applied to the water network of the Petrogal Sines' refinery, with process data obtained through the application of a data reconciliation procedure with outlier mitigation (weighted least squares function followed by robust strategies, using the fair and Cauchy functions). To complete this information, comprehensive water sampling and analysis was also conducted, regarding five major water pollutants. The network optimisation's results achieved a 15.8% in the network's hourly operating costs, a 7% reduction in freshwater consumption, and optimality gap smaller than 5% (for the model's second step), using a mixture of global solvers available in GAMS. This application example demonstrates the successful application of the proposed methodology.

Keywords: Water networks, Process synthesis, Process design, Total site integration

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Optimal Integration of Solar-Aided Hydrogen Production with CO_2 Utilization into Polyurethane

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Abstract

Hydrogen is an important energy carrier in transportation sector and essential industrial feedstock for petroleum refineries. Traditional hydrogen production results in considerable greenhouse gas emissions (Voldsund et al. 2016). Therefore, it is highly desirable to investigate clean and affordable hydrogen production process using renewable energy (Turner *et al*., 2008).

Solar energy for hydrogen production has received significant attention in recent years due to its primary abundance as an energy source. The techno-economic analysis indicates that solar steam methane reforming using molten salt (SSMR-MS) has more potential for large-scale hydrogen production compared to others, due to its unlimited operation hours and lower total annualized cost (Likkasit, 2015). However, CO_2 in flue gas of SSMR-MS is released to atmosphere without capture and further utilization. No optimal integration of SSMR-MS with CO_2 capture and utilization technologies have been presented.

In this work, four process alternatives integrated with amine-based CO_2 capture and further conversion into polyurethane based on the existing SSMR-MS process are investigated. The machine learning-based optimisation framework from Wang et al. (2021) is used to achieve optimal integration where artificial neural network (ANN) is applied to build surrogate models to predict total annualized cost (TAC), hydrogen and polyurethane production rates, and molten salt heat duty. A hybrid global optimisation algorithm GA-SQP is employed to solve the surrogate model. The optimisation results demonstrate that in the best case where pre-reformer is adiabatic, a significant reduction in TAC by 14.9 % ~ 15.1 % can be achieved compared to the existing SSMR-MS (Likkasit, 2015). Solar-related equipment cost is reduced around 28.6% along with molten salt heat duty decreasing from 20.0 MW to 10.2 ~ 10.3MW. With the conversion of CO_2 into polyurethane, direct CO_2 emissions declines about 90.1%.

Keywords: Hydrogen production; Solar energy; CO_2 utilization; Machine learning

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Hierarchical Approach for Solvent Selection in a Circular Economy

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Abstract

Chemical recycling allows upcycling of different grades of polymers from varied value chains into their constituent monomers and/or other valuable chemicals and thereby, contributes to a resource-efficient future. This demands selective depolymerisation of a particular fraction from a mixed waste stream and thus, necessitates the use of selective solvents. The choice of an appropriate solvent not only governs the effective depolymerisation but also influences the sustainability of the process. In several strategies, the tendency of the solvent to dissolve the polymer is considered as the only selection criterion. However, to develop a holistic process, careful consideration should also be given to its sustainability and its interaction with other process reagents.

This research refers to the development of a systematic approach to select some promising solvents suited for a proposed recycling strategy. This hierarchical approach begins with shortlisting potential solvents based on their Hansen solubility parameters relative to the polymer under consideration. Subsequently, these solvents are screened for their sustainability based on the principles of green chemistry. Further, operating constraints resulting from their interactions with other process reagents are considered through a computer-aided molecular design tool and comprehensive literature review (Harper, (2000)). The application of this methodology for developing a recycling strategy for PLA is also illustrated (Majgaonkar, (2021)).

With increasing demand, new polymers tailored for a particular application are entering the market. Amongst a variety of solvents, computing the best-suited choice for recycling a newly developed polymer is quite challenging. By developing a solvent selection guideline, which incorporates a trade-off between multiple factors, this effort attempts to address these complexities and thus, promotes the use of process synthesis in this sector.

Keywords: circular economy, solvent selection, chemical recycling, green solvents, process synthesis.

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A Framework to Facilitate Decision Making for Infrastructure Options Analysis of Distribution and Utilities Systems of Chemical Production Plants

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Abstract

The consequences of investment decisions regarding a chemical plant's distribution and utilities system can be crucial for the operability and thus the success of a chemical plant. This work presents a novel framework for investment decision making regarding distribution and utilities systems of a chemical plant, based on multi-stage infrastructure planning and production scheduling, incorporating all relevant process and material timescales. The literature has classically investigated distribution systems only for a single distribution process material or energy system (J. G. C. Pena et al. 2019) and utilities systems only in terms of heat or work exchange networks and their respective integration (L. V. Pavão et al. 2020). However, the evaluation of several relevant material streams holistically within the distribution system of one chemical plant together with several interconnected utilities, and the incorporation of different timescales has not yet been presented in a decision-making framework. To do so, a mixed-integer linear programming (MILP) to investigate decision making regarding future investment decisions based on multi-stage infrastructure and maintenance planning for chemical plants is formulated. To underline the applicability and capabilities of the developed framework, it is applied to the distribution and utilities system of a chemical plant in South-East Texas.

Keywords: infrastructure planning, production scheduling, multi-scale engineering.

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Optimization and prediction of crude oil blending properties and compatibility assessment using different techniques

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Abstract

Crude oil blending is one of the beneficial ways to improve the final product properties of crude oil. However, blending procedure play a key role in obtaining a promising oil product. If the blending procedure conducted randomly or in nonsystematic manner, impurities such as asphaltenes and wax can precipitate. However, asphaltenes are difficult to re-dissolve quickly after blending in the refinery and pipelines. It also makes it undesirable product in the market. Therefore, this study focused on the possibility of transport three different crude oil blend scenarios and investigate the compatibility and incompatibility of these scenarios. The selected Crude oils for blending denoted by (A, B, C) via a 40" pipeline from oil fields to the export terminal 212 km away. The operating pressure of the blending line which denoted by Z, should not exceed 120 psig due to the limited operating pressure of the pipeline. The objectives aimed at improving some physical properties, increase the revenues and reduce operating costs. The pipeline status under different operating scenarios was studied using OLGA software. Different techniques such as Turbiscan Instrument and Optical Microscopy were used in the prediction of a compatibility scales to avoid phase out and precipitation of asphaltenes. It has been found that the three scenarios under certain operating conditions are compatible However, The initial hydraulic study has been conducted and the results confirmed that the pipeline is capable to transfer the proposed blend for the scenario 1 and 2 within the maximum allowable operating pressure of 114 psi and 105.8 psi, respectively at 83.5 and km189 respectively, but the third scenario cannot be applied due to the risk of wax deposition, as result of wax appearance temperature is above of the lowest temperature located along the pipeline, to overcome this problem the wax inhibiter should be added or increase flow rate at least 134,000 b/d. Further investigation will be conducted to validate the obtained simulated model.

Keywords: Crude oil blending, Compatibility, OLGA, Physical property

Introduction.

The concern of mixed crude oil properties has gained much attention nowadays. Preparation of a blend with different unique characteristics compared to the original oil is one of the major challenges in the oil market because it increases the economic value of the oil demand. It's important to characterize the new physicochemical properties of the produced blend and evaluate the impact of such properties on the refinery and pipelines Tozzi, F. C., et al (2015).

The Ratio between two or more crude oils consider as a key variable in obtaining a favourable and high value blended oil. However, Compatibility and incompatibility characteristics between blended crude oils consider as one of the obstacles in attaining a

unique blended oil. Indeed, Insolubility Number (I_N) and Solubility Blending Number (S_{BN}) are key dependent parameters in the prediction of compatibility and incompatibility phenomena of blend Benmahmoud & Aboujadeed (2017).
The (S_{BN}) and (I_N) were measured crude oils and their blends as shown in Table 3.

Results

Table 1: Physical properties of crude oils and their blends

Description	Crude A	Crude B	Crude C	Blend A+B+C Scenario 1	Blend A+B Scenario 2	Blend B+C Scenario 3
Total production, b/d	110,000	66,000	30,000	206,000	176,000	96,000
API gravity	37.1	41.9	39.5	39.1	39.0	41.3
Wax A.Temp., °F	86	49	24	93.2	93.2	109.4
Total sulphur, wt.%	0.064	0.010	0.339	0.087	0.045	0.115
Pour point, °F	+69.8	+102.2	+53.6	+80.6	+80.	+91.4

Table 2: OLGA Simulation results.

Scenario	Tin, °F	Tmin, °F	MPHS, °F	Tout, °F	Pin, psig	Pmax, psig	Pout, psig
Scenario 1	183	102.8	140	104	39.5	114	97.3
Scenario 2	185	95	140	100	25.7	105.8	97.3
Scenario 3	182.3	95.5	185	95.5	22.3	119	114.2

MPHS: Mid Power Heat Station

Table 3: Solubility blending numbers and insolubility numbers for crude oils and their blends

Description	Crude A	Crude B	Crude C	Scenario 1	Scenario 2	Scenario 3
Stability Index	3.16	1.19	8.41	3.18	2.39	3.40
S_{BN}	38.40	46.32	31.89	39.98	41.17	41.81
I_N	22.16	27.06	29.41	24.78	23.87	27.79
S_{BN}/I_N	1.73	1.71	1.08	1.61	1.72	1.50

Conclusion

Scenario 1 showed that the pipeline is capable to transfer 206,000 b/d of the blend within the maximum allowable operating pressure of 114.0 psig at km 83.5 and the highest temperature at an arrival point of 104°F = 40 °C. On the other hand, results of Scenario 2 revealed that the pipeline is capable to transfer about 176,000 b/d of the blend within the maximum allowable operating pressure of 105.8 psi at km189. In scenario 3, the pipeline could transport 96,000 bbls/d of the blend if the wax inhibiter was added, due to the high percentage of wax content or increase flow rate at least 134,000 b/d. The results were referring that crudes A, C and the three blends were stable and compatible, while crude B wasn't stable and incompatible. It has been found that, the stability of the parent crudes is the key parameter in influencing the status of the blend as compatible or in compatible blend.

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Generalized disjunctive programming model for the optimal design and planning of reliable power generation systems

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Abstract
As evidenced by the Texas power crisis in 2021, power generation systems should be designed to have high reliability to supply uninterrupted electric power to industries. Reliability indicates the probability that a system will perform its required function properly even if one or multiple units fail. One method to improve the reliability of the systems is to add redundant units (i.e., backup units) to prevent the system from completely failing. This approach is known as 'reliability-based design optimization,' and various studies on this topic have been conducted [Chen *et al.,* 2021; Ortiz-Espinoza *et al.,* 2021; Ye *et al.,* 2018]. The authors mainly focus on optimizing the number of redundant units; however, since the power systems operate in unsteady state due to time-varying power demand, the reliability is also influenced by the operational strategies that the systems use. This paper aims to develop a new Generalized Disjunctive Programming (GDP) model for the design and planning of reliable power generation systems. This work optimizes the number of redundant units to maximize the reliability and to minimize the cost by considering operation strategies that can affect the system reliability. We develop a GDP model, which involves Boolean and continuous variables, algebraic equations, and logic propositions, to represent the reliability and expected power production rigorously. The resulting GDP model can be reformulated as a mixed-integer linear programming (MILP) using either Big-M and hull-relaxation methods [Grossmann *et al.,* 2013]. The proposed model is tested with an expansion planning problem of a power generation systems [Lara *et al.,* 2018]. The results show that the proposed optimization model yields the optimal design and operation strategies that establish the trade-off between economics and reliability.

Keywords: Reliability, Power generation systems, Expansion planning

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Application of an ontology-based decision support system for the design of emulsion-based cosmetic products

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Abstract

The decision-making process for the design of formulated products faces different challenges because of its intrinsic complexity. On the one hand, it is not sequential, but iterative due to the fragmented and diverse nature of available information (Zhang *et al.*, 2020). On the other hand, there is not a unique design workflow; it changes from company to company according to its context and specific requirements (Zhang and Wang, 2016). The lack of structure of knowledge for product formulation requires developing a robust knowledge representation to show coherently and explicitly concepts, models, and data. Furthermore, this representation must allow design teams to use it flexibly and to adapt it to specific design contexts. In view of the above, this work proposes an ontology for formulated products with emphasis on cosmetic emulsions. This ontology integrates concepts from emulsion science, cosmetic formulation, expert knowledge, and design heuristics in a systematic and accessible way. It was done based on the recent work of our research group in chemical product design (Arrieta-Escobar *et al.*, 2020; Serna *et al.*, 2021) and its uses, applications and limitations are demonstrated with a case study: the formulation of a skin care cream. As conclusion, it was found that the ontology enables the access to precise information according to design requirements. It is a versatile and useful tool for the design of emulsion-based products.

Keywords: Product design, Cosmetic emulsions, Ontology

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Synthesis of extractive distillation structures for the purification of ethanol

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Abstract

Mixtures forming azeotropes cannot be separated by conventional distillation columns because, at the azeotropic point in equilibrium, the composition of the mixture in vapor and liquid phases are the same. Such is the case of the separation of ethanol/water mixtures. Thus, this work presents a synthesis problem for the separation and purification of Ethanol using extractive distillation. Ethylene glycol was the chosen solvent to separate the azeotropic mixture.

The synthesis problem was based on the Infinite-DimEnsionAl State-space (IDEAS) approach, which can take advantage of the following two features: 1) it considers all process networks without any a priori given set of unit operations, and 2) the optimization formulations result in linear optimization (Drake and Manousiouthakis, 2002). A superstructure representation was used in which distillation modules (i.e., discretized liquid composition subspace) connect to generate an optimal distillation structure. Then, the synthesis problem was formulated as a linear programming (LP) problem in which the utility cost was minimized subject to material and energy balances. Furthermore, the optimal structure was derived without the need to set any preestablish distillation structure. After the optimization problem is solved, the best connection between distillation modules is known. Therefore, a realistic and feasible distillation structure is interpreted at a post-optimization step.

The typical extractive distillation structure is comprised of two columns. The first column concentrates Ethanol above its azeotropic point at the top, while the second column separates water at the top and recycles the solvent at the bottom (Gil, García and Rodríguez, 2014). This work proposes a thermally coupled distillation column with a side stripper in which Ethanol is obtained at the top and ethylene glycol at the bottom of the first column. In the side rectifier, water is obtained at the bottom. The utility cost of the interpreted solution was 67.8 $/h, which was 6.3% less expensive than that of the typical process.

Keywords: Process Synthesis, Extractive Distillation, LP, Process Simulation, Ethanol

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Optimal design for flexible operation with multiple fluctuating input parameters

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Abstract

Chemical process plants are constantly subject to disturbances and need to respond appropriately in order to meet safety, environmental or operational constraints. Early research found that an integrated approach to design and control processes is superior to a sequential one when dealing with these disturbances during operation. However, these integrated design and control strategies were usually developed to maintain an optimal operation around a nominal steady-state operating point. Due to recent developments in chemical engineering, flexible operation of plants has received considerable interest. Flexible operation implies significant changes in the operational conditions and requires a rethinking away from one steady-state operating condition towards a constantly changing process condition. Processes that require flexible operation must be specifically designed and controlled.

In this contribution, we provide a new integrated design and control approach that allows to design processes and their equipment for flexible operation while multiple input parameter intentionally undergo considerable changes. The approach is based on dynamic optimization as an overarching framework. We test the approach on the production of green methanol. The aim is to design a flexible methanol reactor that both operates over a wide range of operating conditions, while providing feasible operation during dynamic transitions. We assume that the required CO_2 is generated by absorption in a fossil power plant that is operated for frequency regulations. The required H_2 on the other hand is produced by a water electrolysis that operates with renewable energies. In this scenario, both parameters fluctuate considerably during operation.

The design approach is based on a worst case test to optimize the multidimensional operating window of the methanol reactor. The operating window that can either be the objective function or a constraint is approximated by a rectangle in the space of the intended changing parameters. In this way, we achieve a reactor that pushes feasibility boundaries, resulting in a design that is most flexible towards both reactant input streams. Furthermore, by considering path constraints during the dynamic transitions, both design and advanced control strategies can be utilized to ensure feasibility. The resulting reactor design allows operation to be maintained when a design for an optimal operating point would fail.

While the focus in this contribution is on a fixed-bed reactor, the approach is of general applicability to chemical processes. It should be noted that a reactor designed specifically for flexible operation will be more conservative than a common reactor designed for an optimal operating condition. The trade-off between flexibility and economics should always be considered and can be incorporated into the design problem.

Keywords: Design optimization; flexibility; power-to-x; dynamic operability; methanol production

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Design and Optimization of Membrane System for Gas Separation

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Abstract

Membrane separation is one of the emerging technologies that can replace conventional energy intensive technologies, and it could have cost benefits and lower environmental footprints. In the process industry, solvent absorption (amine absorption), solid adsorption (pressure swing adsorption) and cryogenic distillations are used to separate gas mixtures (Tock, 2013; Leung et al., 2014). Membrane separation has several advantages over conventional gas separation technologies, e.g., no use of chemicals, mild operating conditions, simple installation and easier operation, and flexibility to integrate with other separation technologies. Recently, gas separation using membranes has received considerable attention for industrial applications, namely post-combustion CO_2 capture and biogas upgradation by CO_2 removal. Several studies have explored post-combustion CO_2 capture from coal and natural gas power plants, using membranes (Kárászov et al., 2020). Sun et al. (2015) reviewed several biogas upgrading technologies, including cryogenic separation, physical and chemical absorptions, pressure swing adsorption, membrane separation, hydrate formation and biological methods.

Post-combustion CO_2 capture and biogas upgradation have challenges in terms of energy consumption, (capital and operating) cost and environmental impacts. The selection of CO_2 removal technology depends on plant location, production capacity and quality specifications. Several membrane processes have been developed to achieve higher purity and recovery. This study uses a generic membrane superstructure (or system) that facilitate all possible inter- and intra-connections among different membrane stages (or units) which are arranged in series-parallel configurations. For separating a mixture of gases, membrane system can choose membranes from a Membrane Database, which has a number of polymeric and inorganic membranes (graphene, carbon molecular sieve, zeolite and MOF membranes). In this work, two industrial case studies of gas separation are considered: post-combustion CO_2 capture and biogas upgradation by removing CO_2. The developed mathematical model for membrane system is a Mixed Integer Non-Linear Programming (MINLP) problem. The mathematical model is implemented in AMPL (A Mathematical Programming Language), and the BARON solver is used to solve it. Multi-objective optimization problem was formulated (*via* ε-constraint method) to quantify tradeoff between energy consumption and cost of the membrane system. The final solution of the membrane system may contain the same or different membranes in the different stages. The separation performance of the membrane system is also evaluated and compared for all membranes (available in Membrane Database), where the same membrane is used in all stages. This study identifies best performing membrane clusters, based on the membrane permeability and selectivity, for post-combustion CO_2 capture and biogas upgradation.

Keywords: CO_2 Capture; Membrane Superstructure, Post-combustion CO_2 Capture, Biogas Upgradation.

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Assessment of Carbon Capture Technologies for Waste-to-Energy

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Abstract

Municipal solid waste (MSW) is a mixture of urban and industrial waste, consisting of biodegradable fractions, such as food waste, waste wood or paper, but also fossil-based fractions, among which plastics, textiles, metals, glass and aluminum. Its sustainable disposal can produce biogas, biofuels, heat, electricity, and recovered metals, depending on the type of waste and its energy content. Process integration and optimization techniques are thus useful in identifying sustainable and cost-effective strategies for waste management (Rizwan et al., 2020). This study focuses on three major waste categories: MSW, biomass and plastic. Anaerobic digestion is used to convert biomass into biogas; the organic material is broken down by bacteria into a methane rich gas in the absence of oxygen. Syngas, on the other hand, is produced by gasification of plastic in the presence of air or steam. Finally, incineration is a thermal treatment for recovering energy of MSW. As both biogenic and fossil carbon are present among waste fractions, the reduction and capture of carbon is crucial in the deployment of sound waste management technologies. Recently, Castro-Amoedo et al. (2021) have studied biowaste valorization along with CO_2 removal from biogas.

There are several physico-chemical CO_2 capture technologies, such as physical adsorption (pressure and temperature swing adsorptions), chemical absorption (amine absorption, ammonia scrubbing, selexol process), membrane separation, and cryogenic technology (Tock, 2013; Sharma and Maréchal, 2019). Each technology has its own benefits, challenges, and limitations. Each technology has some key requirements, namely material, heat and electricity. Further, CO_2 source (biogas, syngas, flue gases) also has some specific characteristics, such as composition, temperature, pressure and impurities. Hence, there is a strong need to evaluate and compare the integration of different CO_2 capture technologies with waste-to-energy. In this study, we have developed a superstructure for waste-to-energy, by incorporating digestion, gasification and incineration as the main waste treatment technologies. The waste-to-energy superstructure includes several options for CO_2 capture, namely amine absorption, pressure swing adsorption, temperature swing adsorption and membranes. The captured CO_2 can be sequestrated, mineralized and/or converted to renewable fuels. This study systematically generates and compares a number of decarbonization options for waste-to-energy. The formulated optimization problem is a mixed integer linear programming (MILP) problem. The energy efficiency, (operating and capital) cost and environmental impacts are considered as performance criteria, for comparing different decarbonizing options.

Keywords: Waste-to-Energy; Anaerobic digestion; Gasification; Incineration; CO_2 Capture and Sequestration.

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Process Integration and Techno-Economic Assessment of a Green Biorefinery Demonstration Scale Platform for Leaf Protein Production

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Abstract

Green biorefinery corresponds to sustainable processing of green biomass, such as grass, clover, and lucerne, as well as agricultural residues. Those plants are rich in multiple products, which include proteins, sugars, and lipids, among other high value-added products in smaller concentrations. This multiple-products system allows developing greener alternatives to conventional products, employing different routes and technologies that are chosen according to the target products. The extraction of proteins from leaves represents an attractive solution to the high European dependency on soybean imports, used as feed for monogastric animals. Knowing that Denmark is the fourth largest pig producer in the EU after Spain, Germany, and France, with 8.5 % of the total pigs, a demonstration facility operates in Foulum, Denmark, intending to precipitate a protein-rich concentrate from green biomass. Besides the manufacture of leaf protein concentrate, the facility also produces a fibrous pulp fraction that can be used for ruminant feed, and a nutrient-rich residual juice, that can be used for biogas production.

The green biorefinery was simulated using Aspen Plus V12 for the processing of grass-clover. The process included the maceration of the harvested biomass; mechanical fractionation into a fiber-rich press cake and a green juice; heat treatment of the green juice for precipitation of soluble leaf proteins; centrifugation and drying of the precipitated protein; and anaerobic digestion of the residual brown juice for biogas production. The simulation was validated based on experimental data obtained in the demonstration plant, resulting in a precipitation of approximately 35 % of the crude protein in the protein concentrate. The feasibility of the implementation of the biorefinery on a commercial scale was calculated using Aspen Process Economic Analyzer.

Keywords: green biorefinery; leaf protein concentrate; process modeling; techno-economic assessment.

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The effect of alternative fuels on calcium-looping

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Abstract

Calcium looping (CaL) is a promising post-combustion CO_2 capturing technology, showing high compatibility with the cement industry, one of the major industrial sources of CO_2 emissions (IEA, 2018). CaL comprehends two circulating fluidized bed reactors, a calciner and a carbonator. The flue gas from the rotary kiln is fed to the carbonator, in which the CO_2 is captured by reacting with CaO to form $CaCO_3$. The carbonation reaction is exothermic and the heat released is used to produce electrical energy through a steam cycle. The $CaCO_3$ formed in the carbonator enters the calciner, to be regenerated to CaO. As the calcination is endothermic, energy must be supplied to the calciner through oxyfuel combustion. The oxygen is usually obtained through an air separation unit (ASU) and the most common fuel used in CaL pilot-plants is still coal (Arias et al., 2018; Hornberger et al., 2017). However, there is an effort to replace it with greener fuels. In fact, in "La Robla" CaL pilot plant, biomass combustion was carried out in a joint combustor/carbonator (Alonso et al., 2014). Nevertheless, the possibility of using other cement kiln alternative fuels in the CaL calciner was not yet evaluated. The goal of this work was to evaluate the influence of using these green fuels in key performance indicators, such as the amount of fuel needed, the electric energy produced, the ASU energy consumptions, and the CO_2 captured in the process. Therefore, a CaL process, including a steam cycle and an ASU, was modeled using Aspen Plus. This model also incorporates a carbonator model developed using Python, which followed the work of (Romano, 2012). The energy requirements of the calciner were fulfilled by supplying petcoke and five alternative fuels: tire chip, waste derived fuels, olive pomace, dangerous liquid residues and cork residues. Different random compositions of each fuel were studied following a Monte-Carlo based approach. The data obtained was analyzed in terms of the key performance indicators and compared with full petcoke utilization.
Keywords: Calcium-looping, cement, CO_2 capture, alternative fuels, process modelling

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Simultaneous Synthesis of Metabolic and Process Engineering for the Production of Muconic Acid

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Abstract

Recent advances in metabolic pathway reconstruction and in silico modelling have enabled the development of microbial strains suitable for efficient cell-factories. Emerging infrastructures of Design-Build-Test-Learn paradigms hold a tremendous promise to innovate with new products, also novel integrated processes that can be intensified for the highest efficiency1. Still, the current Design-Build-Test-Learn (DBTL) cycle approach in biofoundries and biorefineries remains a disconnected sequence of tasks with an undisclosed potential to integrate. Specifically, the genetic modifications of strains are usually driven by the overproduction of target metabolites without considering downstream processing which can account for up to 80% of the overall bio-production cost2. Therefore, there is a need for an inclusive methodical approach that incorporates separation processes in metabolic engineering upstream design.

The paper presents a systems integration approach for the computational strain design workflow for the identification of reaction eliminations that reshape network connectivity in way that both biomass production and revenue are simultaneously maximized by utilizing a bilevel optimization framework. The research expands the outer problem of the bilevel approach that is established in the literature with the use of a superstructure scheme that addresses several design options simultaneously with the several options to select the pathways. The superstructure scheme is laid out to reduce model and optimization complexities. The existence of each process is denoted by binary variables. Our method entails the identification and the categorization of these technologies as well as the insertion of the model equations and their economic parameters into the optimization problem. Separation steps include pretreatment, cell removal, product isolation, concentration, purification and refinement. The superstructure's input stream is a variable determined by the optimization problem and is separated into five components: product, liquid by-product, water, cells, and solid by-product. Each process redistributes the stream's components through linearized model equations. The problem can be constrained based on the specific bio-process characteristics and objectives. The model has been developed in GAMS environment and solved using the BARON global optimization solver.

We assess the effect of the new optimization goal, for varying number of metabolic interventions to the downstream separation network and the bioprocess revenue. We then compare the enriched model to the previous analysis, which only aims to maximize the production of a target metabolite. To showcase the functionality and effectiveness of the developed model we applied the workflow to a muconic acid producing strain of *S.cerevisiae* (iMM904 GEM) that includes the necessary heterologous pathways. Additionally, by utilizing different metabolic engineering tools, it is possible to acquire a variety of promising metabolic interventions that could lead to profitable biorefineries. Overall, this computational framework could be an important step to bridge the gap between strain design and process engineering.

Keywords: Systems Metabolic Engineering, Process Design, Superstructure Optimization

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Renewable hydrogen supply chain for transport application in Corsica island

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Abstract

Most islands and other isolated territories are poorly connected to well-established power grids due to their high cost or technical feasibility (Lamas, 2016). Consequently, they have to meet their electricity needs by using locally available resources or by importing fossil resources. Hydrogen produced via renewable energy sources can be viewed as an "energy vector" that can technically power small islands (Krajačić et al., 2008) by increasing the penetration levels of intermittent renewable sources and purposing a low-carbon fuel for transport sector.

This work presents a methodological framework to determine optimal configurations of hydrogen supply chains for insular territories, based on similar methodologies proposed for other applications (Carrera and Azzaro-Pantel, 2021).
The potential of hydrogen production for Corsican transportation sector with the use of solar and wind electricity and powering electrolyzers (alkaline and proton exchange membrane (PEM)) has been analyzed. The seasonal variation of solar and wind availability was considered in 2030 time period discretization. The approach is based a Mixed-Integer Linear Programming (MILP) formulation, with a multi-period approach, using the CPLEX 12 solver in the GAMS environment. The objective function to be minimized is the total daily cost (TDC). A set of decision variables are involved, such as the number, location and size of production, storage, and distribution units.

The optimal configuration of the hydrogen for Corsica is constituted by a decentralized network where hydrogen can be transported by tube trailers from other neighbouring grids to meet local demands. The exporting area is always equipped with a compressor, and the electrolyzer is only installed in an area where the energy sources are sufficient or pre-assigned by local authorities. The monthly average cost of hydrogen was obtained, with a minimum value of 8 €/kg in August. The model can be improved by diversifying hydrogen demand for other end uses.

Keywords: Hydrogen, optimization, low-carbon fuel, Mixed-Integer Linear Programming

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Assessing the volume flexibility of a bio-electrochemical process

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Abstract

An increasing share of intermittent renewable electricity in the power grid is being deployed. The subsequent intermittency might result in imbalanced grids, increased costs, and lower reliability. As a large power consumer, the chemical industry, especially the electro-chemical sector, seeks solutions to enable production under intermittent electricity supply. A few studies have explicitly studied to what extent electrochemical processes can be operated under varying volume loads caused by fluctuating electricity supply but focused on the conversion units (e.g., Huesman (2020)). Limited works studied the purification of caproic acid from a highly diluted stream (e.g., Woo and Kim (2019)) but did not consider the impact of fluctuating volume loads on the process.

This work aims to evaluate the volume flexibility of a bio-electrochemical process that produces 99 wt.% of caproic acid and identify critical bottlenecks, focusing on the purification units. Volume flexibility is defined here as the ability of a process to handle changes in the volume load while keeping an overall acceptable performance. In this process, the conversion unit is a set of microbial electro-synthesis (MES) stacks with microorganisms as the cathode catalyst. The process is still at an early stage of development but for this work, it was scaled up to a nominal capacity of 10000 t/a. The process was modeled at continuous and steady-state conditions in Aspen Plus v12. In the process, the MES stacks are fed with water, CO_2, and electricity and produce oxygen, acetate, butyrate, and caproate. The dilute outlet stream from the MES stacks is acidified (the titer of carboxylates is 10g/L) in preparation for purification. The purification units consist of liquid-liquid extraction (P1), vacuum solvent removal (P2), water removal (P3), and short-chain carboxylic acids removal (P4) to reach the caproic acid purity of 99 wt.%. The recovered solvent was recycled, and the process loop was closed to achieve higher efficiency. Since the technology readiness level of MES is around 3, it was modeled as a black box in Aspen Plus, based on experimental data from the work of Jourdin, Sousa, Stralen and Strik (2020). The MES stacks were assumed to be flexible against changes in the volume load. Unit P1 was modeled using an extraction column and assumed to be more flexible against fluctuating volume loads than units P2-P4. The volume flexibility was only evaluated for the separation units P2-P4. The process model was initially run assuming fixed equipment size and then was tested by changing the volume load. The volume flexibility test focused on the purification units P2-P4. They were modeled with a single column (without a built-in reboiler or condenser), two heat exchangers

(representing reboiler and condenser), and two splitting units. The internal column dimensions, the heat exchanger area (A), the overall heat transfer coefficient (U), and the minimum temperature approach (ΔT_{min}) were fixed based on the nominal capacity. This allowed fixing the equipment's size and implicitly determined the minimum log-mean temperature difference (LMTD) and minimum heat duty (Q) allowed for the heat exchanger. The volume load was then decreased gradually to assess its impact on the process. The operating parameters adjusted at each volume load were the split fractions representing the reflux and boilup ratios. The aim was to identify the minimum volume load (that is normalized to the nominal load) and corresponding reflux and boilup ratios to maintain caproic acid's purity and recovery rate (ca. 99.5%). Moreover, each tray's operating point was required to be within the hydraulic plots' stable operating region. These were two restricting criteria for selecting eligible volume load and split fractions.

The results indicated that the main bottleneck in terms of volume flexibility was the vacuum solvent removal unit (P2), which showed the smallest eligible load ratio range (82-100%) compared with the other purification units (75-100% for P3 and 48-100% for P4). The root cause was spotted in the reboiler and the selected heating stream of unit P2. At a load ratio of 81%, the reboiler is overdesigned with an overdesign fraction of 110%. It was noted that as the volume load dropped, the boilup ratio in the unit P2 exhibited minor changes when satisfying the two restricting criteria. It was also noticed that the reboiled stream sent back to the column was slightly overheated to maintain the column's temperature profile and thus to obtain the desired product purity and recovery rate. Therefore, though the temperature of the reboiled stream slightly increased, the minimum Q still dropped. The increased temperature of the reboiled stream caused the LMTD and the Q to hit the minimum values imposed by the initial design. It occurred first to this specific heat exchanger because the difference in temperatures of the cold stream (t_{out}) and hot stream (T_{in}) was smaller (ca. 15°C) than that of the other heat exchangers in the purification units (all larger than 20°C).

To increase the volume flexibility, in this case, the hot utility's temperature should be increased, or a heat exchanger that can handle a smaller temperature difference could be used. For further study, design strategies such as installing storage tanks or shifting to a more flexible purification technology to handle the critical bottleneck, i.e., unit P2, will be considered. The internal column dimensions in this work were designed to maintain stable tray hydraulic performance across different volume loads. This could also be studied. Finally, it is essential to highlight the ex-ante nature of this study and, therefore, the need to verify the results experimentally.

Keywords: Process design, Volume flexibility, Separation units

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Computer-aided Design of Biphasic System Comprising Ionic Liquid and Conventional Solvent to Extract α-Tocopherol from Deodorizer Distillate

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Abstract

Ionic liquids (IL) refer to molten salts comprising of organic cation and organic or inorganic anion, of which melting points generally span from negative up to 100 °C. Since their inception in 1914, ILs have been extensively studied in many chemical processes as the replacement of conventional solvents (CS). ILs generally share the merits of thermal stability, nonflammablility, low volatility and designablility etc., and thus harvest plenty of applications in various fields (Lei et al., 2017). Specifically, IL-based extraction is deemed as a promising separation strategy that applies IL or IL-CS combinations to isolate a target molecule from crude products. Although in many separation cases the single IL can receive acceptable extraction performance, the biphasic system constituted by IL and CS have been well-documented to be capable of greatly improving the extraction selectivity, for example, the extraction of α-tocopherol (Toc) from methylated oil deodorizer distillate (MODD) (Cheng et al., 2018; Qin et al., 2022). However, despite the great interests in IL-CS biphasic system (ICBS), most current studies still rely on the experimental trial-and-error method to test different IL-CS combinations while computer-aided methods guiding ICBS design are still scarce. More importantly, for separating compound A from B, the previously reported ICBS only postulated IL as extract phase and CS as raffinate phase, namely{(**IL**+A)+(**CS**+B)}, which neglects the reverse case of {(**IL**+B)+(**CS**+A)}. Therefore, it is significant to develop a rational approach to efficient ICBS design. In this contribution, the extraction of natural Toc from MODD, an abundant by-product in vegetable oil refining, is taken as an industrially relevant case study.

The computer-aided ICBS design framework is proposed in Figure 1a. It consists of two different design strategies including {(**IL**+Toc)+(**CS**+ML)} and {(**IL**+ML)+(**CS**+Toc)}, where ML denotes methyllinoleate as a representative of undesirable MODD components. The initial solvent database covers 7626 CS and 45360 IL combining 420 cations and 108 anions in the COSMObase. First, the infinite dilution activity coefficients of Toc and ML in CS and IL are calculated by COSMO-RS, based on which the infinite dilution capacity (C) and selectivity (S) on the mass basis are obtained. In this step, for ML and Toc extraction, two literature-reported solvents namely hexane and ethyl lactate are employed as CS reference solvents, and the constraints of $S_{ML} > 1$ and $S_{Toc} > 1$ are imposed for IL. Then, the physical properties of CS and IL are assessed. The T_m and T_b of CS are checked according to PubChem and COSMO-RS database to ensure $T_m < 298.15$ K and 323.15 <

T_b < 473.15 K. Due to the negligible vapor pressure of IL, only T_m constraint lower than 298.15 K is considered for IL screening predicted using the group contribution (GC) model (Lazzuś, 2012). Considering CS generally suffer from environmental pollution and health hazards, the environment, health and safety (EHS) properties of CS are further evaluated using a series of quantitative structure-activity relationship (QSAR) models embedded in the VEGA software. Only safe and green CS survived for subsequent steps. Afterwards, the quaternary liquid-liquid equilibria (LLE) constituted by the remained CS and IL are calculated by COSMO-RS to evaluate the extraction performance of different IL-CS combinations. As seen in Figure 1b, the ICBS forming the Pareto front are determined for strategy 1 and strategy 2, respectively, following which the cytotoxicity of the retained IL towards IPC-81 are predicted using the QSAR models (Wang et al., 2020). The IL possessing EC50 value higher than 100 are selected.

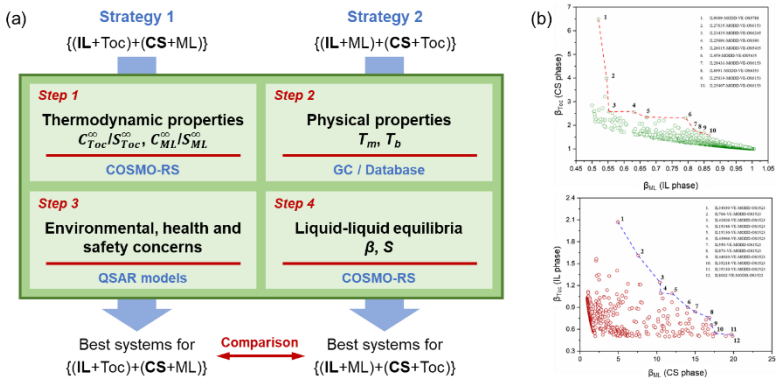

Figure 1. (a) Framework for rational design of ICBS for Toc extraction. (b) ICBS forming the Pareto front after quaternary LLE calculation.

Finally, the best systems for strategy 1 and 2 are screened out and compared to determine the optimal ICBS. From above, it is confirmed that strategy 1 is better than strategy 2 owing to its competitive extractive capacity and much higher selectivity towards Toc. The three ICBS ultimately chosen for Toc extraction consist of CS 2,2-dimethyl-3-pentanone and acetate-based IL (cations are diethyl-methyl-propylammonium, tetraethylammonium and 1-ethyl-1-methylpyrrolidinium), with the Toc selectivity of 11.50, 12.23 and 13.10, respectively. The proposed framework could be readily extended or adjusted to other separation tasks to rationally guide ICBS design prior to laborious experiments.

Keywords: biphasic extraction system, COSMO-RS, α-tocopherol separation

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Optimal configuration of a biodiesel production network using oil from black soldier fly larvae

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Abstract

Before the pandemic, the society was facing challenges respect to the climate change problem as well as the decline in the oil wells production. Now, the sustainable economic recovery represents a bigger challenge. In this context, the development of sustainable biofuels is a key area for the rapid economic recovery. In particular, biodiesel is one of the biofuels most produced worldwide, mainly from vegetable or animal oils (edible, non-edible and wastes); these oil sources have limited availability, especially considering those derived from cultivated crops that compete with lands with edible crops. Thus, the efforts are focused on the search of other oil sources, such the oil derived from black soldier fly larvae (Jung et al., 2022); the cultivation of this insect requires non fertile lands, reduced space, its life cycle is of 24 days, and they can be fed with wastes (as animal manure, restaurant waste, agricultural waste, among others); as result of this insect cultivation, larvae are obtained with high (35-40%) content of lipids (Feng et al., 2018). Therefore, in this work is proposed the analysis of the optimal configuration for a biodiesel production network considering as raw material the oil derived from black soldier fly larvae. Thus, a mathematical model was proposed where all the involved operations required for the biodiesel production supply chain are included, considering to satisfy a B10 mixture for the Mexican demand. As objective functions were considered the environmental aspect, through CO_2 minimization, and the economical aspect, using profit maximization. Results shows that is possible to satisfy current total diesel demand in Mexico using a B10 mixture having a national benefit of 8,106 million USD/y, which represent 0.63% of increase of Mexican Gross Domestic Product; in addition, 94% less emissions are released, in comparison with those generated by conventional diesel use.

Keywords: Biofuels, optimization, supply chain, waste management, circular economy.

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Optimization of Sink Locations in Carbon Integration Networks

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Abstract

The detrimental environmental impacts of climate change that are a result of high atmospheric CO_2 concentrations have prompted global efforts to limit the continuous increase in greenhouse gas (GHG) emissions. Many are now relying on the deployment of various carbon capture, utilization and storage (CCUS) methods which have been found reliable for reducing CO_2 levels in the atmosphere. As a result, various industries are shifting towards the decarbonisation of their operations through the use of a combination of various CCUS activities. This could involve the conversion of CO_2 into value-added chemicals, the utilization of CO_2 for enhanced oil recovery (EOR), the injection of CO_2 into geological formations and/or oceans, the biological fixation of CO_2, and other similar activities. Such operations are often referred to as CO_2 "sinks". It is often crucial for industries to identify which CCUS operations to deploy, especially when faced with many choices, since factors such as the cost of implementation and the sink efficiency play a significant role in the sink selection process. In this work, a mathematical model that helps identify optimal CO_2 sink locations within industrial clusters is developed and utilized. Identifying optimal sink locations is an important factor that needs to be considered as part of a CCUS network planning problem. The proposed model is particularly useful when faced with a number of location choices that could potentially be assigned a selection of CCUS operations. The proposed mathematical model was found to be very useful for identifying optimal CCUS sink selections, and their respective locations. A case study has been carried out to illustrate the proposed model, and key factors that were found to affect the sink location selections have been analyzed and discussed.

Keywords: Carbon Capture Utilization and Storage, Climate Change, Integration, Optimization, Spatial

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Optimization Strategies for Solving Multi-Period Integrated Planning and Scheduling Problems

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Abstract

Due to globalization, liberalization of emerging markets, and population growth, the demand for energy is rapidly increasing. Consequently, energy systems are expanding at the global scale and becoming more and more synergistic at the regional scale. Simultaneously, there has been a societal push towards carbon neutral energy systems Shell Oil Company (2020). To ensure the successful transition to net-zero energy systems will require the use of quantitative decision-making frameworks Demirhan et al. (2020).

The optimal development of energy systems is an extremely computational intensive problem and often requires bespoke techniques to produce quality solutions at the enterprise level Heuberger et al. (2017). This difficulty is further exacerbated when the energy system is expanded over the course of its lifespan as opposed to being completely constructed at the beginning of its operational life. To this end, we expand our previously developed optimization framework to be applicable to multi-period integrated planning and scheduling problems Allen et al. (2021).

In this work, we present an optimization strategy featuring a matheuristic for solving multiperiod integrated planning and scheduling problems that can be integrated into a commercial grade mixed-integer linear programming (MILP) solver. The heuristic utilizes the linear programming relaxation of the problem to construct locally optimal infrastructure planning and operational scheduling decisions. The proposed framework generates high quality solutions in a fraction of time that it takes commercial grade MILP solvers, while simultaneously providing a certificate of optimality.
Keywords: Supply Chain Optimization, Mathematical Programming, Heuristics

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Holistic Capacity Management and Production Planning in the Pharmaceutical Supply Chain

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Abstract

Planning of pharmaceutical manufacturing resources is vital during all stages in the product life cycle. Existing resources can be used to manufacture batches for late-stage clinical trials and for launch and long-term commercial production (Marques et al., 2017). First, continued supply of legacy products must be guaranteed through proper estimation of current and future manufacturing capability including downtime for process adaption and product changeover. Integration of scheduling information in production planning has been highlighted (Maravelias and Sung, 2009)) and mathematical models have been presented for campaign scheduling (Sampat et al., 2020)) and capacity planning (Qi et al., 2017). However, the combined capacity and production planning problem has received limited attention often focused on clinical portfolios or single-stage manufacturing. In this work we aim to bridge this gap through a framework for capacity planning that embeds production planning models for planning of real full-scale manufacturing. The framework consists of four steps: (1) system categorization and data collection, (2) baseline supply capability, (3) exploration of capacity changes and (4) optimal production plans with capacity activations and minimal downtime. The categorization is used to set up a campaign planning model which is populated by data from internal company systems. The model is deterministic, multiperiod, discrete-time, multi-stage, multi-product and handles time- and line dependent capacity, shutdown requirements, ramp-ups and release time. The framework can be used to support decisions on sales & operations planning, location & timing of clinical product campaigns and evaluation of capacity projects. A case study from real pharmaceutical production is used to illustrate the framework and highlight the benefits of data-centric decision support for production and capacity planning on both a strategic and operational level. Future work will focus on adding uncertainty to the framework.
Keywords: MILP, Planning & Scheduling, Pharmaceutical Manufacturing, Capacity

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Towards Resilience in Next-Generation Vaccines and Therapeutics Supply Chains

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Abstract

Promising clinical outcomes of Advanced Therapy Medicinal Products (ATMPs) are highlighting the potential of genetic engineering for preventing and treating life threatening diseases, including cancers. With several gene therapy drugs already been launched over the last few years, the versatility of genetically engineered drug delivery vehicles is also seen in preventive healthcare, with emerging mRNA and viral vector-based vaccine platforms (EMA, 2021). Given the increasing demand and limited manufacturing capacity, ATMPs manufacturers are asked to simultaneously tackle engineering product and process-related challenges, whilst scaling up production under demand uncertainty to ensure clinical availability and patient accessibility when products reach market approval. Furthermore, manufacturers of vector-based Covid-19 vaccines are challenged by rapid and in-risk manufacturing. In this space, there emerges a need for sophisticated tools that can assist responsive decision-making and support supply chain planning under uncertainty (Sarkis et al., 2021).
In this work, we present a novel mixed-integer linear programming (MILP) model for the design and optimisation of supply chains for next-generation therapeutics and vaccines. We focus on a range of pharmaceutical applications for viral vector-based products and their respective demand scales, thereby capturing the emerging paradigm shift from *one-size-fits-all* manufacturing and distribution to targeted healthcare. The formulated optimisation framework considers (i) a set of products and demand scenarios, (ii) scale-dependent capital and operating manufacturing, (iii) storage and shipping costs for sensitive formulated products, (iv) candidate locations over a region of interest for network nodes, namely primary and secondary manufacturing and distribution centres, to identify good candidate supply chain structures, allocate capacity and production plans for multi-product multi-suite facilities, and determine distribution and transportation plans across the network. The resilience of the strategic decisions under demand uncertainty is then assessed, with supply chain performance quantified and compared in terms of (i) cost, (ii) scalability, and (iii) flow time.

Keywords: mathematical programming, supply chain optimisation, advanced therapeutics, pharmaceutical manufacturing

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Network Modeling Approach of Chemical Processing Electrification with Renewable Energy Sources

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Abstract

Wind power is an energy source whose capacity has been increasing significantly in the past years, producing 8.4% of total U.S. utility-scale electricity generation, as published by the U.S. Energy Information Administration (2021). However, cases of under-utilization of the available power are common, with the main issues being the transmission capacity of the wind generation facilities to the main electricity load centers or because of the variability of wind generation, considering the fact that the maximum generation rate usually occurs early in the day, when power demand is low. Infrastructure addition that would only be operational when wind power is at its peak is generally uneconomical. More effective use of wind power could either involve expanded local use of electricity at times of peak wind power generation, or finding ways to store energy at times of peak wind power production. In the case of chemical production (which is a form of expanded use of electricity and energy storage), the main advantage would be to produce chemicals that would be readily compatible with existing fuel transport systems. In this work we aim to identify how wind power generation peaks can be utilized more efficiently to assist in chemical processing electrification. For this goal, we have developed a network model that represents a shale gas processing plant and its surrounding area. The encompassing area contains chemical plants that utilize natural gas liquids (NGLs) and their products, utilities (water, steam, electricity) supplies and a wind power generation capacity. Depending on the electricity production level, chemical production may alternate between the conventional process or an electrified version (electricity used instead of steam or fuel). The model we developed is used to maximize the network's profitability, thus identifying the optimal chemical pathways for the utilization of available wind power.

Keywords: Optimization, Network Modeling, Electrification, Wind Power, Chemical Manufacturing

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MINLP framework for systems analysis of the chemical manufacturing industry using network models

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Abstract

Recent technological advancements in hydraulic fracturing and horizontal drilling have led to rapid increases in U.S. oil and gas production, particularly from shale formations. A side effect of this growth is the significant increase in the production of natural gas liquids (NGLs), which are often abundant in shale gas. NGLs consist mainly of ethane, propane, n-butane, i-butane and (in smaller amounts) C5+. These molecules constitute some of the most important building blocks of the chemical manufacturing industry. Therefore, the increase in the availability of shale gas and associated NGLs has provided a unique opportunity to expand the U.S. chemical manufacturing industry (Siirola, 2014; Yang and You, 2017).

In recent work to assess new technologies for the utilization of NGLs and compare different candidate products for industry expansion, we developed (Skouteris et al., 2021) a nonlinear, optimization-based industry network model that seeks an overall cost minimum for the industry. In this model, in contrast to previous work (e.g., Derosa and Allen, 2015), process costs and material prices are allowed to be variable and respond to external perturbations to the industry network superstructure (e.g., adding a new process). To solve the resulting mixed-integer nonlinear program (MINLP), one option (Skouteris et al., 2021) is to use a successive linear programming (SLP) approach that alternates between solving a constant-cost LP and a special cost-propagation algorithm that updates process costs based on the LP results. In this work, we expand the problem formulation to consider other means to compute material prices. Additionally, we propose new means for efficiently tackling the resulting MINLP and compare them to the original SLP approach. This work will facilitate the solution of nonlinear industry network models for planning the strategic use of NGLs.

Keywords: Optimization, Network modeling, MINLP, Chemical manufacturing, Supply chain

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A Novel Approach for Vehicle Fleet Sizing and Allocation Under Uncertain Demand

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Abstract

The sizing of vehicle fleets and their allocation are key decisions for modern industries that need to meet the demand of geographically distributed operations. Proper fleet planning is a must to guarantee the supply of services, resources and equipment to keep operations running. Planning maintenance tasks in offshore wind farms (Gundegjerde, 2015), sizing and allocating aircraft fleets to airline routes (Repko, 2017) or, in more general terms, optimizing transportation through a network of origin and destination nodes using a fleet of vehicles (List, 2003) are challenging problems proposed in the literature. Fleet planning involves decisions aimed at fulfilling operational schedules that are often subject to uncertainty, usually leading decision-makers to overestimate the number of resources. An efficient procurement and utilization plan requires solving critical trade-offs between fleet acquisition and contracting costs, asset performance decay and penalties for unmet demand, under a wide range of possible scenarios.

The problem addressed in this work can be stated as follows. Given: (i) a set of nodes, (ii) random variables accounting for the trips to be made between the nodes during the time horizon, (iii) the type of vehicle for each trip, (iv) alternative contracts with vehicle suppliers, (v) unit costs for vehicle acquisition, rental, hiring/firing, and (vi) penalty costs for unsatisfied demand; we seek to determine: (a) the fleet size for each type of vehicle; (b) the allocation of vehicles to trips; (c) the service level to be provided, i.e. the probability of meeting demand; and (d) the contracts (vehicles hiring/firing) along the time horizon, in order to minimize the total costs. We propose a novel model based on mixed integer linear programming (MILP) to optimally determine the size and allocation of vehicle fleets under uncertain demand. In contrast to previous works, demand satisfaction is a model decision and any probability distribution can be used to characterize the number of trips required in the network. Furthermore, fleet procurement and contracting decisions for alternative types of vehicles are integrated into the model.

The proposed model solves problems of real dimensions in very low computational times in comparison to previous approaches, from several hours to a couple of minutes. The formulation allows considerably reducing costs due to oversizing and proves adaptability to diverse demand characterizations and contracting terms from different industries. A real-world case study involving maintenance operations in geographically spread assets is addressed to highlight the model capabilities and draw conclusions.

Keywords: fleet sizing, allocation, planning, optimization, uncertainty

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Towards the development of decomposition-based approaches in personalised medicine supply chains

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Abstract

Chimeric Antigen Receptor (CAR) T cell therapy is a type of immunotherapy, where a patient's own immune system is utilised to recognise and kill cancer cells (Sadelain (2015)). Currently, CAR T cells are administered to approximately 1000 patients in the UK. Owing to the promising clinical results of the therapy, patient numbers are estimated to increase rapidly and reach 40,000 people in the next decade (Papathanasiou (2020)). This necessitates agile, responsive distribution networks that will be able to adequately respond to patient needs. Mathematical models can play a significant role in supporting this growing market and optimally coordinate the different tasks to identify robust and responsive solutions. The autologous nature of these therapies challenge the solution of such problems even more. This is primarily as they result into a high number of decision variables and constraints that increase the size of the problem.

We have developed a mixed integer linear problem describing the current distribution network of CAR T cell therapies. To keep the problem computationally tractable for a higher number of therapies, a bi-level decomposition approach is proposed. The original detailed model is decomposed into a relaxed upper-level planning problem responsible for strategic planning decisions and a lower-level scheduling problem (Erdirik-Dogan (2008)). Optimal solutions for the structure and operation of the supply chain network are obtained for demands of up to 5000 therapies per year, in which case the original model contains 68 million constraints and 16 million discrete variables. The performance of the algorithm can be observed by the decrease in the number of constraints. The proposed approach has the potential to decrease the computational time by more than 50% compared to the original, large scale model in cases of more than 1000 patients per year.

Keywords: cell therapy, supply chain optimisation, MILP

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A novel hybrid algorithm for scheduling multipurpose batch plants

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Abstract

Multipurpose batch processes feature on shared facilities and product-specific production routes, for which flexibility provides industrial application prospect, but complexity poses challenges on design of optimization algorithms. A plethora of mathematical programming models have been proposed to schedule multipurpose batch plants, and their capabilities for small-size problems are well established. However, they often fail to solve industrial-scale problems to optimality because appropriate number of time points is unknown a prior and feasible solutions are hard to yield in short time frames. Although various decomposition approaches have been attempted, large computational efforts are still inevitable to obtain near optimal or optimal solutions.
Genetic algorithm (GA) is widely embraced to address industrial-scale problems because it can generate good quality solutions quickly crediting for its strong global search capability and inherent parallelism. However, research works [Han (2021)] show that worse objectives could be obtained for some large-scale examples than MILP models, although computational effort could be significantly reduced. Therefore, the hybrid algorithm combining advantages of GA on fast convergency and mathematical programming approaches on computational accuracy may eliminate limitations of single algorithm and solve challenging large-scale problems.
In this work, we propose a new hybrid algorithm integrating GA and sequence-based MILP model to generate near-optimal or optimal solutions for industrial scheduling problems. We first use GA to obtain good feasible solutions, where chromosomes are constructed to represent sequence, assignment and task repetition based on production recipe. A knowledge-guide search operator is introduced to enhance exploitation by adjusting chromosome using experiential possibility knowledge. Then some strategies are proposed to fix the majority of binary variables related to batching and sequence in MILP model using solutions obtained from GA. Finally, the MILP model is quickly solved to improve solution quality. The results show that the proposed hybrid algorithm can generate the optimal solutions within 3 minutes. It can generate a smaller makespan than the model of Vooradi (2012) and significantly reduce the computational effort by about one order of magnitude compared to the work of Velez (2015).

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Assessment of biomass supply chain design and planning using discrete-event simulation modeling

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Abstract

The dynamic structure of current supply chains poses significant challenges to the implementation of effective decision support systems. This complexity entails the simultaneous assessment of different business criteria for the majority of strategic and operational decisions, with a compromise between all entities to deal with uncertainty. With the advent of digitalization, the development of decision support systems is demanding an enterprise integration with faster decisions. It represents a challenge for the traditional modelling techniques to encompass the tradeoffs of different dimensions, with particular importance to the growing sustainability implications of economic, environmental and social levels.

Within the modeling research of complex systems, the development of Digital Models, Twins or Shadows have been addressed in the fields of planning and control improvement. The scope often aims at high-resolution representations of a physical system or focused on specified traces when fast reaction is crucial. Due to this multi-level decision-support, discrete-event simulation can provide data information and performance indicators (e.g. lead time, makespan, set of resources, capacity utilization), allowing to model uncertainty and evaluate how the system reacts in different scenarios.

It is recognized the growing interest in replacing fossil resources by biomass to produce bioenergy and biomaterials at integrated biorefineries. However, attracting investment requires additional efforts to increase its competitiveness with an efficient supply chain. The challenges concerning its design and planning can include the (1) selection of biomass sources, type, and quantities; (2) storage locations/capacities and preprocessing technologies; (3) processing facilities with technology definition, capacity and location; (4) type of products/byproducts and respective amounts; (5) markets, location and demand to satisfy; or (6) logistic operations at the supply chain nodes. Moreover, the strategic decisions are greatly influenced by the uncertainty on biomass availability and quality, products demand, and the non-mature technologies for preprocessing and processing operations at these biorefineries.

With the proposal of a simulation approach, it is possible to incorporate the dynamics and uncertainty interactions of the real supply chain system by means of an event-based model. Using the SIMIO platform, a 3D visual model accurately simulates the characteristics of the biomass supply chain and evaluates the network performance under alternative scenarios. The results highlight the advantage of the developed model to provide supervision in the design and planning of biomass supply chains, assessing strategic and tactical solutions with more precise liability of its major uncertainty factors.

Keywords: Design, biomass supply chain, discrete-event simulation.

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Design of a three-echelon supply chain under uncertainty in demand and CO_2 allowance prices

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Abstract

Nowadays there is a growing concern regarding greenhouse gas emissions and their consideration in the supply chain design. In this work we present a robust stochastic model for the design of a supply chain under uncertainty of CO_2-allowance prices and market demand. The three-echelon petrochemical supply chain superstructure consists of 7 production plants in Europe, storage associated with these plants and four possible markets. At each plant different products can be produced according to the available technologies. The goal is to maximize the expected net present value (ENPV), while reducing the amount of CO_2 equivalent emissions.

We implemented the carbon cap and trade model from the European Union emissions Trading System, whose goal is to reduce the emission cap over time in order to achieve a climate-neutral EU by 2050. We combine the environmental LCIA data, required to determine the global warming potential, with the forecast of CO2 allowance prices. The problem involves a multi period mixed integer linear program (MILP) formulation, which was implemented in the General Algebraic Modelling System (GAMS) and solved using CPLEX.

To deal with uncertainty in market demand and CO_2-allowance prices, we implemented an ARIMA model and generated multiple scenarios. Since a full discretization of the resulting probability space leads to a number of scenarios that exceeds capacities of state of the art computers with ease, decomposition techniques are applied.

The obtained results show an improvement of the economic performance when compared to the results from the deterministic approach that is being widely used in literature.

Keywords: CO_2 price uncertainty, stochastic model, optimum supply chain management, decomposition methods

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Monetization strategies for the design and planning of sustainable supply chain

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Abstract

Over the years, the need to invest in sustainable development has been a reality so that future generations may not be compromised. As a result, international regulations have come up to ensure that companies' sustainability is considered when managing supply chains. Thus, the design and planning of companies' decisions should include not only the economic concerns, but also the environmental and social ones as well (Barbosa-Póvoa et al., 2018). Considering the complexity associated to the supply chain management towards sustainability, there is the need to develop decision support tools to help decision-makers when managing their supply chain (SC) while considering demand uncertainty (da Silva et al., 2020). In this way, a mixed-integer linear programming (MILP) model is here developed for the design and planning of SC that accounts for the economic, environmental, and social performances. This optimization-based tool intends to translate both supply chains' environmental and social performances in the same monetary unit to optimize the design and planning of economic, environmental, and social performances of the SC in the same unit.

In the model a generic SC is considered. Taking into account the possible set of locations of SC entities, production and remanufacturing technologies, possible transportation modes between entities, and products within the SC, the main objective is to obtain the SC network structure, supply and purchase levels, entities' capacities, transportation network, production, remanufacturing and storage levels, supply flow amounts, and product recovery levels, in order to maximize profit and social performance, while minimizing environmental impact. The MILP model used to solve this problem is based on da Silva et al. (2020), which was extended to also consider the impact of SC social performance. Eq. (1) represents the first objective function, which is the maximization of the expected economic, environmental, and social performances of the SC, namely the expected net present value (Eq. (2)), the expected environmental impact value (Eq. (3)) and the expected social impact value (Eq. (4)).

$$\max\ (e\,NPV_N + e\text{So}\,Impact_N - e\,EnvImpact_N) \tag{1}$$

$$\text{eNPV}_N = \sum_N pb_N \left(\sum_{t\in T} \frac{CF_{Nt}}{(1+ir)^t} - \sum_{\gamma} FCI_\gamma\right) \tag{2}$$

$$\text{eEnvImpact}_N = \sum_N pb_N \left(\sum_{\substack{t\in T \\ (a,m,i,j)\in NetP}} ei_{ac} pw_m d_{ij} X_{maijtN} + \sum_{i\in I_f \cup I_w} ei_{ic} Y_i C_i\right) \tag{3}$$

$$\text{eSoImpact}_N = \sum_N pb_N \left(\sum_{\substack{t\in T \\ i}} MNEmp_{iNt} Y_i \alpha_i \beta_i \gamma_i \delta_i\right) \tag{4}$$

As uncertainty in demand is a reality in SC this is also added into the model through a multistage stochastic approach. Constraints regarding mass balance, capacities, transportation, and technology are considered.
The resulted model is applied to a chemical components' producer whose main production is in Lyon (Silva et.al., 2020). The company's suppliers are also located in Lyon. It supplies three main markets that are in different European countries: Portugal, France, and Germany. Company's decision makers are interested in expanding, to three new markets. The company sells three different types of chemical products that can be sold to different industries. In addition, three technologies may be selected that produce them. Initially, the three goals are considered separately followed by an aggregation in the same objective function, which was possible due to the monetization of both the environmental and social. Thus, four cases are studied: A) analyses the case-study result that represents the optimal economic performance as major goal; B) analyses the case-study result that represents the optimal social performance as major goal; C) analyses the case-study result that represents the optimal environmental performance as major goal, evaluated through EPS; D) analyses the case-study result that represent the optimal equity between social, environmental, and economic performances. As a result, the values for the total expected net present value, social impact, and environmental impact obtained in each case is shown in Table 1.

Table 1 Outcomes for the economic, social, and environmental impacts.

Obj. Function	**Case A** Max eNPV	**Case B** Max eSoImpact	**Case C** Min eEImpact	**Case D** Max (eNPV+eSoImpact-eEnvImpact)
eNPV	$1.52x10^{9}$ €	$1.49x10^{9}$ €	$1.20x10^{9}$ €	$1.51x10^{9}$ €
eSoImpact	$8.17x10^{-12}$ €	$3.12x10^{-11}$ €	$1.61x10^{-11}$ €	$5.26x10^{-12}$ €
eEImpact	$1.01x10^{9}$ €	$1.11x10^{9}$ €	$9.35x10^{8}$ €	$9.82x10^{8}$ €

From the analysis of Table 1, it is clear that results are influenced by social and environmental impacts and thus proving the importance of considering these goals in solving real-life problems. An extension of this work should consider different social indicators and a more comprehensive study of uncertainty to conclude on its adequacy even better.

Keywords: supply chain, sustainability, monetization, uncertainty

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From simulation towards optimisation for petroleum refinery operations in industry 4.0

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Abstract

Although there has been an increasing development and implementation of optimisation-based approaches in the last decades, simulation methods are still widely employed for problems that could instead be optimised. This is especially valid for industrial processes, in which complex, uncertain, and dynamic problems are modelled, solved, and controlled considering process safety, operational requirements, scheduling implementation, and plant-model mismatches.

Simulation relies on achieving feasibility through a trial-and-error procedure and provides meaningful and useful resources to find quick or rigorous solutions in the continuous variable space. On the other hand, optimisation provides the proper capabilities for automatically searching for optimal (and better) solutions. Despite being more computationally expensive, optimisation has been increasingly used with the recent technological improvements and research developments in Industry 4.0. Overall, the decision on using simulation or optimisation depends on the problem, application, complexity, and solution requirements.

Industry 4.0 offers many opportunities of improvement for multiple applications in diverse fields. Automation has become real and necessary, in which faster, more flexible, and more efficient operations achieve minimum costs and higher product/service quality. However, a large number of companies still employ obsolete methods, tools, and techniques in their decision-making process. The main reasons include insufficient knowledge to implement or develop better approaches, lack of trained or qualified employees, fear of change or lack of motivation to do so, lack of proper investments, etc. Hence, most companies either struggle to survive or miss significant opportunities to achieve economic and operational improvements.

In this work we address the importance of optimisation replacing simulation for problems and applications that are optimisable, i.e., suitable to be solved by optimisation-based algorithms and tools rather than simulation-based or trial-and-error procedures. We emphasize the main advantages for industrial operations within computer aided process engineering, and highlight the benefits over a diesel blending and scheduling application. We illustrate how optimisation can be employed for replacing the currently used simulation tools, and which qualitative and quantitative achievements are expected. The main results include significant cost reduction, improved process flexibility, better adaptation against uncertainties and disturbances, and enhanced reliability in the computer aided tools.

Keywords: Optimisation, simulation, petroleum refinery scheduling, blending operations, industry 4.0.

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Dynamic scheduling of customer orders in the order-to-cash process of a chemical supply chain

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Abstract

There are two main approaches to supply chain modeling: the bottom-up and top-down approaches (Shapiro, 1999). The top-down approach is the more traditional approach to supply chain optimization, which focuses on the design, planning, and scheduling of supply chains. On the other hand, the bottom-up approach targets the transactional processes that are present in Enterprise Resource Planning (ERP) systems. In the PSE community, Laínez and Puigjaner (2012) have emphasized the need for a holistic approach to supply chain management, requiring a paradigm shift from operation-based decision support systems to integrated decision frameworks that account for the different areas (e.g., accounting, research and development, sustainability) and flows (material, financial, and information) associated with supply chains. The present work seeks to address this need by merging the two approaches mentioned by Shapiro. As a first step in accomplishing this, a framework is presented to integrate the material flows in a chemical batch plant with the information flows in the order fulfillment or order-to-cash (OTC) supply chain process (Croxton, 2003). Previous work by the authors includes the development of scheduling models to optimize the order transactions in the OTC process (Perez et al. 2021). However, these works focus primarily on the information flows in the supply chain and represent the physical processes as nodes in the transactional process network with a lumped process duration. In this work, we provide a more comprehensive approach, which incorporates manufacturing scheduling models in the OTC process model. This approach provides a more complete and accurate view of the supply chain by accounting for both material and information flows. The use of chemical production and material availability models enables an accurate modeling of the processing times in the chemical manufacturing steps, which in turn allows the optimization models to find better solutions when scheduling customer orders. Thus, this work takes a step forward in the development and management of digital supply chains by coupling information flows captured in the ERP system with material flows in the production processes.

An illustrative example is presented in the context of the order fulfillment business process in the make-to-order batch chemical plant presented in Kondili, et al. (1993). In the plant, three raw materials (A, B, and C) are used to produce two products (P1 and P2), via three intermediates (AB, BC, and E). There are three unit operations in the plant: one heating step (heater), three reaction pathways (small or large reactor), and one distillation step (still). In the illustrative example, orders arrive with stochastic inter-arrival times and are processed by two different transactional agents. A stochastic discrete-event simulation framework is used to dynamically model the system behavior. Optimization events are triggered each time a new order enters the system, at which time a comprehensive State-Task Network model is called to schedule both the order processing steps and the plant operations. Whenever an optimization event is completed, updated order priorities and

queue assignments are passed to the transactional queues in the discrete event simulation, along with the updated production schedule. This closed loop approach allows the system to be optimized without compromising solution quality, as occurs when models focus exclusively on either the transactional system or on the manufacturing system. Purely transactional models can yield suboptimal results because these models do not account for synergies in the manufacturing plant arising from co-production, which allows reducing the order fulfillment lead times. On the other hand, purely physical models can result in schedules that are infeasible. This occurs because the models do not account for bottlenecks in the transactional process, which affect raw material availability at the plant. Thus, the integrated approach finds a solution that is 58% more profitable than the purely transactional one, and corrects for the infeasibilities in the purely physical solution, which erroneously predicts a 19% profit increase, as shown in **Fig. 1**.

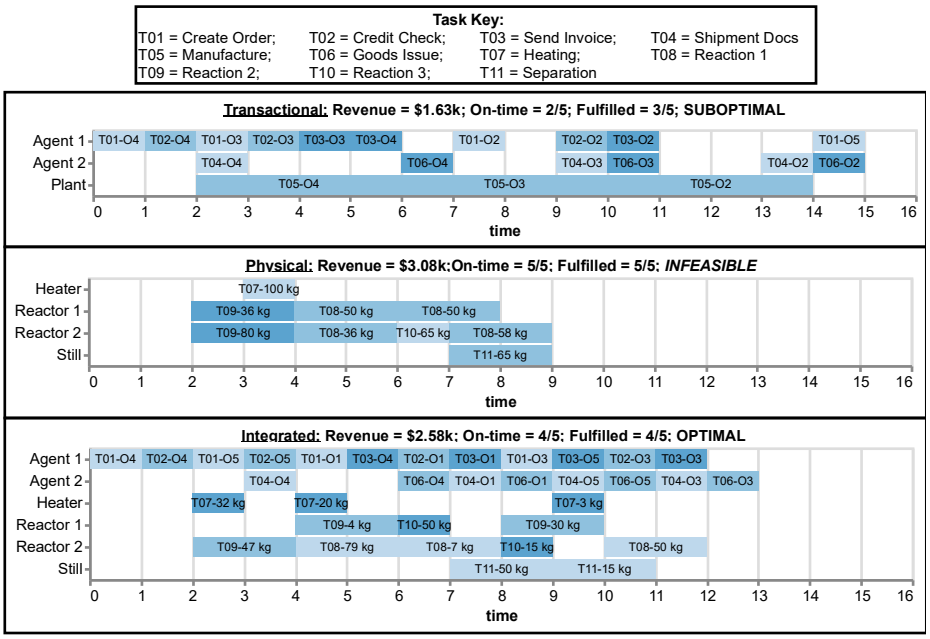

Figure 1. Schedules for each model. Batch sizes and order IDs are indicated in the bars.

Keywords: Scheduling, Business Processes, Supply Chain.

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Decomposition of Two-stage Stochastic Scheduling Problems via Similarity Index

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Abstract

Two-stage stochastic scheduling problems (TSSP) often involve a large number of, both continuous and discrete, variables that are computationally demanding and can be challenging to solve in a monolithic fashion. One alternative is to apply decomposition methods (e.g. Benders, Lagrangian decomposition, etc.) with the idea of splitting the original problem into smaller ones that progressively approach the solution of the monolithic formulation. In the case of two-stage stochastic optimization, the first-stage variables are the link among the decomposed subproblems. Martí et al. (2015) proposed a price-driven decomposition approach for setups that only involve continuous decision variables. However, this method is not directly applicable to mixed-integer optimization problems, especially when the number of binary variables is high. To overcome this limitation, we propose a price-driven decomposition for the above described class of problems, inspired by the so-called Similarity Index (SI).

Palacín et al. (2018) proposed a SI to force discrete recourse variables to approach among scenarios, i.e improving solution robustness without extending the robust horizon in time-discretized TSSP. It was inspired by the idea of fuzzifying discrete decisions for a particular scenario around the neighboring time periods, see Figure 8 in the above reference for a graphical illustration. Then, the SI is finally calculated as the intersection between fuzzified schedules for all scenarios. This concept was successfully applied to formulate the production-maintenance scheduling of an evaporation network.

However, with decomposition in mind, note that this concept of SI could also be applied to first-stage variables. Thus, after solving each scenario independently, the similarity between the first-stage discrete decisions can be measured using the SI concept. Later, the SI can be incorporated into the scenarios' cost functions together with an updatable Lagrange-like multiplier. Of course, a constraint is required such that the solution of the scenario yields the higher SI. Hence, an iterative algorithm could push it forward while resolving the scenarios. Ideally, at the end of the procedure, the SI would reach a value of 100% SI and the solution for the first-stage variables for all scenarios would coincide.

Keywords: Scheduling, Decomposition, Uncertainty, Similarity Index

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Scheduling of Crude Oil Operations

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Abstract

Scheduling of crude oil operations is one of the most critical and challenging problems in petroleum refineries. Crude oil operations have more impact on the profitability of the whole refinery as these operations are the first steps of refinery operations. Also, crude oil operations scheduling is a very complex problem because of depending on continuous, discrete and binary variable optimization, and this type of problem is known as NP-hard (Li-ping & Nai-qi, 2011). In a refinery, a planner tries to schedule all crude oil operations by using a wide variety of complex and very dense data sets. Daily planning is mainly based on manual scheduling by trial and error method and operational experiences. Hence, as a planner, it is extremely important and hard to reach the best solution by handling all the data sets in a short period and in an efficient way. Unfortunately, there is no such tool that can be used efficiently for making the planners' life easier regarding adaptive different refinery scheduling cases.

An efficient scheduling and allocation model is developed for unloading crudes into multiple storage tanks from the tankers arriving at various times, blending crudes, and feeding the crude distillation units from these tanks at various rates over time. Refinery crude oil operations include 2 docking stations, 12 crude oil tanks, 2 crude oil distillation units (CDUs). The objective of the crude oil scheduling problem is to minimize operating cost. The crude oil scheduling problem is formulated with both unloading and loading flow rate constraints due to different level gaps among the crude oil tanks and pumping rate limitations during the transfer. In addition to that, a wide variety of crude oil types also lead to some limitations in blending. Each crude oil has its own unique properties like Sulphur, API, salt etc., and most of the petroleum refineries have some processing and design constraints in terms of these properties. Hence, to tackle the abovementioned limitations effectively, a Mixed Integer Linear Programming (MILP) model is formulated. MILP formula is solved by using GAMS, a high level modelling system for mathematical programming and optimization, and the results are visualized via a dashboard framework. The developed solution helps planners to schedule crude oil operations in a short time.

Keywords: crude oil operations, short-term scheduling, mixed integer linear programming, optimization.

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Optimal design of hydrogen supply chains to decarbonize hard-to-abate industrial sectors

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Abstract

Hydrogen produced with low-carbon emissions has the potential to decarbonize a wide range of sectors. These sectors include so-called hard-to-abate sectors (e.g. chemical industry), where it is proving difficult to reduce CO_2 emissions (Gabrielli et al., 2020b). Over 95% of hydrogen is currently produced via steam methane reforming of natural gas, contributing 2% of the global CO_2 emissions (IEA, 2019). To reduce the carbon-intensity of steam methane reforming, the process can be coupled with carbon capture and storage (CCS). Alternatively, hydrogen can be produced from renewable energy sources (RES) via water electrolysis from renewable electricity, reforming of biogas, or biomass gasification. Hereafter, we refer to this portfolio of options as low-carbon hydrogen. Previous works assess the potential of low-carbon hydrogen for several hard-to abate sectors within Europe and quantify the availability of renewable electricity, and biomass (Kakoulaki et al., 2021; Scarlat et al., 2018, 2019a, 2019b). However, the lack of a European hydrogen and carbon supply chain prevents a widespread use of low-carbon hydrogen. While the optimal design of hydrogen supply chains is investigated in previous works, combined assessments of RES-based hydrogen production and CCS value chains are rare, and the analysis of an optimal and realistic infrastructure evolution is lacking (Gabrielli et al., 2020a).

This work aims to fill this gap and presents an optimization framework for the optimal planning of hydrogen supply chains coupled with CCS. The hydrogen supply chains and CCS value chains are modelled as networks. At each node, hydrogen production technologies can be installed. The available hydrogen production technologies are reforming of biogas and natural gas, biomass gasification, and water electrolysis from electricity. Resulting CO_2 emissions can be reduced by capturing the CO_2 at the point of source when carbonaceous feedstock is used. Different transport technologies are available to connect hydrogen production with hydrogen consumption and CO_2 storage sites, hereby modelling the transport of hydrogen and CO_2 between the nodes. The available transport technologies include ship, truck, and rail. The node-specific demands of the hydrogen consumption sites, the availability of resources, and the location and capacity of CO_2 storage sites are required as input data. Uncertainties in the evolution of future hydrogen demand are considered through investigating different demand scenarios.

The resulting optimization problem is formulated as a mixed-integer linear program that minimizes cost while complying with different demand scenarios for low-carbon hydrogen. The optimization problem determines the optimal location, type, and size of (i) the hydrogen production technologies, (ii) the CO_2 capture technologies, and (iii) the transport technologies. In compliance with mass and energy balances, the (a) input and output streams of the hydrogen production technologies, (b) the flow through the transport technologies, and (c) the required amount of feedstock are computed. All decisions, namely design (i-iii) and operation (a-c), are time-dependent, with a yearly

resolution. The solution of the optimization problem identifies the optimal evolution of the hydrogen supply chains and the CCS value chains over a multi-year time horizon. The hydrogen supply chains connect (1) the available sources of feedstock with the hydrogen production sites, and (2) the hydrogen production sites with the hydrogen consumption sites, so that the spatially and temporally distributed hydrogen demands are satisfied. The connections between the point-source CO_2 capture technologies and the CO_2 storage sites are modeled within the CCS value chains. The goal is to unveil the rationale behind the optimal evolution of hydrogen supply chains, and CCS value chains over a multi-year time horizon and to investigate the interplay between the different production pathways, feedstocks, and energy sources.

The optimization problem is applied to a case study that determines the optimal evolution of a European hydrogen supply chain to decarbonize oil refineries and ammonia production. Oil refineries and ammonia production currently account for 95% of the European hydrogen consumption (Kakoulaki et al., 2021). The case study aims at investigating whether low-carbon hydrogen represents a cost-effective solution to decarbonize oil refineries and ammonia production within the next ten years. Offshore reservoirs such as the Northern Lights project (NO) are considered as potential CO_2 storage sites (Becattini et al., 2021). The selection of production and transport technologies is limited to the commercially mature, and economically viable options as listed above. Pipelines are not viewed as a viable transport option that can be deployed within the next ten years due to technology-specific barriers, such as the high capital investments, long construction times and complex regulatory backgrounds. Hence pipelines are not considered here.

Keywords: hydrogen supply chains, carbon capture and storage, energy networks, optimization, chemical industry.

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Multiperiod optimization model for CO2 capture, storage and utilization, Colombian case study

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Abstract

Colombia is formulating policies to accelerate the energy transition, decarbonize its industries and decrease its dependency on fossil fuels. In this context, the design of infrastructure for carbon capture, use and storage (CCUS) plays a key role to reach out the target on reduction of greenhouse gas emissions (GHG) (Garcia et al., 2016 and Nordhaus, 2020). To the best of our knowledge, previous works on CCUS design are focused on modelling one echelon of the infrastructure, considering CO2 transport by pipeline and the temporal base is uniperiod. This feature is the main drawback to show how the topology evolves and how the investments should be made from one time period to the next. In this work we present a novel optimization framework for the CCUS design applied to the Colombian case. The model considers technologies for carbon capture, multimodal transportation, CO2 utilization for enhanced oil recovery (CO2-EOR) and geological storage to meet a given target on GHG at minimum cost of the infrastructure. The model provides insights regarding investments on carbon capture technologies such as timing, sizing, location, and type of technology. Furthermore, the model determines the optimal transportation mode considering on-shore (pipelines, and trucks) and offshore (pipelines, river fleet routes, and maritime vessels). One novelty of this work is the integration of the CCUS design with the oil field development for CO2-EOR. The model considers oil production profiles, petrophysical properties and economic data to determine the optimal petroleum production campaign (i.e., production wells for CO2 injection). We tested the model on a long-term planning horizon (25 years), considering 14 CO2 emissions sources temporally and geographically distributed across the country, 2 types of commercial carbon capture technologies, 3 different plant sizes (small, medium, and large), 3 potential oil fields for CO2-EOR and 2 for geological storage, and 3 multimodal transportation modes. Results shown a carbon capture cost between 40 – 80 USD/t, with a cost breakdown of 70%, 20% and 10% allocated into the carbon capture processes, CO2 transportation and CO2 injection respectively. This proportion does not change despite increasing the GHG mitigation target to 50% and 80%. Furthermore, results shown that scale economy on the CCUS infrastructure leads to significant cost reduction. Future research may focus on considering a more detailed model representation for designing the CO2 pipeline transportation network. This challenge would lead to solve a nonlinear system of equations, and second, to investigate the impact of injection pressure on the production wells. These are now the main concern of the ongoing research, which would require the formulation of novel modelling approaches to manage nonconvexities.

Keywords: supply chain, design, capture, storage, utilization, Dioxide Carbon, CCUS.

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Towards improved rescheduling operations: small time-steps and long time-horizon

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Abstract

Scheduling operations in industrial processes are often inefficient in terms of decision-making methodology and solution approaches. Industrial operations are subject to multiple sources of uncertainties that bring difficulties for an efficient decision-making. Noises, disturbances, and other unforeseen events happen over time and result in plant-model mismatches. The scheduling operations often become suboptimal or even infeasible, which affects the economics and operations of the plant. Rescheduling the incumbent process conditions can properly update the state of the system and quickly and accurately adjust the model to match the ongoing scenario in the plant. However, this requires a continuous cycle of optimisation with periodic or event-triggered rescheduling. This is especially important under complex processing environments that often require integrated plant-model environments for exchange of data, update of information, and accurate tracking of quality information (i.e., properties of streams) throughout the process network. In this context, the properly selection of modelling and optimisation parameters such as time-step size and time-horizon length becomes especially important. Small time-steps are fundamental within efficient rescheduling approaches whereas long time-horizon can significantly enhance the scheduling solutions.

Although the literature on the topic indicates the importance of addressing small time-steps and long time-horizon for improved scheduling operations, to the best of our knowledge there are no works that provide comprehensive quantitative analyses and results on the impact of these features on the scheduling economics and operations. In this work, we address the influence of the time-step and time-horizon lengths in the scheduling solutions. Two industrial-sized product blending examples are employed, whereby the operational scheduling and economic value of the process are investigated over distinct scheduling conditions.

Keywords: Scheduling optimisation, Rescheduling features, industrial processes, industry 4.0.

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"Pharmaceutical industry supply chains: planning vaccines' distribution"

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Abstract

Pharmaceutical supply chains tend to be complex, and its management faces several challenges. Decision-makers often struggle with the high levels of uncertainty. This, together with the need to consider sustainability principles in supply chain management, have greatly increased the complexity of the network's management in this sector. Addressing equity in access has proven to be a critical concern in pharmaceutical supply chains, in particular when dealing with vaccines' distribution, thus being important to consider availability and affordability when designing and planning a vaccine' supply chain.

A decision-support tool is presented following the work developed by (Mota *et al.*, 2018), where a multi-objective mixed integer linear programming model is proposed, aiming to integrate several strategical-tactical decisions while considering the three pillars of sustainability, which are addressed as objective functions. Decisions such as factory and warehouse location, capacity installation, inventory and production planning and transportation network definition are included in the model. The economic assessment is performed through the Net Present Value. The environmental impact assessment follows the Life Cycle Analysis methodology. Accessibility of pharmaceutical products is the major focus for the social assessment, aiming to provide an equal distribution by making products both available and affordable among countries. Thus, the social evaluation is made through a DALY-based metric. Moreover, while the social objective function aims to maximize equity in access, a social constraint is also used to respect a satisficing level of equity.

The model is applied to a real base case study aiming to discuss different optimization scenarios and to study trade-offs among the three pillars of sustainability. Apart from the understanding of the effect of decisions on each performance indicators, the model also enables the comprehension of connections among different supply chain activities, providing an opportunity to better understand the performance of the combined indicators across the supply chain. Therefore, the results can be used to better craft and perform strategic and tactical decisions, envisioning the achievement of economic, environmental, and social objectives.

Keywords: Pharmaceutical Industry, Sustainable supply chains, Equity, Mixed-integer linear programming

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Multi-fidelity Approaches for Simulation-Optimization in Industrial Make-and-Pack Process Scheduling

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Abstract

This work deals with the simulation-optimization based short-term production scheduling of a two-stage industrial make-and-pack process that consists of a formulation stage and a packaging stage (Klanke et al. (2021)). Several features, such as a high combinatorial complexity due to the large number of products and production lines to be scheduled, render its scheduling very challenging. A buffer decouples the two production stages to increase the flexibility in the routing of products, which increases the overall productivity of the plant, but also necessitates to model detailed mass balances. Besides the buffer, the case study at hand is characterized by a large number of products in several product families, product-specific deadlines, product-dependent processing times and sequence-dependent changeover times.

Although those features were considered in the MILP model that is presented in Klanke et al. (2021), several extended features that have to be considered for the daily operation of the industrial plant had to be left out due to limitations in the flexibility of the mathematical formulation. Those features include a limited number of operators in each stage that perform the changeovers, an upstream raw material delivery with limited buffering capacity and frequent refilling as well as packaging line maintenance. The inclusion of these features is indispensable to ensure the feasibility of the production schedules. Therefore a detailed Discrete-Event Simulation (DES) model, denoted high-fidelity (HF) model, was set up with an industrial-strength simulation software that provides the necessary expressiveness to represent all features of the production process.

The goal is to optimize the solution quality of the schedules as it results from their simulation using the HF model. For the optimization of scheduling models that are formulated as a DES, it is a natural choice to use a simulation-optimization approach (Piana and Engell (2010)). An Evolutionary Algorithm (EA), is used as the optimizer that iteratively improves the allocation and sequencing decisions of the schedules.

Since the simulation times are high for the HF model, we propose to use an additional low fidelity (LF) model, which only needs a fraction of the runtime of the HF model, to steer the search in promising regions and then to perform a polishing step using the HF model. We refrain from using the MILP model as LF model and use a custom schedule builder, as the decomposition-assisted solution procedure proposed in Klanke et al. (2021) only yields a single solution. Due to the differences in the LF and HF simulation model, it is unlikely that this single solution coincides with the best HF solution and it is necessary to explore multiple LF solutions to increase the probability of finding solutions of high quality for the HF model. Within a simulation-optimization framework where both LF and HF models are available, the research question arises how to optimally distribute the total available time budget to evaluations of the two simulation models. Using the LF model only potentially drives the optimization towards a sub-optimal solution, as not all features are represented, but exclusively evaluating the HF model is time-consuming and high-quality solutions may not be found at all before the time budget is exhausted.

Several strategies are investigated in this work to distribute the available time budget among LF and HF evaluations. The first approach (LastGenHF) is that all evaluations by the EA are LF evaluations and the individuals from the last generation are evaluated with the HF simulation model only once and the best solution is applied. The second approach (BlockHF) interleaves evaluations of the LF and the HF models, where after a certain fraction of the total simulation time budget, the evaluations are switched from LF to HF simulations. Using only the HF evaluations (OnlyHF) serves as a benchmark. Finally, we propose an ordinal transformation EA (EAOT), that is applicable to parallelized, generational EAs. In ordinal transformation, the solutions are ranked according to their LF solution quality and grouped into sets of solutions of similar ranks, from which solutions are selected for the evaluation using the HF model. A similar strategy, denoted GAOT, was proposed by Chiu et al. (2016), where mostly LF simulations are performed, but some solutions are chosen for reevalution using the HF model in every generation. The EAOT proposed here differs from GAOT as we apply the same ranking procedure for the selection of survivors, but we keep a record of all ever evaluated LF individuals and reevaluate the best individuals that have not been simulated with the HF simulation model yet every N generations. The HF simulations are performed as a parallelized evaluation of a complete generation of individuals.
In Table 1 a comparison of the results of the four investigated strategies is shown in terms of the best-in-run objective function values and the number of LF and HF evaluations. The results are averaged over 5 independent repetitions each having 3600 s of available computational time. The objective that was optimized was the completion time (CT) of the packaging lines, i.e. the sum of the finishing times of the last packaging operation on all packaging lines.

Table 1: Results of the completion time optimization with the proposed strategies.

Strategy	Mean of CT [h]	Std. dev. of CT [h]	# of HF evals.	# of LF evals.
LastGenHF	284.14	5.39	40	2360
BlockHF	285.85	3.23	120	1760
EAOT, $N = 3$	273.80	2.65	260	820
OnlyHF	274.91	5.00	320	0

The results demonstrate that the additional intermediate evaluation of the HF model in the EAOT algorithm, significantly improves the mean of the best-in-run completion times of the packaging stage compared to LastGenHF and BlockHF. Comparing EAOT to OnlyHF, the observed improvements are smaller, but are achieved with a smaller overall number of expensive HF simulations which becomes important for even more detailed HF models. The limited improvements point to the existence of significant differences in the LF and the HF models. This will be analyzed in more detail in upcoming work.

Keywords: Multi-fidelity Optimization, Make-and-Pack Processes, Industrial Short-Term Scheduling, Simulation Optimization, Evolutionary Algorithm

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Development of EMS with MERLIN: application to a solar thermal power plant with heat storage

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Background and motivation

While 90% of electricity production in France is decarbonised, 80% of heat is still produced from fossil fuels. In a context, using alternative technologies to produce heat and optimal management of utilities are therefore important lever in the fight against climate change but also, a major economic challenge for industry. The incentives to promote renewable energies and waste heat valorization in the energy mix have led to different energy chains. To overcome intermittency and asynchrony of sources and sinks, these energy networks have to include heat storage solution, for which various technological responses are now available. Nevertheless, a common and classical issue when implementing these networks is:

- in the *design phase*, to scale them as accurately as possible, taking into account the dynamics of the overall system in which they will evolve,
- in the *operating phase*, to have appropriate management software, including advanced planning functions, to take full advantage of them.

To meet these expectations, the LGC/PSI has designed a software environment for the implementation of general *CAPE* tools suitable for the optimization and management of systems including *thermal battery*.

Methodology

From a theoretical point of view, the introduction of such features requires the implementation of a *digital twin* of the system under consideration. With this objective in mind, the main challenge of the MERLIN environment is to propose a modelling/optimization methodology articulated around a *description model* allowing the modelling of the material/energy flows and a generic *execution model*. More precisely, one of the founding principles of this work (Thery & al., 2012, Mallier & al., 2021) is to automatically instantiate the mathematical model based on a *MILP* (*Mixed Integer Linear Programming*) formulation from a formal graphical model specified by means of the *ERTN* (*Extended Resource Task Network*). The interest of this level of abstraction is to make the interface between the business representation and the mathematical model used for the resolution and avoids to a large extent the rewriting of the fundamental dynamic equations common to any industrial process.

From a software point of view, the resulting numerical kernel can be either used to realize *what-if* analyses or integrated into new generation *EMS* (*Energy Management Systems*) in order to build real decision-making tools. Indeed, most of the applications available on the market offer real-time monitoring functions (visualization, evaluation of performance indicators), but few of them still include planning functions, which is essential to really optimize the energy performance of such systems.

Problem statement of the case study

The capability and applicability of MERLIN environment have been proven through the implementation of several applications (Mallier & al., 2021) in various industrial sectors. In this paper, we present works concerning the design and the operation of a solar thermal power plant (based on a Fresnel mirror concentrator) coupled with a heat storage (containing a granular porous medium) to compensate for the intermittence of the solar source and thus, offer flexibility in production (figure 1). In order to limit the environmental impact and production costs, the main challenge is to substitute all or part of the carbonised heat consumed by a drying furnace of the food industry with decarbonised renewable heat.

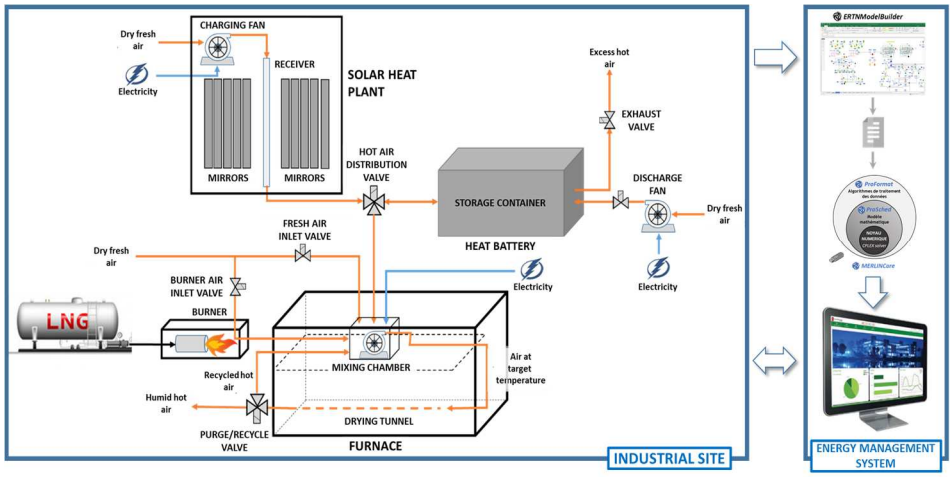

Figure 1 : synopsis of the system

Conclusion

The application developed in this study achieved several operational objectives:

- size the receiver and the thermal battery in a dynamic context, i.e. taking into account the meteorological conditions and the production plans,
- define the decision-making process and the *Energy Management System* of this installation in order to optimally plan and control the whole site,
- obtain significant gains in terms of economics, operational management, energy and avoided CO_2.

Keywords: Energy Management System, Thermal solar power plant, MILP optimization model, graphical modelling formalism.

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Evaluation and comparison of safety criteria on different reactions kinetics

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Abstract

Thermal runaway is one of the biggest issues in chemical reaction engineering. Prevention, detection and control of that event is crucial in order to maintain safety operations in chemical industries.

In order to position the thermal runaway and highlight the importance of studying it. We must illuminate the occurrence of that event. According to (Balasubramanian and Louvar, 2002), more than 26% of accidents in the petrochemical industry are due to the thermal runaway. Moreover, (Dakkoune et al., 2018) analyzed 169 accidental events involving French chemical industries. According to them, thermal runaway was responsible of 25% of the accidents. It seems obvious that these events must be avoided, this can be done, for example, by applying preventive measures based on the use of different runaway criterions capable of predicting the thermal runaway in a system (Zaldívar et al., 2003) (Westerterp et al., 2014) (Guo et al., 2016), therefore the safe and unsafe regions can be conducted for a specific initial and operating conditions of a chemical reaction process. Also, they can be applied in order to specify the optimal operating conditions.

The main objective of the present work is to study the thermal runaway phenomena for a reacting system under batch operating mode by applying various thermal runaway criterions reported in the literature. For a better evaluation of the criterions, two different reaction systems were used for this purpose under different operating conditions. The two reactions were chosen because of their fast reaction rate and high exothermicity, which make them a good model for safety studies.

The calculation software Matlab was used to simulate the process. The ordinary differential equations (ODEs) which represent the mass and energy balance are numerically solved using the Runge-Kutta integration method. In this work, various runaway criterions have been applied to the simulated data and the results obtained have been compared.

According to the results, criterions provide good prediction for thermal runaway but only for specific conditions. Nevertheless, they are too conservative under certain operating conditions and they cannot be applied for the control of industrial reactors. Indeed, they may lead to unnecessary shutdowns. In this work, we found that there was a lack of experimental data on the use of these criteria. For this reason, in our future work, it seems necessary to carry out a safe conduct of a reactor by proposing a reliable criterion based on the previous studies. Of course, a validation of the simulation results by experimental tests on a pilot reactor is in progress.

Keywords: Thermal runaway, modelling, runaway criterion, chemical reactor, safety.

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On-line control of chemical reactor under safe and cost-effective operating conditions.

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Abstract

Different causes have led to major accidents in the chemical industry within which the main percentage is due to thermal runaway in chemical reactors (Dakkoune et al., 2018 https://doi.org/10.1016/j.ssci.2018.02.003). This phenomenon is characterized by an increase in temperature that increases the reaction rate, and that reciprocally produces an increase in the reaction temperature. The main consequences of loss of temperature control are the interruption of operations, destruction of facilities, deaths, injuries, and emissions to the outside. Despite all efforts to avoid these accidents (design of inherently safe processes, hazard analysis, safety barriers, modification of operating procedures), they still occur.

The aim of our work is to reduce the consequences of incidents through on-line control of chemical synthesis processes. In a previous work, the influence of input parameters (reactant concentrations, inlet temperatures and flow rates) on the maximum temperature in continuous reactors (with temperature sensors at many points) has been studied by (Vernieres-Hassimi et al., 2015, https://doi.org/10.1080/00986445.2014.973943). However, in our case we use models to anticipate dangerous situations from reduced information.
The first step of our method is based on the early detection of the loss of thermal control, in a second step we proceed to the isolation of the main causes that triggered it. In this way, (Dakkoune et al., 2020, https://doi.org/10.1016/j.compchemeng.2020.106908) we have developed a method for detecting and isolating faults when a situation arises that could lead to thermal runaway. In order to be representative of a wide variety of real-life situations, we use this method on processes in batch and continuous reactors. We have also developed models of exothermic reactions with different kinetics (fast and slow).
Criteria for the return to stable and safe operating conditions have been defined. The impact on product quality and the cost of the actions taken must also be monitored. Indeed, a desired characteristic is that the quality of the product is not affected by the measures taken to maintain safe conditions. Similarly, the strategy used to ensure the best performance under safe conditions must be economically viable. A decision must be made during the course of the reaction based on the results of this analysis.
It appears that the conditions are very different depending on the kinetics or the type of reactor.

A difficulty for on-line control is the change of model when control actions result in changes of hydrodynamic regime or heat and mass transfer. This last point is the subject of our future improvements.

Keywords: safety, operations conditions, thermal runaway, chemical reactor.

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Plantwide control strategy for a biodiesel production process from *Jatropha curcas* oil with variable composition

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Abstract

Biodiesel is a biofuel composed by fatty acid alkyl esters. It is commonly produced by transesterification of triglycerides and esterification of free fatty acids; both are main components of vegetable oils and animal fats. There is a wide variety of potential oil sources for biodiesel production. The second-generation sources are non-edible sources which avoid competition with human food. Among such raw materials, *Jatropha curcas* oil can be mentioned. An important aspect to consider when designing a biodiesel production process is that each raw material has a different lipid profile and different free fatty acids content. Even for the same kind of oil, the kind of triglycerides and their composition may vary from one batch to the other. This may affect the performance of the production process. Nevertheless, with a proper design-control strategy, a given process can be able to handle with the variations on the composition of the raw material, maintaining the quality of the product. In this work, a strategy for the design and control of a process to produce biodiesel from *Jatropha curcas* oil with variations in the composition of triglycerides of the raw material. First, the process is designed assuming steady state, using the process simulation Aspen Plus V. 8.8, for a representative composition of oil, with 95.5 wt% of triglycerides and 4.5 wt% of free fatty acids. The process includes an acid pretreatment step, followed by neutralization steps. Then, the basic transesterification takes place. A sensitivity analysis is performed for the units with degrees of freedom. Once the steady-state design has been obtained, the simulation is exported to Aspen Dynamics. For the base case, control loops are stablished and disturbances of ±10% are applied to the feed flowrate to test the proposed loops and the parameters of the controllers Then, the compositions on the feed streams are varied, maintaining the same design for the process, i.e., same volume for the reactors and same number of stages and feed stages for the distillation columns. This modification implies that the composition of the *Jatropha curcas* oil changes due to variation in its origin. The effect of these variation on the operation of the process is assessed, and the capability of the proposed control structure to stabilize the process while maintaining the product quality is verified. In general terms, the proposed control structure allows keeping the product with the desired quality in terms of the standard EN 14214.

Keywords: biodiesel, controllability, feed composition disturbance.

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Cascade fuzzy control of a tubular chemical reactor

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Abstract

A comparative study of the cascade control of a tubular chemical reactor using classical fuzzy controllers, type-2 fuzzy controllers, and PID controllers is reported. The main goal is to show that in a cascade control, fuzzy controllers and especially type-2 fuzzy controllers can guarantee energy savings and better performance compared to conventional PID controllers.

Tubular chemical reactors have negative properties from the control viewpoint, as nonlinearity, time delay, asymmetric dynamics, or presence of uncertainty. They are also energy intensive processes, and it is necessary to develop innovative advanced control strategies for them.

Cascade control represents one of the complex control structures, in which advanced controllers can be used. The advantage of fuzzy control is that it can be used successfully for the control of non-linear processes and processes that are difficult to model. The type-2 fuzzy logic controllers were developed to handle uncertainty, which can be due to noise, dynamic changes in the environment, or imprecisions in the process model. The rule base for the interval type-2 fuzzy controller is the same as for the classical fuzzy controller, only its membership functions are represented by the type-2 interval fuzzy sets and a reducer is used prior defuzzification, see e.g. Mendel (2018).

Cascade control with the fuzzy controllers, type-2 fuzzy controllers, or PID controllers was designed for a tubular chemical reactor. The primary controller was a fuzzy PID, a type-2 fuzzy PID, or a conventional PID controller. The secondary controller was a fuzzy P, a type-2 fuzzy P or a conventional P controller. The control performance was evaluated via the integral absolute error IAE and the integral square error ISE. The coolant consumption during control assessed the energy effectiveness of control.

Based on simulation results and values of quality criteria, it can be stated that cascade control with both types of fuzzy controllers assured better results. Application of the type-2 fuzzy controllers guaranteed the most efficient operation of the investigated tubular chemical reactor. The IAE, ISE, and coolant consumption increased only by 1 % exploiting the classical fuzzy controllers. The IAE increased by 37%, ISE by 2 %, and the coolant consumption by 9 % using the conventional P and PID controllers tuned by the Cohen-Coon method.

The type-2 fuzzy cascade control strategy is promising for implementation in practice.

Keywords: cascade control, fuzzy control, PID control, tubular chemical reactor.

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Design and Implementation of an Advanced Optimal Control Framework for Post-combustion CO_2 Capture Proces

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Abstract

The global Greenhouse Gas (GHG) emissions need to peak now and be reduced to net-zero by 2050 to fulfil the Paris agreement [1]. The high penetration of renewable sources into major GHG emitters such as fossil fuel-based thermal power plants will demand for operational flexibility with Carbon Capture and Storage (CCS) to produce clean form of energy soon [2]. Post-combustion CO_2 capture (PCC) processes using chemical absorption of CO_2 in flue gas need to cope with flexible operation and the effect of controlling the CO_2 capture rate under fluctuating flue gas conditions should be studied [2, 3]. Additionally, the development of control approaches accounting for strong interactions among multiple process variables associated with highly nonlinear models of energy systems with PCC is a necessity of the time [4]. To fill this gap, in this work, an advanced optimal control framework is proposed and implemented on PCC with monoethanolamine (MEA)-based CO_2 capture process model simulation in Aspen HYSYS. A two-input-two-output control structure is selected from PCC that consist of flue gas flow rate and lean MEA flow rate as the input/manipulated variables while CO_2 capture rate and reboiler duty are considered as the output/controlled variables. Open-loop simulations are performed in which simulated step tests are designed by individually moving the input variables as steps and collecting the resulting data for the output variables. The classical autoregressive model with exogenous inputs (ARX) method is used for deriving the data-driven simplified dynamic model that can be embedded inside the gradient-based optimal control solver named dynopt (DYNamic OPTimization) in MATLAB to compute control moves via total discretization with orthogonal collocations on finite elements for simultaneous control of both output variables. The obtained control laws are implemented as the setpoints for Proportional-Integral-Derivative (PID) controllers of the input variables existed in the simulation by employing MATLAB-Aspen HYSYS link. The results are compared to the standalone PID controller implementations in terms of the time required to reach new steady state and the output setpoint tracking error. The proposed approach improves the overall performance of the process resulting in faster and flexible setpoint tracking during hypothetical load variation when PCC is integrated with power plant and thus providing a promising alternative.

Keywords: CCS, Process Control, Energy Systems.

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Data Driven Process Monitoring, from Fault Detection and Diagnosis Points of View, in Industry 4.0 Context

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Abstract

Industry 4.0 context refers to robust computation mainly via employing networked information-based technologies. It is considered the last revolutionary step in industrial history that significantly enhances the process quality and products.
Process monitoring has been a critical mission in the industrial chronicle and may include a wide distinct range of actions and reactions through simple statistical models to advanced complex hybrid frameworks. Traditional process monitoring methods cannot efficiently deal with the huge, diverse, and heterogeneous data produced rapidly due to employing industry 4.0. Process monitoring methods need revolutionary enhancement in the accuracy, computational capacity, and flexibility to handle Big Data to keep up with newly emerged technologies.
In this paper, the Fault Detection and Diagnosis (FDD) scheme, as a core part of the process monitoring system considering industry 4.0 requirements, is reviewed. Furthermore, to represent the adequate industry 4.0 FDD framework, different applied technologies related to industry 4.0 are studied.

Keywords: Industry 4.0, Process Monitoring, Big Data Analytic.

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Safe Reinforcement Learning for Batch Process Control and Optimization

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Abstract

Reinforcement Learning (RL) controllers have attracted a lot of interest within the control community with case study demonstrating application in the domains of control, online optimization, production scheduling and supply chain. The main allure of RL controllers relative to existing methods is their ability to optimize uncertain systems independently of explicit assumption of process uncertainty or the manner in which it propagates as the process evolves. Recent focus within the control and process systems community has been in the domain of safe RL. Safe RL primarily considers the satisfaction of constraints, process model-mismatch and epistemic uncertainty in the control function. Previous methods have translated the concept of constraint tightening from the domain of stochastic model predictive control for constraint satisfaction. Here, these approaches are further extended to consider plant-model mismatch. In particular, we propose a data-driven approach that leverages Gaussian processes for the offline simulation. It is proposed to leverage the posterior uncertainty prediction to synchronously account for joint chance constraints and plant-model mismatch. The method is benchmarked against nonlinear model predictive control in case study. The results demonstrate the ability of the methodology to account for process uncertainty, enabling satisfaction of joint chance constraints even in the presence of plant-model mismatch.

Keywords: Safe Reinforcement Learning, Optimal Control, Dynamic Optimization, Bioprocess Operation, Machine Learning.

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Support Vector Machine-based Design of Multi-model Inferential Sensors

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Abstract

Nowadays, there is an increasing need for the monitoring of industrial variables by linear inferential (soft) sensors. Complexity and non-linear behavior of the processes usually reduce the prediction accuracy of the sensors. Thus often, a single soft-sensor model cannot explain the behavior of the desired variable. In such a situation, designing a multi-model inferential sensor is a way to increase the sensor prediction accuracy and to preserve its linear structure. This research aims to develop an effective design method of multi-model soft-sensors together with the switching logic between the models. As a guiding example, we design a sensor to infer the value of pressure compensated temperature that is often used in the petrochemical industry (King, 2016).

A standard methodology (Shuang and Gu, 2016) approaches the problem in a sequential manner. In the first step, an unsupervised machine learning algorithm (e.g., *k*-means clustering (Forgy, 1965)) is used to classify the available data into training subsets of the desired number of models. In the second step, a supervised machine learning algorithm (e.g., support vector machine (SVM) (Boser et al., 1992; Bredensteiner and Bennett, 1999)) is used to determine the regions of validity (switching logic) of the models, and each model is finally trained. The main disadvantage lies in the use of unsupervised learning that does not take into account final model accuracy.

In this research, we introduce a simultaneous approach, which finds the SVM-based classifier and the models of the inferential sensor in one shot. The resulting multi-model sensor is optimal. The mathematical formulation relies on mixed-integer quadratic programming (MIQP). The increased problem complexity, compared to the sequential approach, is the price to pay for the more accurate sensor. The effectiveness of the multi-model inferential sensors design is investigated in two scenarios; the measurements are easy (scenario A) and difficult (scenario B) to classify into the models of the inferential sensor. The results demonstrate that the inferential sensors with multiple models are more accurate than the single model sensor. Moreover, the simultaneous inferential sensor design outperforms the prediction accuracy of the sequential approach.

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Data-driven robust model predictive control for the greenhouse adjustment and crop production under uncertainty

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Abstract

Greenhouse cultivation targets providing protection to the plantations from severe weather and become a way to achieve controlled agricultural production. The appropriate control of the climate within the greenhouse can lead to the growth of potential yields and the extension of the growing season. (Bennis et al., 2008). Model predictive control (MPC) has been acknowledged as a suitable control strategy to solve the problem of regulating the climate and growth processes, plus MPC can also guarantee the fulfillment of the constraints specification (Camacho and Alba, 2013). On the other hand, robust MPC (RMPC) can be built to deal with uncertainty. One of the promising methods is from (Ning and You, 2018), which constructed the data-driven robust optimization framework using principal component analysis (PCA) in conjunction with kernel density estimation (KDE). PCA is capable of capturing the correlations between uncertain parameters and identifying the uncertainty sources. Meanwhile, KDE can help in extracting distributional information of latent uncertainties which are projected onto each principal component (Ning and You, 2018). In this work, we propose a novel data-driven RMPC framework that minimizes greenhouse energy consumption and maximizes crop production under uncertain disturbances. To develop the state-space model (SSM) required for the proposed MPC, we start by studying the dynamics of the greenhouse based on the building geometry and dynamics. Afterward, we use data-driven techniques and system identification methods to construct the SSM and then incorporate the SSM into the proposed data-driven RMPC framework. Based on the proposed dynamic SSM model and the data-driven uncertainty set, we propose a novel data-driven RMPC framework, which is capable of controlling the greenhouse's temperature, humidity, CO_2, and light.

Keywords: Robust Model Predictive Control, Greenhouse, Uncertainty

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Study on the noise contents of different measurements in industrial process and their impact on process monitoring

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Abstract

As a large amount of industrial data is acquired by distributed control system (DCS), data-driven process monitoring methods have attracted a significant research interest. However, various types of noise are also collected with signal together from process, instruments and data transformation, which could compromise the information of signal itself and provide a huge challenge for data analysis and modeling. Moreover, noise contents of different measurements such as temperature measurements, pressure measurements, flow measurements, and etc., may be also varied in industrial process. Therefore, the selection of decomposition scale has a great influence on the denoising effect, while among methods reported in the literature, the decomposition scale is usually constant for all measurements in a process.

In this research, a novel standard to characterize an optimal denoising depth for each measurement is proposed. wavelet decomposition is first selected to extract the high-frequency features of signals in different measurements for its ability to retain the local characteristics of signals in both time and frequency domains. Then information entropy is applied as a standard to characterize the depth of wavelet decomposition. An optimal decomposition scale is determined by maximizing the retention of original signal information in each measurement. According to this standard, signal in each measurement can be processed individually according to its optimal decomposition scale. Then the processed data can be further applied to a multivariate statistics method for a more effective process monitoring. In order to verify the effectiveness of this method. The research is implemented on an industrial naphtha cracking process. The results show that abnormal operational conditions can be detected earlier on the basis of a lower false alarm rate compared to other methods, by which the difference in noise characteristics of each type of measurement isn't considered.

Keywords: wavelet denoising, process monitoring, information entropy, naphtha cracking process

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A Comparative Study on the Influence of Different Prediction Models on the Performance of Residual-based Monitoring Methods

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Abstract

As a representation of the difference between observed and expected behaviors, residual has been widely used in monitoring methods based on the mechanism models, but the accurate mechanism models of certain complex processes are hard to obtain. With the rapid development of artificial intelligence, the accuracy of data-driven prediction models has been significantly improved, which makes it possible to reflect a certain status of the process by data-driven models instead of mechanism models. The residuals between status estimates of data-driven models and observations can be calculated to indicate status changes in the process. Therefore, residual-based multivariate statistical models are established for faults detection. Quite a few data-driven monitoring methods based on predicted residuals have been proposed (T. Lan, C. D. Tong & H. Z. Yu, 2020; C. D. Tong, T. Lan & H. Z. Yu, 2019; S. F. Alvar, B.F. Javier, S. P. G. Ismael, B. J. Manuel & F. M. Chemometrics, 2018). However, the influence of different prediction models on prediction residuals and monitoring performance hasn't been fully discussed. Referring to the above issue, various data-driven prediction models including PLS, SVM, and LSTM are applied in the Tennessee Eastman (TE) process and a real industrial case to study the influence of prediction models, evaluation indicators, distribution of prediction residuals on monitoring performance. A statistical analysis on corresponding residuals is also conducted to investigate its impact to monitoring performance. Accordingly, a select strategy of prediction models is carried out to improve the performance of residual-based monitoring methods. Based on the proposed strategy, the prediction model is confirmed and integrated with monitoring methods based on prediction residuals to achieve the best performance.

Keywords: Multivariate linear regression, Time series modelling by LSTM, SVM (Support Vector Machine), Selection strategy of prediction models, Statistical feature of residuals

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Optimal operation of parallel mini-bioreactors in bioprocess development using Multi-Stage MPC

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Abstract

Bioprocess development is commonly characterized by long development times, especially in the early screening phase. After promising candidates have been pre-selected in screening campaigns, an optimal operating strategy has to be found and verified under conditions similar to production. Cultivating cells with pulse based feeding and thus exposing them to oscillating feast and famine phases has shown to be a powerful approach to study microorganisms closer to industrial bioreactor conditions. In view of the large number of strains and the process conditions to be tested, high-throughput cultivation systems provide an essential tool to sample the large design space in short time. We have recently presented a comprehensive platform, consisting of two liquid handling stations coupled with a model based experimental design and operation framework to increase the efficiency in High Throughput bioprocess development. Using calibrated macro-kinetic growth models, the platform has been successfully used for the development of scale-down fed-batch cultivations in parallel mini-bioreactor systems. However, it has also been shown that parametric uncertainties in the models can significantly affect the prediction accuracy and thus the reliability of optimized cultivation strategies. To tackle this issue, we implemented a multi-stage Model Predictive Control (MPC) strategy to fulfill the experimental objectives under tight constraints despite the uncertainty in the parameters and the measurements. Dealing with uncertainties in the parameters is of major importance, since constraint violation would easily occur otherwise, which in turn could have adverse effects on the quality of the heterologous protein produced. Multi-stage approaches build up a scenario tree, considering the uncertainties and calculate optimal inputs considering the model uncertainties. Using the feedback information gained through the evolution along the tree, the control approach is significantly more robust than standard MPC approaches. We show in this study that the application of multi-stage MPC can increase the number of successful experiments, by applying this methodology to 24 mini-bioreactors cultivated in parallel.

Keywords: high-throughput, model-predictive control, scale-down, multi-stage

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Platform for online system identification and diagnosis of dynamic ultrafiltration systems

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Abstract

Dynamic Micro/Ultra-filtration technology has shown its potential to achieve remarkable separation performance (i.e., selectivity or throughput). Still, the main challenge is how to operate it optimally due to its time-variant nature, occasioned by concentration polarization and membrane fouling, the no-measured high-variance inlet disturbances, and the dynamic system operation. Extensive experiments have been performed for produced water treatment with dynamic ultrafiltration at real field conditions, aiming to determine critical flux operating conditions which sometimes cannot be reliably estimated [Prado-Rubio, O.A. (2012)]. Off-line modelling approaches have shown to be useful for process design but have limitations for optimal operation/control at real conditions [Grisales Díaz, 2017]. Therefore, there is a need for tools to determine the membrane fouling state during operation and thus have a chance to optimize the relatively high energy demanding operation. The purpose of this work is to develop a user-friendly platform (GUI – Matlab®) for monitoring and diagnosis based on online system identification capable of providing a real-time representation of the system, focused on the time-variant fouling rate. The platform uses the Recursive least squared with forgetting factor method to correlate operating conditions (i.e., pressure, flow rates and inlet concentrations) with the obtained membrane flux, thus permeability. The above-mentioned experimental datasets are used for parameter estimation, where data are provided at real sampling time to tune the model. Results indicate that the system identification can be performed in real-time and model prediction have a high degree of experimental data reproduction under different operating strategies (~4% average prediction error). Current efforts focus on investigating the model predictive window and interpreting the results to develop the diagnostic guidelines, relevant to build the tool which can estimate a sustainable membrane system operation.

Keywords: Dynamic Ultrafiltration, online system identification, diagnosis

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Development of a virtual sensor for real-time prediction of granule flow properties

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Abstract

Monitoring the flowability of granules in real-time is critical to producing high quality tablets in a continuous dry granulation line; the granules produced by the roller compactor need to be able to flow consistently into the die of the tablet press. (Becker-Hardt, 2018) Since there is currently no sensor available that can directly measure flowability, monitoring is focused on the density of the compacted ribbon before it is milled into granules. While reasonable, this is not a very comprehensive solution. Other parameters like the configuration and condition of the subsequent milling operation need to be considered, as they can have a significant influence on the final granule properties. To circumvent this problem, the granules need to be measured directly albeit via different properties that are measurable in real-time. These properties need to be highly correlated with flowability, so they can serve as predictor variables together with ribbon density.

In this work, we explore the potential of granule size and shape distribution to be flowability predictors, since they can be measured in real-time using direct imaging techniques, and they have been established to strongly determine powder behavior under stress.(Fu et al., 2012) Flowability will be measured from several methods: shear cell testing, powder rheometery, powder avalanching, flow through an orifice, and tapped density measurements. The diversity of methods is necessary because accurate characterization requires the test conditions to match the expected process conditions experienced by the granules.(Schwedes, 2003) In the case of the tablet press, quasistatic and dynamic flow conditions occur inside the tablet press hopper and the feed frame respectively. This work will proceed in two phases. The first phase will explore the use of data-driven models such as Partial Least Squares Regression to predict the flowability of granules produced by wet granulation; the predictor variables will be granule size and shape distributions measured at-line by a direct imaging particle analyzer. Then, the monitoring effectiveness of the resulting sensor model will be tested in the second phase by configuring the same tool to take continuous in-line measurements of granules exiting a roller compactor.

Keywords: virtual sensor, monitoring, flowability, machine learning, size and shape distribution

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A Hierarchical Approach to Monitoring Control Performance and Plant-Model Mismatch

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Abstract

Controllers are often tuned during plant commissioning, with a fixed process model. However, over time degradation can be expected in both the process model and controller, making it necessary to either re-tune the controller or re-identify the process model. Authors have proposed a variety of approaches to identify plant-model mismatch and control performance degradation. These include transfer function-based approaches by Wang et al. (2012), partial correlation coefficient (PCC)-based approaches by Chen and Ierapetritou (2020), covariance-based approaches by Yu and Qin (2008), and control strategies that also include estimation, e.g., moving horizon estimation-based nonlinear model predictive control (MHE-NMPC) frameworks by Huang et al. (2010) to further handle plant-model-mismatch. While each approach may have their own advantages and disadvantages, it is important to note that they are designed to function on different time scales. Transfer function-based approaches require model re-identification in order to determine loop robustness through analytical studies, and are time-consuming and may only be feasible during periodically scheduled maintenance. It is therefore essential to utilize alternative approaches that can be implemented on shorter time scales using closed loop operating data to identify control performance degradation and plant-model mismatch, e.g., the PCC-based and covariance-based approaches. Applications with quicker dynamics, e.g., continuous pharmaceutical manufacturing lines, require immediate action on an even shorter time scale to handle plant-model mismatch caused by uncertain model parameters, and this can be achieved through efficient control frameworks, i.e., MHE-NMPC. The differing time scales result in the need for a 3-level hierarchical approach to monitor, detect, and manage plant-model mismatch and control performance degradation, as illustrated through a continuous pharmaceutical manufacturing application, i.e., a direct compression tablet manufacturing process. This work also highlights the need for index-based metrics to allow the impact of plant-model mismatch and control performance degradation to be quantified in order to carry out fault diagnosis through root cause analysis to guide maintenance decisions for continuous manufacturing industries.

Keywords: control performance monitoring, plant-model mismatch, nonlinear model predictive control, process monitoring and control

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Optimal Control Policies of a Crystallization Process Using Inverse Reinforcement Learning

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Abstract

Crystallization is widely used in the pharmaceutical industry to purify reaction intermediates and final active pharmaceutical ingredients. Efficient control of crystal properties such as: size distribution, purity, and polymorphism is critical to ensure the targeted quality and efficacy of the final pharmaceutical product (Benyahia, 2018). Despite the significant advancements in crystallization process control, there is still an increasing demand for more robust and versatile control strategies that can deal with uncertainties and deliver self-optimizing capabilities. Such motivations have been the driving factor for the implementation of AI-based and data-driven techniques such as: Reinforcement Learning (RL) and Inverse Reinforcement Learning (IRL) combined with Transfer Learning (TL) and Apprenticeship Learning (AL) approaches (Petsagkourakis et al., 2020; Mowbray et al., 2021). In this work, we consider the implementation of an IRL approach where an agent observes the expert's demonstration of the control task and attempt to mimic its performance. In essence, an apprenticeship learning setup was developed where an expert demonstrates the control task to the IRL agent to help attain near optimal performance when compared to the expert. This is achieved through repeated execution of "exploitation policies" that simply maximizes the rewards over the consecutive RL training episodes. The cooling crystallization of paracetamol is used as a case study and both proportional integral derivative (PID) and Model Predictive Control (MPC) strategies were considered as expert systems. A model-based IRL technique is implemented to achieve effective trajectory tracking which ensures final crystal size, considered as the critical quality attributes, by reducing the deviation from the optimal reference trajectories namely process temperature, supersaturation, and particle size. The performance of the trained IRL agent was validated against the PID and MPC and tested in presence of noisy measurements and model uncertainties.

Keywords: Apprenticeship Learning; Transfer Learning; Reinforcement Learning; Inverse Reinforcement Learning; Batch Crystallization.

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Comparative study of optimal operation strategies for an industrial bio-production case

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Abstract

The interest in the industrialization of bio-production is increasing due to the search of alternatives to fossil feed-stocks. Bio-production is mainly performed in fed-batch cultures to ensure sterile conditions and achieve good performances by the controlled manipulation of feeding profiles, which have an impact on yield, liquid volume, productivity and fermentation times Ashoori et al. (2009). Kinetic models can be of great use to help with the scale-up of fermentation and, at the same time, provide information about the microbial kinetics Riascos and Pinto (2004). In this work, we have studied the bio-production of a chemical of interest (D), which is produced after two sequential phases. First, the microorganism X grows in a carbon substrate S (e.g. sugar) to be later used as a catalyzer to convert a substrate A into a product D following the pathway: $C \rightleftharpoons A \longrightarrow B \longrightarrow D$.

A dynamical model was developed to describe the kinetics of the growth and conversion phases. This model is based on the data obtained from laboratory experiments. The experiments were performed at controlled temperature, pH and oxygen conditions. The model is developed using mass balances and kinetic expressions to describe the dynamic behavior of the most important variables of the process (e.g., inputs/outputs). Furthermore, the microorganism in the system exhibits a certain particularity such that the production of the chemical slows down and almost stops when the cell is saturated with the product. The moment of saturation is called the tipping point, at which the intermediate products B and C are formed hampering the enhancement of the production of the chemical (D). The dynamic model considers Monod kinetics with down regulation kinetics for the bio-production of the chemical Bernard (2011) for the reactions going from A to D in order to detect the tipping point. The kinetic terms have the form $r = r^{max} \frac{A}{K_A + A} \left(1 - \frac{D/X}{\alpha}\right)$, where r^{max} and K_A are the maximal production rate and the saturation constant, respectively; and α indicates the value of the ratio D/X at which the tipping point occurs. Independent experimental data sets were used to calibrate and validate the model parameters. Model simulations have proved to be useful to understand and to predict the tipping point. Given that overfeeding can saturate the microorganism and inhibit the production of the main chemical while inducing the formation of undesirable by-products, control laws have been developed to avoid the occurrence of the tipping point. Different configurations have been tested in simulation to maximize the concentration and productivity of the chemical. The optimization was performed in two steps: (i) maximization of biomass in a growth phase (regulation of the input of S) and (ii) maximization of the chemical (D) in a conversion phase (feeding of S and A). Four options have been tested considering larger scales. The model was adapted to a larger scale to consider higher input flows under the assumption that the mass transfer coefficient ($k_L a$) was constant. The tests considered a growth phase (GP) either in batch conditions or in fed-batch operation with maximization of biomass followed

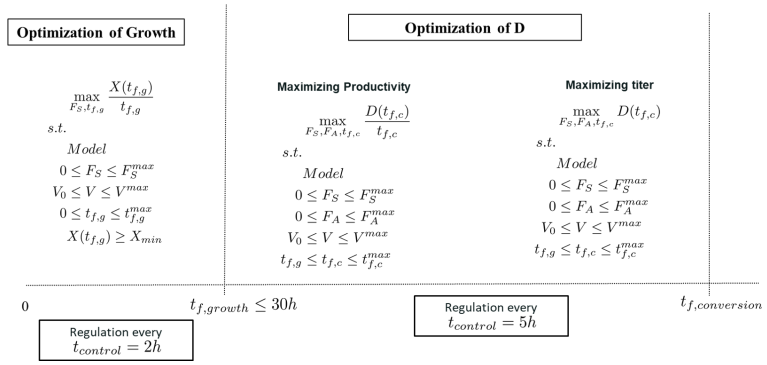

Figure 1: Optimization approach.

Table 1: Results of optimization

		Units	Opt 1	Opt 2	Opt 3	Opt 4
Biomass after growth	X_g	(gX)	22.69	20.85	22.69	20.85
Time of growth	t_g	(h)	22.44	24.96	22.44	24.96
Final time	t_f	(h)	98.5	118.97	92.49	102.97
Concentration	$D(t_{f,c})$	$(mmolD/L)$	172.49	177.09	170.24	172.24
Productivity	$D(t_{f,c})/t_{f,c}$	$(mmolD/L-h)$	11.22	9.54	11.79	10.71
Total sugar	S_{Total}	$(Kg\ S)$	14296	10994	9287.8	10394
Total A	A_{Total}	$(kmolA)$	782.55	802.48	754.92	778.95
Final Volume	V_f	(m^3)	748.64	749.83	725.22	736.75

by the maximization of either the titer or the productivity of *D*. The cases were: (Op1) GP in fed-batch + maximization of titer; (Op2) GP in batch + maximization of titer; (Op3) GP in fed-batch + maximization of productivity; and (Op4) GP in batch + maximization of productivity. Simulations for the optimization were carried out to solve the control objectives displayed in Figure 1 subject to the specific constrains on each step. The obtained optimal inputs were applied to the system for a period of $t_{control}$ until a final time (t_f 120h), the maximum volume (V^{max}) or the tipping point is achieved. The results reported in Table 1 have shown that the best option was Op3 which includes maximization of productivity starting with more biomass from the growth phase. This implies less time, more product and lower utilization of substrates. Each of the analyzed options present a different feeding profile for both inputs in which the saturation of the cell is always avoided. In most of the results, the final batch time (t_f) was the time at which the tipping point occur. The feeding of both inputs stops at t_f to avoid the formation of by-products. However, in real application a longer operation time must be considered to deal with the emptying of the bioreactor. Although the study is implemented for a large lab scale process, it also provides insights for large scale production.

Keywords: bio-production, optimization, feeding profiles, cell saturation

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Dynamic Real–Time Optimization with Closed-Loop Prediction for Nonlinear MPC–Controlled Plants

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Abstract

Current trends toward globalization and electricity market deregulation are requiring increasingly dynamic operation of chemical processes. Single and two-layer approaches have been proposed for economic optimization of the plant performance (Ellis et al., 2014). In the former, computation of the control action and economic optimization are performed simultaneously, whereas in the latter, economic optimization is performed by a dynamic real–time optimization (DRTO) module that provides set-points to an underlying regulatory control system, typically model predictive control (MPC). Jamaludin and Swartz (2017) propose a two-layer DRTO formulation in which the closed-loop dynamics of the plant under the action of constrained MPC are taken into account at the DRTO level, resulting in improved economic performance. Most two–layer approaches assume that the plant is controlled by linear MPC. However, linear controllers may perform poorly for highly nonlinear processes and large transitions, for which cases nonlinear model predictive control (NMPC) is generally considered a better choice.

In this paper, we develop a DRTO formulation for plants controlled by NMPC. It utilizes a prediction of the plant under the action of constrained NMPC. At every prediction time-step, an NMPC problem is solved to compute the control action used in the dynamic process model. This representation yields a multilevel optimization problem that is reformulated as a single-layer problem by replacing the embedded NMPC subproblems by their Karush-Kuhn-Tucker (KKT) conditions. However, this solution approach assumes convexity of the NMPC problem, which we analyze for a class of single–input single–output NMPC problems that utilize a quadratic objective function, and for which the dynamic models are affine in the inputs. We show conditions under which the first-order KKT conditions are both necessary and sufficient for optimality.

Performance of the proposed method is demonstrated through case studies. The equivalence of the NMPC solution using the KKT conditions versus that generated via direct optimization of the primal problem is established, and the performance of two-layer DRTO with embedded NMPC subproblems for set-point target tracking as well as economic optimization is demonstrated. Avenues for future work are identified.

Keywords: NMPC, DRTO, convexity, economic optimization, KKT conditions

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Dynamic Real-Time Optimization of a solar thermal plant during daytime

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Abstract

Solar thermal plants are operated in a complex environment, where both the energy source and demand are time-varying. Solar resource is intermittent, with daily and seasonal variations. The meteorological conditions are difficult to predict accurately and have a great impact on the solar heat production. Furthermore, there is a time gap between the production and the consumption of solar heat in most applications such as domestic hot water, space heating and industrial use. A storage tank can be added to the solar field in order to improve the flexibility of the plant and to transform solar heat into a dispatchable energy. However, this supplemental degrees of freedom further increase the complexity of the operation of a solar thermal plant.

Economic dynamic optimization has been used to find the best operation of a solar thermal plant, based on weather and load forecasts. For transient systems, with unknown disturbances, Dynamic Real-Time Optimization (DRTO) seems better suited. DRTO is well known in the chemical engineering community and has been used to optimize processes that never reach steady-state, such as batch reactors. However, this approach is fairly new in the field of solar energy. Since solar systems are always in transient behavior, DRTO is a promising method to operate them. If this methodology has been implemented in order to optimize the operation of a concentrated solar field, it has never been applied to a solar thermal plant. The latter operates at lower temperatures, uses a different technology to collect solar radiation and sells heat instead of electricity. Moreover, a non-concentrating solar field presents slower dynamics. This contribution will fill this gap and show the benefits of using an economic DRTO to operate the solar field of a solar thermal plant.

A physical model solved in Matlab is used to represent the real solar thermal plant, subject to disturbances. It regularly calls a second model, used for the dynamic optimization and implemented in the Gams environment. The dynamic optimization solves a NLP problem obtained by temporal discretization of the model equations, through Orthogonal Collocation on Finite Elements. The optimal trajectories for the controlled variables are sent to the controllers of the simulation which track the reference trajectories and reject disturbances as they appear in the process. Before each new optimization run, the state of the system as well as the current weather data are sent to the optimizer.

This work presents the first results obtained for the DRTO of the solar thermal plant during daytime. They show an improvement of the quantity of heat delivered and the economic benefits achieved, compared to the classic operation of the plant and the offline dynamic optimization. These results provide good perspectives for the implementation of DRTO over a longer time period.

Keywords: Dynamic real-time optimization, solar thermal energy, simulation

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Online Bayesian Re-design of Parallel Experiments based on Asynchronous Posterior Sampling

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Abstract

Aim and Scope - In bioprocess development, dynamic modeling should face significant levels of epistemic uncertainty in both structure and parameters which makes probabilistic models of the bioreactor the alternative of choice (Martinez, et al. 2021). High Throughput mini-bioreactor systems for intensive experimentation help gathering informative data sets to achieve different modeling or optimization goals by resorting to on-line redesign of asynchronous parallel experiments (Cruz Bournazou et al., 2016).
Study Design / Methods/Case Study - In a Bayesian setting, a probabilistic (causal) model is learned based on data gathered in a sequence of planed interactions between a Bayesian modeling agent and a biological system. Based on its beliefs about the parameter distributions and model structure, the agent only takes the first action of the planned sequence to maximize the information content of probable future states in the most rewarded state trajectories. In this work, a novel algorithm that combines Asynchronous Thompson Sampling (ATS) of model parameter distributions with Bayesian Optimization is proposed. Once new data are available, model parameter distributions are first updated using variational inference. Posterior Thompson sampling is then used to propagate beliefs to assess the expected information gain of changing the cultivation conditions in different bioreactors. A recombinant E. coli expressing a fluorescent protein is used as a model organism. The chosen goal for re-designing an experiment is biasing operating conditions to maximize productivity.
Major Results / Findings - Results obtained demonstrate that combining Bayesian optimization with asynchronous Thompson sampling is an efficient alternative for balancing exploration with exploitation in parallel on-line experimental re-design.
Conclusion - Simulation results obtained for a robotic platform with 48 parallel mini-bioreactors highlight that on-line redesign decisions aim to explore aggressively initially when the variances in parameter distributions are large. As more informative data are available, most of parallel experiments are steered towards process optimization.

Keywords: Bayesian inference, Bioprocess optimization, Experimental re-design, Posterior sampling, Probabilistic Models.

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Dynamic optimisation and comparative analysis of perfusion and fed-batch bioreactor performance for monoclonal antibody (mAb) manufacturing

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Abstract

Integrated continuous bioprocessing (ICB) holds great promise towards achieving higher efficiency, a critical target for ensuring the advent of biopharmaceutical manufacturing. Culture productivity must be drastically improved to reduce production cost projections, especially in comparison to traditional fed-batch process platforms (Pollock et al., 2017).

The present paper explores the benefits of continuous bioprocessing, employing dynamic optimisation of upstream fermentation for production of monoclonal antibodies (mAb). Industry-standard cultures of Chinese Hamster Ovary (CHO) cells have been used to develop models of mAb bioreactor operation (Karst et al., 2017; Kishishita et al., 2015). These models tracks several state variable trajectories of interest, including concentration profiles for CHO cells, substrates, by-products and biopharmaceutical targets (mAbs).

Dynamic optimisation of both operation modes (fed-batch and perfusion bioreactors) has been undertaken, with the objective function of maximizing the final mAb product titers and comparatively analyse optimal feeding strategies for improved culture proliferation. The clear differences in terms of reactor space (capital costs) and time (operating costs) are highlighted, and a fair comparison basis is established so as to evaluate performance. For both modes of operation, a technoeconomic analysis illustrates the implications of optimal bioreactor designs, with a view to systematic decision making in mAb ventures.

Keywords: Biopharmaceutical manufacturing; monoclonal antibodies; dynamic optimisation.

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Control of an industrial packed extraction column for biodiesel washing

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Abstract

A recent trend in the biodiesel industry is the increasing incorporation of waste cooking oil and other low-quality fatty materials motivated by economic and regulatory factors. This trend causes the formulations of raw oil to change significantly, requiring process flexibility and adequate control systems to maintain the product within strict quality standards and prevent operational problems.

In the homogeneous alkali processes, currently the most common in the industry, the separation stage includes the water washing of biodiesel to extend the removal of glycerol, methanol, and acylglycerols (Zhang et al., 2003; Granjo et al., 2017). This operation is accomplished in an extraction column. In practice, subtle changes in the oil composition (i.e., incomplete reaction, soaps, or fine solids in suspension) can promote the formation of stable emulsions that need to be handled before causing shutdowns and extra manufacturing costs. Consequently, a high-fidelity dynamic model of the extraction column is valuable for control and troubleshooting.

The present contribution addresses the design of feedback controllers and model predictive control for a packed extraction column for biodiesel washing based on a pseudo-homogeneous dispersion model. This dynamic model was developed in gPROMS® ModelBuilder and validated against data from an industrial unit.

The operation of the extraction column was simulated for the following scenarios: change in biodiesel composition; contamination in biodiesel inlet; and change in glycerol concentration in the washing water inlet. The impact of these disturbances on the column hydrodynamics (e.g., the existence of flooding, phase inversion) and product quality was analyzed. Finally, the performance of the conventional and predictive control approaches was compared by testing the system in closed-loop.

Keywords: Biodiesel, Liquid-liquid extraction, Process Control, Dynamic simulation

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Development of mechanistic reduced order models (ROMs) for NMPC control applications in continuous manufacturing of pharmaceutical solid-dosage forms

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Abstract

As the pharmaceutical industry transitions from batch to continuous manufacturing, real-time monitoring and mechanistic model-based control are essential to conform to FDA quality standards. Glidants and lubricants are known to affect the Critical Quality Attributes (CQAs) of a tablet such as tensile strength, tablet porosity and dissolution profile (Razavi et al. (2018), Apeji and Olowosulu (2020)). Quantitative models for predicting these effects are essential for enabling centralized control strategies of lubricant and glidant feeding and blending in direct compression tableting lines. This work presents the development of mechanistic reduced order models to capture the effects of lubricant (Magnesium Stearate) and glidant (silica) on CQAs and Critical Process Parameters (CPPs). A Latin Hypercube experimental campaign with thirty different mixing conditions of silica with MCC (Avicel PH200) and APAP (Acetaminophen) was carried out using a Natoli NP400 tablet press and a SOTAX AT4 tablet tester. Experiments show that the tensile strength and blend bulk density are significantly affected by the mixing conditions of silica. Similarly, adding Magnesium Stearate (MgSt) changes the bulk density of the blend, compaction force required to form a tablet, and tensile strength of tablet, depending on the lubrication conditions (Mehrotra et al. (2007), Razavi et al. (2018)). The models were calibrated with the experimental data and then implemented in an NMPC framework to demonstrate the potential of integrating glidant feeder/blender and tableting to control tablet CQAs in continuous manufacturing. This integration also helps to achieve process steady state conditions faster, and minimizes off-specification tablets during transient processing conditions.

Keywords: Lubricant effects, glidant effects, Model Predictive Control, continuous pharmaceutical
manufacturing

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Health-aware controller using hybrid models applied to a gas-lifted oil well network

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Abstract

In subsea oil and gas production systems, unexpected breakdowns and maintenance interventions are costly. To avoid equipment wear, engineers often adopt a conservative production strategy leading to profit loss (Verheyleweghen and J¨aschke, 2017) . Hence, there is a trade-off between maximizing production and minimizing equipment degradation in subsea production systems that needs to be addressed such that optimal operation from an economic point of view is guaranteed.

This paper uses a health-aware controller (HAC) (Escobet et al., 2012) strategy to deal with this problem. In HAC, prognostics and health monitoring (PHM) are integrated into the control structure to avoid conservative operation by actively steering plant degradation and preventing violation of health constraints. In the subsea oil wells, choke valves are the critical equipment. Obtaining accurate first-principle models for PHM of these valves is challenging (DNV, 2015). We then propose a hybrid HAC that combines first-principle transport phenomenon models with the data-driven valve PHM models from Jahren et al. (2021), which use different pressure, flow and temperature measurements along the wells for predicting the current valve degradation state.

The hybrid HAC is applied to a synthetic case study of an oil and gas well network with artificial gas-lifting. We test two different data-driven model structures, a simple linear regression and a neural network model. We investigate their performance in open-loop, carrying out an uncertainty analysis using historical data to check the effect of poor degradation diagnosis (i.e. degradation estimates used as the controller state observer), as well as in closed-loop. The simulation results show that hybrid HAC is a possible alternative for dealing with the mentioned trade-off. However, plant-model mismatch had a detrimental effect on its performance. The main conclusion is that HAC's performance is dependent on the type of data-driven PHM model and the quality of the feedback from diagnostics. Nevertheless, the complexity of the chosen data-driven models does not necessarily give a better overall result.

Keywords: Model predictive control; Hybrid Modeling; Diagnostics and prognostics

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Applying Ecological Interface Design for Modular Plants: Safety-Demonstrator Case Study

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Abstract

A promising approach to reduce the time to market of chemical products is the application of modular plants, which are composed of standardized, previously developed Process Equipment Assemblies (PEAs) (Mädler et al., 2021). As this approach goes along with process intensification as well as continuous and highly autonomous operation, human operator performance might benefit from a more structured guidance to fully understand the system and interact with it whenever it is necessary. With the major goal of reducing human error, Vicente and Rasmussen (1992) introduced the Ecological Interface Design (EID), suggesting that an interface should provide a virtual ecology, connecting the work domain to the human operator. EID is based on a 2-dimensional Abstraction-Decomposition Space (ADS), resulting in a structural decomposition of the plant, and also categorized information about the actual phenomena taking place in the process (which explains how each component in modular plant is working).

In this study, the effects of applying EID for modular plants is investigated. To this end, a pilot modular plant, namely Safety-Demonstrator, is considered as the use case, which consists of a total of two PEAs: one for dosing the reactants and the other one for the reaction (Pelzer et al., 2021). Considering the fact that each PEA is a separable process, we can develop an ADS for it, and then connecting them to get the ADS for the whole process. This developed ADS, which also consists of the explanation of the phenomena taking place in each component, not only helps operator understanding the system and making better decisions in challenging situations, but also facilitate exploiting the changeability feature of MPs and selecting the best PEAs for a specific function of the process.

Keywords: Modular Plants; Ecological Interface Design; Safety-Demonstrator Case Study

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Feature engineering for machine learning-based oscillation detection in process industries

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Abstract

Process industries frequently encounter oscillations in control loops. Oscillations often indicate a more severe problem than irregular variability. The presence of oscillations in a control loop increases the deviations from the setpoint of the process variables, thus causing inferior products, larger rejection rates, increased energy consumption and reduced average throughput. Several machine learning (ML)-based techniques have been proposed for oscillation detection and diagnosis. Dambros et al. (2019) presents a deep feedforward network for automatic oscillation detection using frequency domain data as input features and has gained popularity in the recent years. Although the technique is shown to have high accuracy in detecting oscillations, the ML model uses 4097 input features and thus have a very large set of weights making it a computationally expensive method. Optimization of hyperparameters is also difficult due to large size of neural network. In this article, various feature engineering and feature selection strategies are adopted to reduce the computational efforts of ML-based approaches for oscillation detection. Feature selection based on peaks in the frequency domain data is used. Further, a sensitivity study is conducted to find the optimal number of input feature. The outcome shows that the accuracy and confusion matrix saturate after optimum number of input features (401) and is computationally more efficient as compared to taking entire deep feedforward network. It was observed that there is negligible reduction in accuracy by reducing the input features from 4097 to 401. Feature selection using the same approach was carried out for the quantification of number of periods and oscillation amplitude. Further, the accuracy in detecting oscillations were improved by including various features like zero crossings, FFT (Fast Fourier Transform) of ACF (Autocorrelation function), variance in data etc.

Keywords: Oscillation detection, Feature selection, Feature engineering, Machine learning, Neural network

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Multiparametric Model Predictive Control Strategies for Evaporation Processes in Pharmaceutical Industries

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Abstract

Due to their complex nature, pharmaceutical plants are required to operate near operational constraints with very strict product quality specifications and deal with complex and highly integrated processes, varying production targets, raw material variability and process/model uncertainty (Ierapetritou, Muzzio et al. 2016, Su, Ganesh et al. 2019). Using model based control approaches greatly affects the time and resource utilization for the development process; certain pharmaceutical process design problems, under assumptions, can be transformed into process control problems(Nascu, Diangelakis et al. 2016). If we consider a pre-existing pharmaceutical process in which a new molecule comes in, i.e. in the form of a newly developed active pharmaceutical ingredient (API). The standard approach requires a series of Design of Experiments (DoE) to be performed for the new process to be designed. However, only information regarding the material properties of the new molecule are required. A model based, material properties aware controller can make the necessary adjustment to adapt to the new molecule thus alleviating the need of computationally expensive and time consuming DoE's.

In this work we set the foundation for advanced multiparametric model predictive control (mp-MPC) systems for a continuous evaporation process that are designed to work with different molecules without repeating the process design and process control design steps. The first step is to design a model of the process for one molecule type. This model will be then used to design advanced mp-MPCs for different molecules. The performances and limits of the designed control schemes are tested on the model developed within the gPROMS platform for varying operating targets and process disturbances. The designed methodologies show good performances: fast settling time and no significant overshoot or undershoot. Moreover, this work represents the first step towards the development of advanced MPCs that are designed to work with different molecules and different thermodynamics scenarios without redoing the process design and process control steps.

Keywords: pharmaceuticals, process control, PID, mp-MPC

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Process as a battery: Electricity price based optimal operation of zeolite crystallization in a COBR

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Abstract

The electrification of the energy supply requires major changes in the process industry, which poses new challenges and possibilities for the operation of processes. At the same time, the total energy grid mix is in a constant change from fossil to renewable energy sources, which will increase the fluctuations in production and price. The resulting problems are firstly the destabilization of the energy grid and secondly strongly varying energy prices. To ensure an economically efficient operation of electrified processes, the flexible dynamic operation of continuous processes is considered. Similar approaches were already demonstrated for scheduling problems e.g. by Leo and Engell (2018). This has two main advantages, firstly the economic benefit of using less energy at higher price levels and secondly the stabilization of the electric energy grid.

The dynamic energy price driven operation is shown for the continuous hydrothermal synthesis of zeolites in a Continuous Oscillatory Baffled Reactor (COBR). Zeolites are widely used inorganic crystalline products. Possessing large pore volumes and surface areas, zeolites are used as catalysts and absorbents in industrial and consumer applications. The hydrothermal synthesis of zeolites requires long processing times at elevated temperatures, which poses a challenge for the economical efficiency at fluctuating energy costs. The usage of model based optimizing control techniques circumvents this problem and enables a flexible energy price based zeolite production. The throughput and the heating power are optimized based on the variation of the price of electric power, such that the energy cost of the process is minimal while guaranteeing the required average product quality and throughput.

The paper presents a first principle dynamic model describing heat and mass transfer and the crystallization reaction. The concept of optimal operation of the COBR is introduced and the performance is investigated in simulation studies that demonstrate the enhanced flexibility of the process. The economical advantages of this enhanced flexibility are shown for varying energy prices based on data from the day-ahead energy market.

Keywords: dynamic optimization, energy price based operation, Continuous Oscillatory Baffled Reactor, fluctuating energy prices, optimal operation

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Leveraging Deep Learning for Efficient Explicit MPC of High-Dimensional and Highly Non-linear Chemical Processes

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Abstract

Model predictive control (MPC) is one of the most common control methods used in Chemical Engineering, due to its advantageous of handling multivariate systems and hard constraints on control and state variables [1]. However, MPC faces the challenge of the high computational resources required for running its expensive online computations. At each sampling period, MPC solves a dynamic optimization problem that entails repetitive evaluations of a dynamic process model [1]. So, MPC applications become infeasible for processes characterized by high-dimensional state, high nonlinearity and/or fast dynamics [2]. To tackle this challenge, explicit MPC methods have been developed which solve the MPC problem, offline, providing simple mathematical expressions that describe the future values of the optimal control variables as a function of the current state variables. Then, these mathematical laws are used, online, to control the process, thus alleviating the computational bottleneck problem. Still, the explicit MPC applications are limited to linear discrete-time state-space models with moderate dimensionality/nonlinearity [1]. Recently, the use of Machine Learning (ML) has been proposed to extend these constraints by exploiting their universal approximation capabilities to develop accurate and computationally efficient data-driven control laws [2]. However, most of these methods have been applied to simple test cases and lack comprehensive validation metrics to guarantee their effectiveness. In this direction, our work contributes with an efficient Deep Learning (DL) based method for explicit MPC of high-dimensional and highly nonlinear processes, which employs DL models for offline development of control laws that accurately approximate the relation between the future values of the optimal control variables and the current state variables. The training data is generated by solving the MPC problem considering different initial values of the state variables selected by design of computer experiment techniques. The obtained ML-based laws are then integrated into a closed-loop for online control of the process. A validation procedure is used to assess the obtained control laws, providing efficient performance metrics in terms of open-loop response accuracy, closed-loop response accuracy, final-state accuracy, and computational cost. The method is applied to case studies from the literature [1], to which the direct application of explicit MPC is not possible due to their high dimensionality and nonlinearity. Numerical results show high performance of the proposed method and significant reduction in the solution procedure complexity of mathematical explicit MPC.
Keywords: Explicit MPC; Chemical Processes; Deep Learning.

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Incorporation of error propagation into an elemental balancing based soft-sensor for improved online monitoring of microbial fed-batch processes

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Abstract

Monitoring and control of biological processes is still mainly limited to only a few physical and chemical properties that can be measured online with relatively low efforts. Important parameters and variables of a bioprocess are predominantly determined by offline sampling as they are difficult to accurately measure online. Therefore closed-loop control of those critical process variables poses great difficulties to the bioprocessing industry. To overcome this challenge state estimation techniques can be used. For their proper function they need observable process models, which are still not available for every bioprocess.

In this work a first principle based soft-sensor is presented which allows for real-time estimation

of biomass and specific reaction rates for cell growth, substrate uptake, O_2 consumption and CO_2 formation in biotechnological production processes. The proposed algorithm utilizes elemental balancing of the carbon flux alongside the degree of reduction balance to incorporate gross error detection and data reconciliation between the two balances. The functionality of gross error detection and data reconciliation strongly rely on the errors of the used measurements. Recent works employed elemental balancing for state estimation considering only constant measurement errors over time. The high dynamic range during fed-batch operation as well as the carbon evolution and oxygen uptake rates being calculated from several measurements necessitates a proper and dynamic error propagation procedure.

We successfully applied an adaptive propagation of measurement uncertainties to substrate limited fed-batch cultivations of recombinant Escherichia coli. The novel soft-sensor algorithm led to a reduction of the biomass estimation error from formerly 22% to 11% NRMSE. Especially the consideration of additional uncertainty derived from supplemented pure oxygen increased data reconciliation effectiveness, which can be seen by smooth rate estimates. In addition gross error detection is more sensitive to better indicate sensor faults or mismatches between carbon and degree of reduction balances. Elemental balancing including true measurement errors and error propagation is a valuable tool to estimate biomass and biomass specific reaction rates of microbial fed-batch processes. The basis on the law of mass conservation rather than on very specific process models makes it a generically applicable soft-sensor with reduced efforts for implementation and measurement needs.

Keywords: bioprocessing, soft sensor, process analytical technology, state estimation, online process monitoring

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Iterative Learning Control in Chromatographic Polishing of Biopharmaceuticals

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Abstract

As downstream processes for production of biopharmaceuticals move towards integrated continuous processes with cyclically operating process steps, a need arises to monitor and control each individual step. The ion-exchange (IEX) polishing in an integrated periodic counter-current chromatography (PCC) process is an example of one such step (Gomis-Fons et al., 2020). A method of maintaining consistent operation between process cycles is desired. The cyclic nature of these processes makes iterative learning control (ILC) a promising candidate to achieve this. ILC is a control technique that has been thoroughly researched in the field of robotics as a method of maintaining a consistent output in repeated processes. It has previously been successfully applied to batch processes in the field of chemical engineering (Lee and Lee, 1997).

The purpose of this study was to apply ILC on the separation of two proteins in an IEX chromatography column. The retention times of the proteins were used as measurement signals, while the start and end values of the slope of the linear salt gradient in the elution phase were used as the control signals. The study was performed in-silico, using a convection-dispersion chromatography model with a Langmuir mobile phase modulator. The ILC algorithm was based on an ILC design using a quadratic-criterion objective function (Lee and Lee, 1997), which uses a linear model of the process to tune the control parameters. This linear model was computed by running three simulations and computing a Jacobian matrix using their results. The three simulations were generated automatically using the process set point, resulting in an automatic tuning of the controller.

The ILC performance was evaluated by running simulations with two different disturbances: a change in set point for the retention times and a change in concentration of salt in the elution buffer. The suggested ILC design could compensate for changes in set point within 1 cycle, and for a change in buffer concentration within 3 cycles. This shows that ILC is capable of controlling retention times in simulated IEX chromatography, and so the natural next step is to apply this controller in the laboratory. One limitation of this study is that disturbances that cause a change in the process dynamics, such as the pH of the buffers, were not tested. Such a study could potentially inform the use of adaptive process model estimations, where the model updates between each cycle using the gathered process data.

Keywords: preparative chromatography, process control, iterative learning control, ion-exchange

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Application of Real-Time Optimization with Modifier Adaptation to the Reactive Extrusion of Hydrophobically Modified Ethoxylated Urethanes

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Abstract

Hydrophobically modified ethoxylated urethanes (HEUR) are a group of polymers mainly used as rheology modifiers in paints and coatings, conventionally produced in batches of several cubic meters. Within SIMPLIFY the production of these paint thickeners by reactive extrusion on a twin-screw extruder is investigated, offering numerous advantages. Although to operate the process at the economic and ecologic optimum, an advanced process control strategy is required. Applying classical model-based control methods such as conventional real-time optimization would lead to suboptimal performance as the optimal set-point of the model does not coincide with the optimal point of the real process due to the plant-model mismatch. To overcome this mismatch, realtime optimization with modifier adaptation has been proposed [Gao and Engell (2005)]. Here the formulation for both objective function and constraints are extended by the addition of the difference of the plant and model gradients with respect to the inputs multiplied by the input change. For this reactive extrusion process, the plant gradients are available: The process is robust, can be artificially exited, reaches a steady state within 5 minutes and is overall safety uncritical regarding the processing conditions. Additionally all contributions to the cost function can be accessed directly by measurements. The plant model used in this work is a mechanistic twin-screw extruder model [Eitzlmayr et al. (2014)]. This model accounts for the flows within the extruder caused by various screw geometries. Furthermore, this model discretizes the extruder into finite volumes in which the polymerization is occurring. During the polymerization, the viscosity of the processed material increases, amplifying the energy dissipation and affecting the internal flows. The application of real-time optimization with modifier adaptation with a plant-model mismatch in the reaction and the rheological model is studied in this work. It can be shown that the controller can overcome the plant-model mismatch and drive the process to the true economic optimum.

Keywords: RTO, Reactive Extrusion, Model-Based Control, Plant-Model Mismatch

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A New Solution Strategy for Multiparametric Quadratic Programming

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Abstract

- Background: The solutions of multiparametric quadratic programming (mp-QP) problems frequently include a large number of critical regions, where no persistent patterns on their sizes and shapes can be detected (Pistikopoulos et al. (2020)). In particular, and as the number of inequality constraints increase, an exponential explosion on the number of critical regions is often observed, and limiting the practical utilization of the mp-QP architecture up to problems of a given size.

- Methods: A new framework for the analysis of mp-QP problems is presented. It is made possible by: (i) a transformation of the original vector of parameters, and (ii) a relaxation of the corresponding parameter space. All transformed parameters become associated with a unique inequality constraint, enabling insightful examinations of the solutions of these problems. A study on the occurrence of critical regions and optimizers in this class of problems is presented.

- Major Results: The proposed parameter transformation and relaxation steps lead to a significant re-organization of critical regions. In the new transformed space of parameters, all critical regions share a common vertex, and all are supported on a set of $2p$ 1-dimensional edges, where p denotes the number of inequality constraints. As a result, all critical regions may now be described via a set of $2p+1$ vectors of size p, including the fundamental information of critical regions maps, instead of deriving explicit solutions, as is the common practice in the field. The proposed critical region representation defines in fact a Linear Complementary Problem, although its principles and interpretation are to a great extent different from the classic formulation of such problems (Murty and Yu (2010)). A similar approach is applicable to the calculation of optimizer functions, and mp-QP solutions can now be obtained in a very compact form and with minimal effort, regardless of the number of constraints. The strategy was applied to 15 mp-QP problems, ranging in the total number of inequality constraints between 1 and 15: execution times and solution sizes from the state-of-the art mp-QP algorithms (Oberdieck et al. (2017)) grow exponentially with the number of constraints, while the proposed strategy exhibits an approximately linear dependency with respect to the number of constraints. This strategy also avoids the difficulties commonly reported on parameter space exploration.

- Conclusion: This framework enables major computational advantages to the state-of-the art mp-QP algorithms. It is of particular significance for problems of large size, which can now be solved with minimal effort and thus presenting a key development in the field. Additional work to fully explore these developments are identified as the top priority in future research. This includes the calculation of online solutions for instance in quadratic control problems, and adapting this framework for general nonlinear problems.

Keywords: Multiparametric programming, quadratic programming

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Model-based state estimation and adaptive feed control for automated parallel *Escherichia coli* mini-bioreactor experiments

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Abstract

Screening a large number of candidate mutants and operating strategies in cultivations that mimic industrial conditions is essential to speed up the development of bioprocesses. Robotic facilities that allow High Throughput Screenings (HTS) are widely used to allow for rapid and automated testing of many samples in parallel. In order to maximise bioprocess understanding, real-time monitoring of these systems is essential for efficient screening, control, and process optimisation. Unfortunately, many critical variables in biotechnological systems cannot be measured directly. Concentration measurements, for example, often require a complex and time-consuming treatment prior to their spectroscopic analysis and, thus, are only available atline. Due to the high number of parallel experiments of HTS systems the number of possible atline measurements for each reactor is very limited, either by costs or practicability. Furthermore, sample collection, as well as liquid additions are carried out via robotic needles resulting in a pulse-wise feeding in the fed-batch phase of a fermentation. This introduces very fast dynamics to the system that not only makes numerical simulations extremely challenging, but also stresses the organisms and can, therefore, drastically change the metabolism. Additionally, biological models often lack of sufficient structural identifiability due to their complexity and high parameter correlations (López et al., 2013), and, in the context of metabolic changes, some parameter or even parts of the model structure need to be adapted throughout the time evolution of the process.

Here, we present an approach for model-based, nonlinear parameter and state estimation, specifically tailored for parallel mini-bioreactor cultivation systems (Haby et al., 2019) using only basic online data. A sigma-point Kalman filter (Julier et al., 1995) is implemented to estimate biomass, glucose, acetic acid, and dissolved oxygen tension (DOT). *Escherichia coli* producing antibody fragments is monitored in a platform with 24 parallel experiments in the mL-scale. A macrokinetic model is used to predict growth, glucose consumption, and acetic acid production (Anane et al., 2017). An accurate estimation of the biomass is crucial to compute the specific rates governing the dynamics of the model, for which a software sensor is used to link the cumulative ammonia addition with the total biomass formed (Sundström and Enfors, 2008). Ammonia consumed by the organisms as nitrogen source causes a drop in the pH value, that in turn is compensated for by the pH-controller to keep the pH at a constant level. We show that together with the DOT measurements this method provides valuable information for the state estimation procedure. Additionally, the yield of biomass on glucose excluding maintenance $Y_{X/S,em}$ is estimated to account for metabolic changes during the fermentation. The feed is then adapted online, based on the state

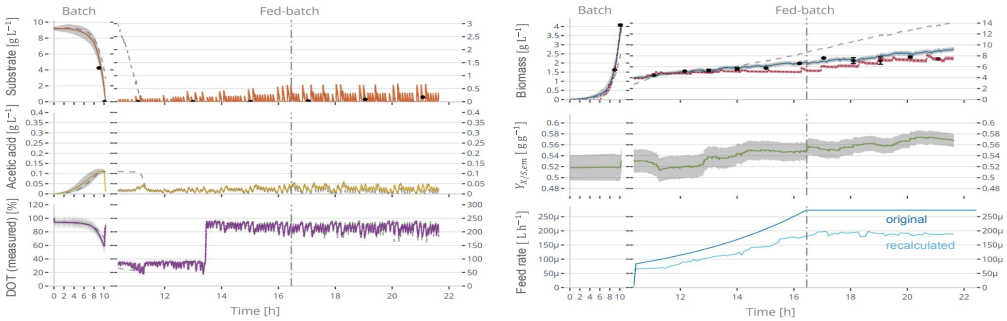

Figure 1: Comparison of model simulation (grey broken line) and state estimation (coloured line). The estimation shows good agreement with atline measurements (dots). Biomass determination via ammonia addition (red line) and estimated standard deviations for each state (grey and red area) are represented, as well as a comparison between online recalculated feed rate (light blue) and predefined static feed rate (dark blue).

and parameter estimates, where an exponential feed rate is recalculated every 15 minutes to match the predicted glucose uptake and to set a specific growth rate.

As depicted in figure 1, state estimates show good agreement to all atline measurements. The biomass determination via ammonia addition successfully provides continuous online information about the current biomass concentration leading to very good estimation results and a high reliability in the batch end forecast. The start of the feeding is crucial to avoid starvation that can cause stress responses and a high metabolic burden. The adaptive framework managed to properly decrease the feed rate to respond to a lower biomass than expected and, thus, ensures a more optimal feeding than with the commonly used predefined exponential feed. Even more importantly, the framework is able to detect and counteract overfeeding so that an unwanted feed accumulation can be avoided. This approach enables for close monitoring of growth and substrate consumption rates in the presence of fast system dynamics and metabolic changes that are difficult to predict. It therefore allows for the screening of optimal conditions for growth and product formation under controlled cultivation conditions in a HTS system, whereby a more optimal feeding is guaranteed.

Keywords: *Escherichia coli*, sigma-point Kalman filter, model-based state estimation, automated parallel mini-bioreactor experiments, adaptive feed control

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Development of a virtual platform for the metaheuristic optimization of heat exchangers

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Abstract

Heat exchangers are indispensable equipment in almost every industry. Different types of heat exchangers can be used depending on aspects such as operating conditions, frequency of maintenance and cleaning, available installation space, properties of the involved fluids, among others. Regardless of the type of heat exchanger to be installed, it is necessary to find its best configuration. From an optimization perspective, the heat exchanger design methods are complex due to the presence of non-linear, non-continuous and non-differentiable equations. Additionally, the design method depends on continuous and discrete decision variables. Thus, it is necessary to implement suitable optimization methods. In this work, the development and performance testing of a virtual environment for the metaheuristic optimization of a variety of heat exchangers is presented. In its current state, the platform allows performing the optimization of shelland-tube heat exchangers, plate-and-frame heat exchangers and plate-fin heat exchangers. Furthermore, the platform allows to use the type of exchanger as a decision variable. Several metaheuristic optimization methods can be selected to perform the optimization, as differential evolution, grey wolf algorithm, particle swarm algorithm, among others. Additionally, a comparison among the optimal designs of each kind of exchangers for a given task can be obtained using statistical information generated in multiple runs. In general terms, the best results have been obtained by optimizing the heat exchangers through the differential evolution method.

Keywords: metaheuristic optimization, shell-and-tube heat exchangers, plate-and-frame heat exchangers, virtual platform.

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A framework combining optimization and life cycle assessment for designing low-carbon energy systems

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Abstract

The energy transition depends on the supply of low-carbon energy in all sectors. In this context, the integration of low-carbon electricity from renewable sources is key to reduce greenhouse gas emissions but also leads to new challenges for decision-making when designing energy systems:

- Local and temporal fluctuation in energy supply.
- Synergetic effects through sector-coupling among energy sectors as well between industrial production and energy systems.
- Burden shifting from climate change to other environmental impacts.

To cope with the resulting complexity, the development of effective energy system designs for reducing greenhouse gas emissions is usually based on mathematical modeling and optimization methods. The underlying models need to address the above challenges that thus have to be reflected when designing optimization methods and software frameworks. Although many models have been developed for the transition to low-carbon energy systems, reusability is limited when these models are not openly available to the research community. Generalized and modular open-source frameworks ensure reusability and, hence, contribute to accelerating transparent research.

SecMOD is an open framework for linear multi-sector optimization of models with flexible spatial and temporal resolution. The object-oriented framework considers energy converters, storage, transport of electricity, and product transport. Hence, SecMOD can identify synergies between different technology options in multi-sector systems. We consider environmental impacts by the full integration of life cycle assessment into the optimization framework. The developed framework can be applied flexibly to energy systems across scales: from industrial to national energy systems.

In this work, we present the SecMOD framework and apply it to an industrial case study, demonstrating the modeling features, such as modular applicability and integration of the life cycle assessment in the optimization problem. We optimize energy converters and storage, identifying the transition pathway to an industrial low-carbon system. Finally, we demonstrate the flexibility of SecMOD by discussing further fields of application, such as large-scale national energy systems.

Acknowledgments

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Robust Scheduling of Distributed Energy Systems Considering Grid Rejection

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Abstract

With persisting efforts to integrate more small-scale renewable energy resources and improve network resilience, a global growth in community distributed energy systems (DES) and microgrids has been predicted. The Energy Management System (EMS) is at the heart of a functioning DES, ensuring the optimal operation of generation and storage technologies within the DES while accounting for network, technology, and cost-related constraints. It is usually formulated and solved as a day-ahead deterministic Mixed Integer Linear Programming (MILP) problem. However, Robust Optimisation (RO) and Stochastic Programming (SP) modelling frameworks are increasingly used to inherently account for the presence of uncertainty in the inputs to these models, such as demand, pricing, and weather forecasts, and produce more realistic operational strategies and costings (Wang et al., 2015). These have assumed that the external electrical grid is an infinite sink to which all excess electricity produced by the DES can be sold. In reality, the grid can choose to reject excess power generated when demand does not match supply or when network constraints are violated. With many decentralised generators at play, electricity service providers that manage the external grid are also in the process of introducing bidding systems which can influence selling prices. If grid acceptance/rejection is not introduced as an uncertain input in these models, it can lead to excessive generation curtailment, energy wastage, and underestimates of operational costs. Some day-ahead models have specifically considered generation curtailment but this alone is insufficient as curtailment is a result of the uncertainty surrounding grid rejection. For the first time, this study considers grid rejection within an uncertainty framework for the optimal operation of a grid-connected community DES. Both RO and SP formulations are proposed and applied within an overarching MILP rolling-horizon framework, while also accounting for other uncertainties related to pricing, demand, and weather forecasts. Benefits and challenges of implementing the two approaches are compared extensively. Results highlight that grid rejection has a significant impact on the conservativeness of day-ahead solutions, particularly in the RO approach, while the SP approach is less conservative but more computationally expensive. Overall, the study contributes to the development of more robust day-ahead models that can be utilised within the EMS and support wider growth of DES and microgrids.

Keywords: Distributed energy system, uncertainty, robust optimisation, stochastic, programming.

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SCR: a novel surrogate-based global optimization algorithm for constrained black-box problems

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Abstract

This paper proposes a novel optimization algorithm for constrained black-box problems, where the objective function and some constraints are computed by a simulation code. The basic idea of the optimization algorithm, referred to as SCR (Surrogate-CMAES-RQLIF), is to (i) build separate Kriging surrogates (Lophaven et al. (2002)) for the objective function and black-box constraints, (ii) use the global search algorithm CMAES (Hansen and Kern (2004)), a well-known evolutionary algorithm, to find the global optimum region of the surrogate, (iii) if the global optimum found by CMAES lies in the same region as the previous iteration, use the recent local search algorithm RQLIF (Manno et al. (2020)), a hybrid implicit filtering – model-based algorithm, to refine the search locally, (iv) use all the points sampled by RQLIF and additional points within the optimal region located by CMAES to update the surrogate model . For problems with black-box constraint functions, while state-of-the-art black-box algorithms handle directly the penalized objective function, the original idea of SCR is to build separate surrogates for the objective function and black-box constraints. This allows generating more accurate surrogates (the penalized objective function is more difficult to approximate due to the steep slope and strong curvature of the penalty term) and avoid ill-conditioning issues. The performance of SCR was tested on 21 constrained test problems and 25 unconstraint test problems with 3-15 variables and compared with other state-of-the-art optimization algorithms, namely NOMAD (Le Digabel (2011)) and plain CMAES. SCR outperforms the benchmark algorithms in terms of fraction of problems solved for both constrained and unconstrained problems. The relative advantage compared to the tested algorithms is more evident at low function evaluations (< 300), range of major interest for computationally expensive simulation-based problems.

Keywords: process optimization, surrogate-based optimization, Black-box optimization, Global optimization.

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Comparative Life Cycle Assessment of Demand-Side Management Processes via Operational Optimization

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Abstract

Due to the volatile nature of renewable energy sources, balancing electricity generation and consumption in electricity systems becomes more challenging with an increasing share of renewable generation technologies. One option to face fluctuations in the electricity grid is demand-side management, the adjustment of electricity consumption driven by varying electricity prices. To assess the environmental impacts of demand-side management processes, the holistic method of life cycle assessment can be applied. Life cycle assessment determines various environmental impacts over the complete life cycle of a process. In literature, the life cycle assessment of demand-side management processes receives increased attention. However, the definition of the functional unit is not consistent. Walzberg et al. (2019) define the products of their system as the functional unit and only consider flexible electricity consumption as an option to benefit from cost savings. In contrast, Milovanoff et al. (2018) consider the flexible electricity consumption as their functional unit. In our view, both the products and the flexible electricity consumption of a process can be critical functions. Thus, a combined approach is necessary. In this paper, we aim to close this gap by jointly considering products and flexibility in the functional unit of demand-side management processes. For comparative life cycle assessment, we define the steady-state process to provide the same products. Furthermore, we expand the reference system with energy storage technologies, providing flexibility in electricity consumption. We quantify the flexible electricity consumption of the demand-side management process by operational optimization. Based on the results of the operational optimization, we determine the parameters of flexibility. These parameters are used to optimize the storage power and capacity in the reference system. Finally, we determine the environmental impacts of both systems.
We demonstrate the assessment of demand-side management processes on the switchable chloralkali electrolysis, using hourly electricity prices and emission factors. We consider the standard electrolysis with a vanadium redox flow battery and a power-to-methane plant for the reference system.
Keywords: life cycle assessment, demand-side management, operational optimization.

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Process mining-based analysis of operator actions towards automated operator decisions

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Abstract

This paper discusses the applicability of sequential pattern mining in the goal-oriented filtering of the alarm & event-log files of chemical plants to gain the different operator action series models with process mining tools. Process mining is a widely used technique to understand and explore processes (Aalst (2011)). However, it was meant to be a tool to understand business processes in the beginning, the field of application was getting wider and wider. With the growing variance of processes, the shortcomings and limitations of the methods have come to light. One of the challenges in exploring operator actions is that parallel processes can exist, as the same trigger event can result in different operator action strategies. Using the whole log file, we assume that all events are related, which is not valid in many cases, especially in alarm management. Once we prepared our log file, such connections and rules are added (in the form of traces), which cannot be removed anymore; no split or partitioning will give a satisfactory sub-process model. More precise process models can be discovered by identifying these strategies and grouping them in separate sub-log files extracted from the original log file. Frequent sequence mining-based machine learning models can provide a well-validated model of the process events (Lucke (2019)). Identifying and eliminating "ineffective" action series (which can be derived from bad historical practice or insufficient training) can lower the workload of the operators (Dörgő (2018)) and improve the overall production performance from HSE (Health, Safety & Environment) and financial points of view. This approach is in line with the digital and green transition goals of the European Union, also known as Industry 5.0.

This work highlights how efficiently this method supports the filtering of traces in log files. This phase of process exploration assumes that our traces are already identified. Partitioning our log file to focus on relevant processes takes two steps:

- we search for traces where a specific group or sequence of events occurs, and we analyze only these,
- then we filter out non-frequent events from our remaining traces.

The suggested method was applied to the alarm management database of an industrial hydrofluoric acid alkylation (HFA) plant. The used itemset mining algorithm was AproioriClose from the SPMF toolkit. The processes were explored with the open-source python-based process mining package, *pm4py*. A wide range of process mining tools, including Heuristic Miner, Inductive Miner, or Directly Follows Graph, supports understanding the different operator reactions triggered by the same event. With their

additional attributes (frequency of events/transitions or the average elapsed time between two consecutive events), deep insight into the processes becomes available.

A correlation heatmap using the support values of frequent itemsets can support selecting proper items for trace filtering (Figure 1). The heatmap can be split into different sections, highlighting the alarm-alarm, alarm-operator action, and operator action-operator action relations. Indirectly, non-frequent items can be extracted. Removing them results in an even more compact process model. Events ending with A are alarms, ending with O are operator actions. The end pairs of alarms (return to normal events, noted with N) were removed before the frequent pattern mining, as they always occur with the alarm, this way, they are redundant information. Usage of frequent sequences instead of itemsets results in an even more specific process model.

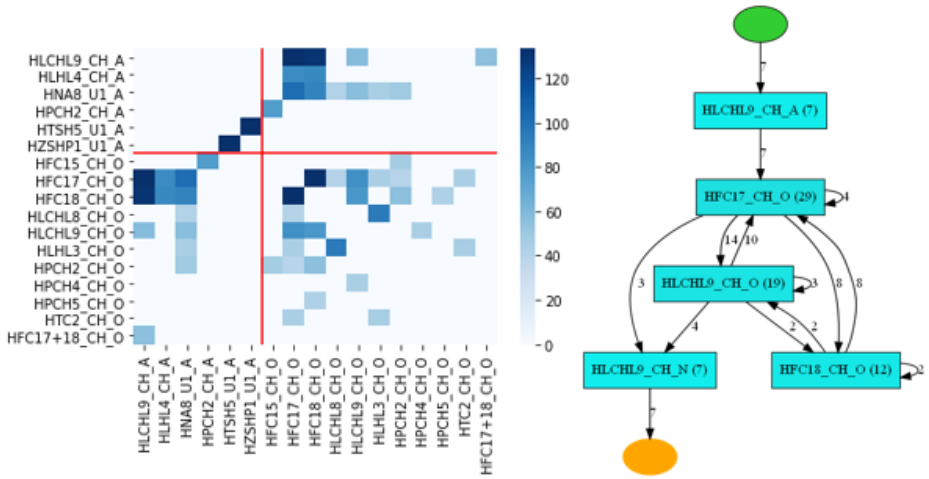

Figure 1: Correlation heatmap of items and the gained process model after filtering the log file. Event name coding: TagName_Unit_EventType.

Our case study proved the method to be an effective tool for targeted process discovery, primarily when parallel and overlapping processes exist in our system. Besides identifying flawed process handling practices, these results can base an operator KPI (Key Performance Indicator) and an automated decision-making-based process control system project. Additionally, with some considerations, this method can validate the definition of traces, which is undoubtedly one of the most critical tasks in process mining.

Keywords: Process control, Operator, Decision-making, Process mining, Sequential pattern mining

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Optimal Design of an Innovative Solar Power Plant

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Abstract

The EU-funded project Next-CSP aims at demonstrating an innovative concept of Concentrated Solar Power (CSP) plant. It uses fluidized particles of olivine as both heat transfer fluid (absorbing heat from the sun's concentrated beams) and storage medium (enabling the power plant to produce even when the sun is not visible) (Zhang et al., 2017). In such a plant, the heat collected from the sun is converted into power *via* a combined cycle: an open air Brayton cycle with two reheats, whose exhaust air feeds a bottoming steam cycle. At industrial scale, such a plant is expected to exhibit a lower Levelized Cost Of Electricity (LCOE) than similar state-of-the-art CSP plants. While some parts of the plant can be considered mature and well-known, the three particle-to-air heat exchangers used as a primary heat source for the thermodynamic cycle have no industrial example and their performance can affect significantly the design of the rest of the plant. A physical model of such an exchanger was therefore produced, enabling a simplified mechanical design and the assessment of the exchanger's cost.

In that model, the exchanger is assumed to be a shell-and-tubes component, with a shell of rectangular cross-section. The pressurized working air of the topping Brayton cycle flows in the tubes, while the particles fluidized near atmospheric pressure flow in the shell through several baffles, overall counter-current to the air.
The inputs of the model are the desired temperatures (particle and air at the inlet and outlet of the heat exchanger), the inlet pressure and flowrate of working air and some geometric parameters of the heat exchanger (tube diameters, total width of the exchanger, height). With those inputs, the model computes the average air speed in the tubes, the particle flowrate and the heat transfer coefficients on both sides of the tubes.
Finally, the main outputs of the model are (i) the length of tubes necessary to achieve the desired heat transfer, as well as (ii) the pressure loss of the working air across the tubes. Tube length (i) allows to compute a total mass of metal, then via a cost correlation, the CAPEX of the heat exchanger. Pressure drop across the tubes (ii) has a very direct impact on the overall efficiency of the Brayton cycle, therefore on the overall plant's conversion efficiency.

System-level performance models were used to compute the rest of the plant's heat and mass balance. Cost models from the literature and Next-CSP project partners were adapted and used for the open air Brayton topping cycle and the solar loop.
A simplified description of the steam cycle was used, as that part is by far the most mature and well-known of the innovative plant being designed. Based on EDF's engineering experience, eleven recovery steam cycles were designed for air turbine exhaust temperatures ranging from 550 to 650°C, using the reference engineering software GT PRO 26 from Thermoflow (Valentin et al., 2019). From those designs, a least squares regression led to the expression of a linear relationship between the steam cycle's net power output and the exhaust air's temperature and flowrate.

The calculation of the plant's heat and mass balance and its CAPEX were entirely computed in Python 3.6, every component model being validated against commercial software like Themoflow's Thermoflex, to the exception of the fluidized-bed heat exchanger model for which only a thorough verification was performed as no experimental data or validated model could be used for that component.
The CAPEX estimation, associated with assumptions on the OPEX and the annual dispatch of the plant, allowed the estimation of such a plant's Levelized Cost Of Electricity (LCOE). That LCOE served as an objective function for a global optimization of both process (pressure ratios across the air turbines, air temperature at the inlet of every turbine, temperature difference at the cold end of each fluidized bed heat exchanger) and geometric variables (width and tube diameters in the fluidized bed heat exchangers, that is a total of 15 variables. 5 inequality constraints were formulated in order to remain within reasonable pressure drops in the fluidized bed heat exchangers and to respect pressure and thermal balance along the topping Brayton cycle.

Due to the complex objective function that already uses the iterative resolution of algebraic and differential equations, the optimization problem was solved using the Python library PYGMO (Biscani et al., 2018; Biscani and Izzo, 2020) with the heuristic "harmony search" algorithm (Mahdavi et al., 2007). Like in genetic algorithms, the two main parameters of that method are the number of generations and the population of each generation. Several runs were performed, using a population of 50 individuals and up to 50 000 generations. The resulting LCOE was always the same within a +/- 0.1% margin. The decrease in objective function usually became very marginal above 20 000 generations. Compared to a previous design (Valentin et al., 2019) of the thermodynamic cycle, using rough assumptions on the particle-to-air exchangers' performance, the present study leads to a very different compromise between temperature difference and pressure loss across the heat exchangers: while the former doubles, the latter is approximately halved, leading to an overall better efficiency.

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Keywords: renewables, solar power, global optimization, energetics

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A rigorous synthesis and optimal design methodology for chemical and biochemical processes

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Abstract

Process synthesis is an established methodology to determine the best process flowsheet considering different criteria like energy, economy, environment, and social aspects. The use of superstructure approach has allowed to identify the best option among diverse process pathways, but most of the time they lack of rigorous thermodynamic analysis. Thereby, the objective of this research was to create and implement, a new methodology based on a genetic algorithm for the optimization of superstructures, integrating two computational programs through an interface: Aspen Plus (AP) and Matlab. This allowed the use of a rigorous thermodynamic approach and combine computer-aided tools, to find the best configuration of a biorefinery considering different processing routes to obtain high value biofuels and chemical products. The biomass used as raw material was agave bagasse, since it is a natural residue from the production of tequila and mezcal in the region. Fig. 1 illustrates the general steps of the proposed methodology.

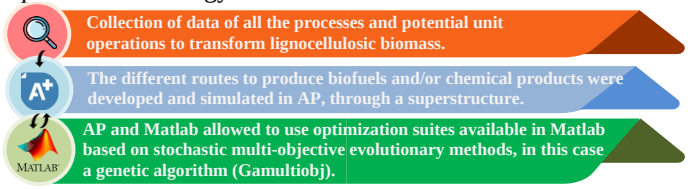

Fig. 1. Methodology for rigorous synthesis and optimal design of (bio)chemical processes.

Different optimizations were evaluated varying the individuals (from 50-100) and generations (from 1-20) of the algorithm, using as decision variables the treated mass fractions of biomass in the different sections such as, pretreatment, saccharification, fermentation and, primary and secondary products synthesis. Optimization results show similar products in the process routes, but they differ in the amount of mass distributed to each stage. Among the 36 optimal process layouts, the best obtained route was to produce furfural, 2,5-furandicarboxylic acid and hydroxymethylfurfural, employing 100 individuals and 20 generations. As final remarks, it has been possible to design and implement a methodology with different scope from the conventional ones, for the optimal synthesis of a biorefinery with a superstructure approach. This allowed optimizing the best configuration for the transformation of biomass into chemical products. A satisfactory integration between computational programs, AP and Matlab, has been carried out, which has permitted a multi-objective optimization, considering the economic objective as well as the energy objective using a rigorous approach in the calculation of thermodynamic properties, through appropriate equation of states and activity coefficient models that consider the non-idealities of the mixtures involved.

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Renewables-Based Multigeneration System for District Energy Supply

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Abstract

District energy systems (DES) provide electric and thermal energies to a developed area from a central plant through underground distribution networks. Fossil-fuels are widely used as a primary energy source in DES. In 2021, energy-related CO2 emissions from residential and commercial buildings reached 10 % worldwide. In this paper, a renewables-based multigeneration system is proposed as a sustainable alternative for DES. The conventional system is based on gas-fired combined cycle turbine and an absorption cooling system (ACS). The proposed renewables-based system utilizes biomass and solar thermal energies together with an ACS for the provision of district electricity, heating and cooling. A process model is developed for both systems and a techno-economic assessment is performed to compare the levelised cost of energy (LCOE) and evaluate the anticipated reduction of the environmental footprint. Results show that although the LCOE of the proposed system is higher than the conventional system, the reduction in CO2 emissions convert directly into annual savings in districts that are covered by a carbon tax regime.

Keywords: Carbon tax, District energy systems, Multigeneration, Renewable energy, Techno-economic Assessment.

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Integrated Material ModellingWorkflows

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Abstract

Motivation: Product design in the light of a business requires information from the business and physical domains, which, from a computational engineering perspective, implies integrating business decision tools with process and material simulation processes to form an overall workflow. The integration is not only in the coupling of the tools but also in the exchange of data. The business workflow management systems must communicate with analysis tools, optimization and decision support systems, some of which require process simulations. The process simulation, in turn, will, in general, model several layers of time scales, which may range from quantum mechanics to the finished product's mechanical properties.
Approach: A workflow describes how one has to combine logically different activities to achieve the overall goal. Tools like CAMUNDA are based on the Business Process Modelling concept, and they are well established and easy to use. In contrast, workflows for the simulation of physical systems are rarer and require expert knowledge to establish. A typical example is multi-scale modelling, where the problem of interest covers any sub-range from quantum mechanics to macroscopic product properties. For some years, NTNU developed a modelling/simulation suite that is ontology-based, ProMo, for Process Modelling. Reductionism forms the background, and processes are represented as a network of mass/energy/momentum interacting networks. Like BPM tools, we use a visual language to model processes.
Paper & Presentation: We will discuss the use of workflows on an industrial example being the object in the VIPCOAT EU project. CAMUNDA is used to model the business layer, and the ProMo technology is employed to construct the process model. We shall address the issue of synchronising the different activities in workflows using Petri-net technology. We will also discuss the challenges with exchanging information between different workflow representations, different levels of workflows and separate workflows. We address the data exchange problem by employing a shared dataspace as a unified knowledge base, managing different data sources containing variables, configurations, accumulated data, and data representations (meta-data and ontologies).

Keywords: Computational engineering, modelling, multi-scale, ontologies

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Investigation of optimal blending of typical livestock manures in Qatar to produce biocrude via hydrothermal liquefaction

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Abstract

Livestock manure is a key agro-waste in Qatar, with more than 1.5 million tonnes generated every year. Most of the manures are landfilled or used as fertilizers, which raises concerns associated with the limited land areas in the country and the possible pollution of air and contamination of groundwater. Meanwhile, Hydrothermal liquefaction is attracting growing attention to valorize wet wastes as an alternative to anaerobic digestion to produce value-added energy products. Livestock manures differ in terms of their composition, availability, and cost; therefore, an optimal blending of multiple livestock manures for liquefaction is expected to yield biocrude with superior properties and contribute to process efficiency improvement and cost reduction. As such, this study evaluates the effect of different blending ratios of five typical Qatar's livestock manures (dairy, camel, sheep, chicken, and horse manures) on biocrude's yield, heating value, composition, and cost. The proximate and elemental analyses of manure samples are conducted in the laboratory, while the liquefaction process is simulated using Aspen Plus®. Besides, Aspen Process Economic Analyzer® is utilized to conduct an economic assessment for the different scenarios. In addition, a mathematical optimization model is developed and will be solved using the Genetic Algorithm of MATLAB to determine the optimal blending scenarios that satisfy both technical and economic preferences.

Keywords: Livestock manure, Liquefaction, Blending ratio, Biocrude, Simulation.

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Synthesis of industrial parks with risk management

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Abstract

With the urgent need to drastically reduce greenhouse gases, industrial parks which capture emissions and systematically utilize or store them are crucial to combat climate change. Industrial ecology and circular economy enable these parks to realize profitable and sustainable circularity through process integration. While many approaches such as those by Lovelady and El-Halwagi (2009), Chae et al. (2010), and Al-Mohannadi and Linke (2016) integrate resources such as water, energy, and carbon individually, Ahmed et al. (2020) proposed an approach that integrates both material and energy resources simultaneously. Carbon Capture Utilization and Storage (CCUS) strategies analyze different carbon sources and sinks, for instance, through graphical techniques that utilize source-sink allocations (Lameh et al., 2020) and marginal abatement costs (Lameh et al., 2021). These techniques, however, only look to a limited number of materials at a time, Multi resource integration allows for greater circularity through the optimization of all resource flows including both material and energy. The approach developed by Ahmed et al. (2020) uses a simple mixed-integer linear programming (MILP) model based on a novel representation that accounts for any resources and processes within an industrial park through resource lines. The flow of resource inputs, outputs, and exchanges, along with the existence and capacities of processes in the network, are identified through this model. The approach was further developed to design carbon negative industrial parks, where utilities are imported (Abraham et al., 2021) or produced in-house (Abraham et al., 2021). Furthermore, the multi-resource integration approach was extended to develop a multi-objective approach that considered economic and environmental trade-offs (Ahmed et al., 2021) and a multi-period approach that considered multiple time periods (Abraham et al., 2021). Thus, process integration that considers all involved resources, both material and energy, are essential in creating sustainable systems.

Although the premise of process integration allows industrial parks to improve their efficiencies and obtain greater collective benefits, they inherently entail a degree of risk. The operational risks that arise from the individual operation of its members and the exchange of resources between them can alter the operation, and ultimately the cash flows of the industrial parks. Simply put, the individual operation of any park member carries a certain degree of operational risk regardless of its participation in a cluster. However, the risk that arises from exchanging a resource only occurs when an industrial park is established. The exchange between park members thus brings greater operational risk than traditional stand-alone facilities since, in addition to the failure of either the receiving or supplying park members, the failure of the connection itself can interrupt operation. The importance of managing these inherent risks is evident in the indisputable reservations that exist with the implementation of industrial parks, albeit with their increased material and energy efficiency. Gong and You (2018) developed a general framework for resilience optimization that quantifies resilience as a ratio of the number of products manufactured with disruption to that without disruption. A multi-objective two-stage adaptive robust mixed-integer fractional programming model was formulated

in their work where the first and second stages determined design before and after the occurrence of identified disruptive events. The disruption and recovery studied here does not incorporate operating expenditures, which is a practical limitation to their work.
To integrate risk management in industrial parks for resilient design and operations, the risks for each member and all possible exchanges must first be identified and quantified. With the risks determined, different pathways by which each risk can be reduced, for example, either through parallel or backup strategies, are established. When a risk reduction pathway is integrated with its respective park member or exchange infrastructure, their quantitative risk measure calculated prior to integration will decrease. Suppose every park member, resource exchange infrastructure, and their respective risk reduction pathways can be represented as input/output process modules in this manner. In that case, it is highly plausible that risk can be effectively managed by formulating an optimization problem. Developing a quantitative measure of risk is crucial for risk management, where a low-risk design is expected to yield greater capital and operating costs. In an industrial park, park members can be dependent on external feedstocks, other park members, or both. Thus, it is crucial to understand the likelihood and severity of each disruptive event and its respective cause when quantifying the risk, so that the trade-offs between risk management and cost efficiency can be strategically assessed. By managing the risks within industrial parks, a true understanding on the validity of the uncertainties associated with their deployment can be warranted.

Keywords: Eco-industrial Parks, Optimization, Operational Risk, Sustainability, Circular Economy.

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Systematic Pairing Selection for Economic-oriented Constraint Control

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Abstract

This work considers the problem of minimizing economic losses due to system-wide production systems, where different subsystems share hard coupling constraints. The hard coupling constraints need to be tightly controlled, and it is important that it is done in a way that the overall system remains close to optimal in the time it takes for the much slower optimization layer to implement the required input changes. The particular application that we study is a large-scale subsea gas-lifted oil production network, where different subsystems have a local objective and the shared constraint can be a common compressor, but the method has general applicability to any system with time-scale separation between control and optimization layers.

Repeatedly solving numerical problem between slower and subsystems layers can be computationally extensive. Morari et al. (1980) proposed to eliminates the numerical optimization problems by indirectly moving the problem into the control layer. Recently, a method called distributed feedback-based real-time optimization is applied to a subsea gas-lifted oil well production system (Dirza et al., 2021) to avoid solving the numerical problem online. However, this approach has several limitations in practical aspects, and one of them is no economic-oriented self-optimizing strategy in the time window between the 'time-point' when the slower layer updates the shadow prices. This case happens when the disturbance is faster than the slower layer's sampling time. Knowing that constraint control plays important role in minimizing loss (Skogestad, 2000), this work contributes in addressing this issue by answering the question of 'Which manipulated variable (MV) is economically best to be paired with constrained variables in that time window?'.

To pair the constrained variables and an MV, we propose a pairing procedures that are based on MV's sensitivities to its local disturbances, assuming that there is no saturation issues in the possible MVs, no back-off problem, and equal value of constraints - MVs gain. Meanwhile, the remaining MVs control their self-optimizing variables. The simulation results of the application show that the proposal is able to avoid steady-state violation and reduce more profit loss than other pairings.

Keywords: Production Optimization, Self-optimizing Control, Active Constraint Control

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Quality assessment for dynamic, hybrid semi-parametric state observers

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Abstract

Simulation models as part of software and further as part of smart equipment are envisioned to become increasingly important for smart, modern plants as part of Industry 4.0. More flexible production cycles require simulation models to be adapted frequently because of changes to the plant structure, process settings or system and to be quality assured accordingly. Since the underlying processes for the simulation models are often not completely understood, hybrid and data-driven methods are a promising approach to combine process knowledge with process data for more reliable and precise simulation models (von Stosch et al., 2014).

In this paper, the conducted quality assessment utilizes the framework proposed by Mädler et al. (2021) for quality assurance of black-box models and is applied to hybrid simulations models. The quality model is revised and expanded to include quality factors, criteria and metrics for dynamic, hybrid semi-parametric simulation models. The use case is a state observer for the estimation of key process parameters that are not easily measurable online or can only be measured offline (cf. Kadlec et al., 2009). The applicability of the state observer is demonstrated on the example of a fermentation process. For this several hybrid models of the fermentation with differing levels of detail are identified and coupled with an extended kalman filter.

It was found that the quality model for hybrid semi-parametric models can successfully be used to assess quality differences in different types of hybrid state observers. The quality model allows a structured and quick assessment of not only the first principles and data-driven components of the model but also the used data and is therefore able to show e.g. the performance improvement of the hybrid model coupled with an extended kalman filter in comparison to a solely parametric model. With the extension of the quality model to hybrid state observers and therefore the quality assessment framework, a broader range of simulations models can be automatically assessed within the framework.

Keywords: Quality assessment, hybrid semi-parametric models, state observer, extended kalman filter.

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ANN-assisted optimization-based design of energy-integrated distillation processes

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Abstract

The design of downstream processes is a critical task since they account for 40 - 90% of the overall expenditures of most chemical plants (Haan et al., 2020). Especially distillation-based processes have received considerable attention in the development of optimization-based design methods. However, due to the complexity of accurate thermodynamic, cost, and sizing models, the resulting non-convex mixed-integer nonlinear programming (MINLP) problems are usually solved by local optimization techniques. This is particularly true for highly integrated distillation processes, for which process feasibility depends strongly on the provision of good initial solutions.
To overcome the limitations of a direct solution of the complex MINLP problems, various strategies have been proposed, which utilize machine learning methods for the generation of simpler but accurate surrogate models. Therefore, especially Gaussian processes and artificial neural networks (ANNs) have been used to replace either parts of the original process model, such as the complex phase equilibrium models, or the overall column models (McBride et al., 2020). Further, global optimization of ANNs in a reduced-space formulation has been illustrated even for full process flowsheets (Schweidtmann et al., 2019). However, application of such methods usually requires numerically robust simulation models, which enable an efficient sampling of the search space.
In this work, a different approach with ANNs is proposed to exploit an efficient and robust local deterministic optimization approach overcoming the limitations of local solutions. Therefore, the ANN acts like a top-level metaheuristic providing valuable initial values for a subset of design variables in combination with a sufficient exploration of the design space, similar to the hybrid optimization approach by Skiborowski et al. (2015).
The applicability of the algorithm to highly nonlinear and multimodal problems is verified on several test functions, while considering an adaptive sampling procedure with different measurements for the exploration and exploitation progress as well as the model variance. Finally, the hybrid algorithm was successfully applied to the design of a direct column sequence for the separation of benzene, toluene, and xylene considering the possibility of direct heat integration, thermal coupling, and the application of a dividing wall column.

Keywords: optimization, artificial neural networks, distillation, energy integration

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Application of multiplicative homomorphic encryption in process industry

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Abstract

Flexibility and mobility of modern value chains have created a necessity of continuous information exchange between involved chain parties. In such process industries, many companies share their assets with each other and consequently provide control over them. By this means, some sensitive essential information about operations and control methods could be leaked from the asset provider to the user and vice versa. Therefore, such information sharing raises confidentiality concerns between the service provider and its operator. The goal of this work is to present a confidentiality-preserving information sharing model for the time series use case in process industry. There are various ways to maintain privacy of the sensitive information such as anonymization and encryption. To preserve control for the user and to allow data gathering about the asset operation by the vendor, homomorphic encryption methods could be implemented. Homomorphic encryption allows to preserve confidentiality of the data while enabling computations on the encrypted data. The main focus of this study is an investigation of homomorphic encryptions with multiplicative properties, such as RSA and ElGamal which can be applied to exchange process data related information. This approach is based on the simulation of the use case between asset vendor and asset operator. The confidentiality model of the information exchange sustains the zero-knowledge proof between involved value chain partners. Thus, the comparison between applications of two homomorphic cryptosystems with multiplicative properties is conducted. This research investigates the probabilistic and the deterministic homomorphic algorithms with respective differences in encryption and decryption speeds. The result implies the major differences in the implementation of both methods within the privacy-preserving sharing model. This study is limited to the use case with application of partial homomorphic cryptosystems in the process industry. The outcome highlights the necessity for further confidentiality improvements by predictive estimation of encryption efficiency.

Keywords: confidentiality, homomorphic encryption, value chains, process systems, secure information exchange

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PPOPT - A new solver for Explicit Model Predictive Control

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Abstract

Multiparametric programming is the mathematical optimization methodology of solving an optimization problem explicitly and offline to reduce the real-time optimization's computational burden. Multiparametric Model Predictive Controllers (mpMPC) is a class of Model Predictive Controllers (MPC) where the entire MPC optimization problem is solved offline Pistikopoulos et al. (2015). Multiparametric programming-based algorithms have been formulated to solve control Pistikopoulos et al. (2015), multilevel optimization Avraamidou and Pistikopoulos (2019), and robust optimization problems Avraamidou and Pistikopoulos (2020) . The current state-of-theart multiparametric solvers are POP from Oberdieck et al. (2016) and MPT3 from Herceg et al. (2013). However, neither solver leverages parallel algorithms and does not scale with hardware innovations, such as multiple cores.

In this work, we describe the PPOPT (Python Parametric OPTimization) package for an open source multiparametric solver written in Python. It is a general-purpose package that features: A) Efficient and parallel implementations of multiparametric programming algorithms, with strong scaling performance with greater than 25 cores, B) Problem reformulation to reduce the computational overhead and increase numerical stability, C) Multiparametric solution code generation to export solutions for multiple different platforms. The speed and scaling behavior of PPOPT are explored with computational studies on the MPQP1 and MPLP1 problem libraries and with explicit MPC controller design. PPOPT is compared to the current state-of-the-art multiparametric solvers: POP and MPT3. Additionally, the exported solutions are benchmarked on a wide array of platforms, including microcontrollers, single-board computers, and desktop computers.

Keywords: Multiparametric Programming, Real Time Optimization, Mathematical Programming, Model Predictive Control, Explicit Programming

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Parallel Simulated Annealing approach for optimal process plants instrumentation

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Abstract

Process information is the foundation upon which other plant activities (monitoring, control, optimization, planning and scheduling, fault diagnosis, etc.) are based. To fulfill information requirements regarding its quality and availability is essential to install an appropriate sensor network (SN) in the plant, and also data reconciliation and SN maintenance tasks should be executed during process operation Carnero et al. (2018); Rameh (2018). The SN designer should decide to measure each process variable or not. These decisions are mathematically formulated in terms of binary variables. A combinatorial optimization problem results, which is usually multimodal and involves many binary variables. Its solution has been addressed using tree search algorithms, MILP techniques, and heuristics procedures. It is known that in this type of NP-hard problems, heuristics are an appropriate resolution approach. For real chemical plants, this may require solving very large instances, which implies high computational costs. To reduce the computation time, parallelization techniques have been applied, achieving a substantial improvement in the performance of the implementation. In this work, a parallel Simulated Annealing (SA) Kirkpatrick et al. (1983); Cicirello (2017) algorithm is proposed to optimize the SN design problem. In this model, many self-contained SA algorithms are launched in parallel. They may or may not cooperate to solve the target optimization problem. When the cooperation is carried out, the self-contained SA exchanges information to improve the quality solutions and enhance efficiency. Furthermore, this kind of model offers a problem-independent parallelization. Case studies of incremental size are used as application examples. Moreover, a large instance over a well-known problem in chemical engineering literature is tackled.

Keywords: Simulated Annealing, parallel computing, sensor network design; combinatorial optimization; metaheuristics

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A sparse polynomial surrogate model for the shrinking core model in phosphate ore digestion

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Abstract

In the phosphate industry, phosphoric acid is a major component in the manufacture of fertilizers. The optimization of its process performances is very challenging and aims to extract the maximum amount of P_2O_5 from the ore, crystallize and precipitate a gypsum with optimum filterability and washing characteristics, and produce the purest phosphoric acid possible, at a lower cost and with limited impact on the environment. The mathematical formulation of optimization problems is generally based on a first-principles process model. However, such process model usually involves many ODEs and PDEs which are time consuming to integrate, thus making the optimization algorithm very slow. A high-fidelity surrogate model to compute the required outputs from the inputs faster than the phenomenological model is therefore needed.

In the present communication, an accurate surrogate model is derived from a shrinking core model developed for the dissolution of phosphate ore in an industrial digestion tank (Elmisaoui et al., 2021). The surrogate model allows to compute the time-varying profiles of concentrations of different components involved in the liquid bulk and in the ore particles, particles radius, and thickness of the liquid film surrounding the ore particles. The main model inputs are temperature, initial radius of particles, initial acid concentration and hydrodynamic conditions. The surrogate model is based on sparse multi-variate polynomial interpolation (Rabhi et al., 2018) generalized to approximate a time dependent vector-valued quantity of interest. To ensure the physical coherence of the surrogate model, particularly in preserving specific properties of the phenomenological model (monotony, positivity of some outputs, etc.), the properties which are always kept by the surrogate model and those which are only preserved at the limit of infinite interpolation points are established. Therefore, increasing the number of points ensures that these properties are checked up to a small convergence error. As an example, the evolution of the particle radius should be strictly decreasing but this is not 'automatically' satisfied by an interpolating surrogate model. In this work, we present effective strategies to ensure the physical properties without refining the interpolation. The predictions of the resulting surrogate model are in very good agreement with those of the first-principles model, and the computation time is drastically reduced, i.e., only 2% of the CPU time required to solve the first-principles model.

Keywords: Digestion, Shrinking core model, Surrogate model, Sparse polynomial interpolation.

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Global Superstructure Optimization with Nonconvex Models: Comparison of MINLP Formulations

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Abstract

Superstructure problems are typically solved as mixed-integer nonlinear programs in either the Big-M or Convex Hull formulations. However, for global optimization of problems that already contain nonconvex terms in the unit operation models or the objective, alternative formulations that introduce additional nonconvex terms but enable smaller optimization problems could be a promising alternative. We compare such formulations in both full-space and reduced-space formulations in BARON and our open-source solver MAiNGO and show they can be faster to solve than the conventional ones.

Keywords: Branch-and-bound, mixed-integer, convex hull, Big-M, reduced-space

1. Introduction

Superstructure optimization is a powerful tool for process design. Superstructure problems are typically solved as mixed-integer nonlinear programs (MINLPs), which are either formulated directly or as reformulations of generalized disjunctive programs (GDP) (Grossmann & Trespalacios, 2013). Common formulations for these MINLPs include the Big-M and Convex Hull formulations. These have desirable properties in case the constraints describing the unit operations and the objective are linear or convex: they avoid nonconvex terms in the problem altogether. Thus, they result in mixed-integer linear programs or MINLPs with convex functions, both of which can be solved rather efficiently in practice. However, in case the model already contains nonconvex terms, the resulting problem is inevitably an MINLP with nonconvex functions, which requires deterministic global optimization to guarantee optimal solutions. In this case, it is not clear whether the Big-M or Convex Hull formulations are the most suitable ones to enable short computational times. In this work, we compare these established formulations with less conventional ones for the special case of selection between alternative units.

2. Formulations

We consider the choice between alternative processing units from a set D. The flow rate through each unit $i \in D$ is F_i, and $\sum_{i \in D} F_i = F$, where F is the overall flow rate through the units. We assume that each unit i contributes to the objective through a term that goes to zero as the flow rate F_i goes to zero as well as through a constant term.
In common MINLP formulations, each unit is associated with a binary variable y_i and the exclusive choice is enforced as $\sum_{i \in D} y_i = 1$. In the *Big-M* formulation, the remaining expressions for individual units are (de-)activated using the y_i and suitable parameters $\boldsymbol{M}$ in inequality constraints. In the *Convex Hull* formulation, copies of the continuous

variables are introduced for each i along with linear inequalities forcing the copies in inactive disjuncts to zero via the y_i. Nonlinear constraints are tightened through the perspective function. The Convex Hull formulation is known to be tighter than Big-M, but in its conventional form, it has more variables (Grossmann & Trespalacios, 2013).
As an alternative, we consider a *Bilinear MINLP* formulation that calculates the unit flow rates as $F_i = Fy_i, i \in D$, which potentially introduces new nonconvex terms beyond those already present in the unit operation models or the objective. The constant terms in the objective function from each i are also multiplied by y_i to disable them for inactive units. This formulation has as many variables as Big-M, but fewer constraints.
Finally, we can avoid introducing binary variables altogether through an *MPEC* formulation that models the exclusive choice through as $F_i F_j = 0, i \neq j$. To deactivate the constant terms in the objective function, we use the step function (or a smooth approximation) taking the corresponding F_i as argument. Instead of the bilinear MPEC constraint, one can also use the so-called *Plus* function, $F_i - \max(0, F_i - F_j) = 0, i \neq j$.
Each of these formulations can also be written as a *reduced-space (RS) formulation* (Byrne & Bogle, 2000), which we have shown to be beneficial for flowsheet optimization (Bongartz & Mitsos, 2017). In these RS formulations, equality constraints are used to eliminate variables from the problem. In the RS formulations, Big-M and ConvexHull often have the same number of variables – in contrast to their conventional (full-space) counterparts. The MPEC, Plus, and Bilinear MINLP formulations often have even fewer variables in RS than Big-M and Convex Hull.

3. Case Studies

To compare the formulations, we have solved simple illustrative examples both with our open-source solver MAiNGO (Bongartz et al., 2018) and with BARON (Kılınç & Sahinidis, 2017). The MPEC, Plus, and Bilinear MINLP formulations were often similarly fast or faster to solve than Big-M and Convex Hull. Especially for MAiNGO, the RS formulations significantly reduced computational time, which can be attributed to the McCormick relaxations used in MAiNGO. For Big-M and Convex Hull, BARON outperformed MAiNGO thanks to its more sophisticated integer handling.

4. Conclusion

We show that for global optimization of superstructure problems with nonconvex models, unconventional formulations that introduce nonconvex terms can be a promising alternative. These formulations can be smaller and faster to solve than Big-M or Convex Hull formulations while also enabling rather intuitive modelling.

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On the use of data engineering and machine learning in global optimization applications with cutting plane approximations

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Abstract

This work explores data analytics in the development of optimization methodology for global optimization, as applied through decomposition methods and cutting plane algorithms. It capitalizes and builds on innovations by Baltean-Lugojan et al. (2019), that focus on a generic and effective outer approximation method suitable for semidefinite relaxations. Cutting planes are treated as data populations, generated at each iteration of the algorithm; population elements are renewed based on the incumbent solution. Data technology is subsequently applied to measure fathom and screen planes, also to represent data spaces of the dual problem. The geometry of space is explored through various metrics, aiming to evaluate correlations in the solution space. The key element of the referenced work is the decomposition of high-dimensional cutting planes into their low-dimensional counterparts. Such method results in a combinatorial explosion of available cutting planes for the separation problem and thus novel selection measures have been introduced based on feasibility violation and improvement of the objective function. In this paper, the separation problem is examined using clustering techniques. The data approach is tested against a library of quadratic and box constrained optimization problems, that feature varying sparsity and density patterns. The affinity metric is introduced, to efficiently evaluate and screen cutting planes generated from different sub spaces. The cosine similarity examines the direction in which the objective function is driven. Among other methods, spectral clustering is applied with a twofold objective: visualize the solution space and represent the data in the dual space. Overall, analytics are found to dramatically improve the duality gap and the quality of the solution, consistently in all the problems tested. As the complexity of the problems increases, the gap closure is widened and the proposed clustering techniques outperform the Reference algorithm. The best performance is observed by the use of the affinity metric followed by Hybrid1. In conclusion, the geometrical interpretation of the dual space holds the most promising lines for future work.

Keywords: global optimization, cutting planes, cut selection, data analytics

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A systematic approach for the processing of experimental data from anaerobic syngas fermentations

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Abstract

The development of the large-scale anaerobic syngas fermentor requires the design of mathematical models that are able to reproduce the *i)* characteristics of mass transfer from the gas to the liquid and the *ii)* microbial metabolic responses to the stimulus provided by the extracellular environment. The collection and adequate processing of experimental substance concentrations are the main source of information about the state of bacteria during fermentations.

This study describes a methodological framework designed for the systematic processing of experimental syngas fermentation data for its use by metabolic models at pseudo-steady state and at transient state. The developed approach allows the use of not only own experimental data but also from experiments reported in literature which employ a wide range of gas feed compositions (from pure CO to a mixture between H_2 and CO_2), different pH values, two different bacterial strains and bioreactor configurations (stirred tanks and bubble columns).

The developed data processing framework includes *i)* the smoothing of time-dependent concentrations data (using moving averages and statistical methods that reduce the relevance of outliers), *ii)* the reconciliation of net conversion rates such that mass balances are satisfied from a black-box perspective (using minimizations), and *iii)* the estimation of dissolved concentrations of the syngas components (CO, H_2 and CO_2) in the fermentation broth (using mass transfer models). Special care has been given such that the framework allows the estimation of missing or unreported net conversion data and metabolite concentrations at the intra or extracellular spaces (considering that there is availability of at least two replicate experiments) through the use of approximative kinetic equations.

The metabolite concentrations and conversion rates obtained through the application of the proposed framework has allowed *i)* the parameterization of metabolic models at pseudo-steady state and transient state and *ii)* through the use of those models, the assessment of the distribution of carbon and electrons inside cells.

Keywords: Syngas fermentation, experimental data processing, fermentation data reconstruction, data reconciliation.

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Techno-economic optimization of plastic waste pyrolysis oil hydrotreatment under parametric uncertainty

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Abstract

Motivation: Driven by the increasing public attention to plastic waste and associated problems, there is a growing interest in new methods for recycling plastics as an alternative for mechanical recycling. One of those methods is pyrolysis by which oils can be produced with many potential applications. This research specifically focused on pyrolysis oils derived from waste polyolefins (PE, PP) which typically consist of paraffins and olefins that are contaminated with oxygen and/or nitrogen-containing organic molecules (oxygenates and nitrogenates). These contaminations originate from food residues, paper fibers, additives and other (non-polyolefin) polymers. In this work, the emphasis was on the removal of oxygenates from pyrolysis oils as these are undesired due to the negative impacts, such as non-volatility, corrosiveness and thermal instability. Therefore the purification of this mixture is inevitable to provide a higher quality product.

Methods: In this research, the hydrotreatment of pyrolysis oil has been optimized with respect to a techno-economic analysis inspired objective function (integrating capital costs and operational costs) in MATLAB® using a pattern search algorithm and the model from Gracida-Alvarez et al. (2019). The model is based on the pyrolysis of HDPE which results in a mixture of methane, ethylene, propylene, aromatics, which all are separated through distillation units and low/high molecular weight hydrocarbons that are hydrotreated. The operating cost of hydrotreatment is high because of the high hydrogen cost with a price of 2,83 USD per kg as a base case (Gracida-Alvarez et al. (2019)). The hydrotreatment process in this model uses 330 kg hydrogen every hour to convert 12046 kg unsaturated hydrocarbons, Figure 1. A 100% conversion for alkenes/alkadienes and a 50% conversion for aromatics is assumed.

Results: Hydrotreatment is a cost intensive process, the operating costs are 90% of the total costs. The total operating cost of the studied process is mainly determined by the hydrogen consumption (934 USD/h) which amounts to 70% of the total cost. The other operating expenses are mainly originating from the hydrotreatment reactor which uses a catalyst and works at 150°C and 1 atm. Catalyst costs

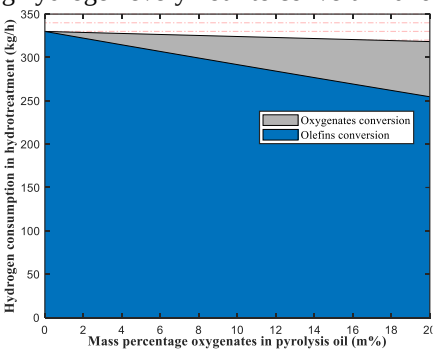

Figure 1: Effect of the increasing mass percentage of oxygenates in pyrolysis oil on the hydrogen consumption in hydrotreatment

amount to 15% of the total cost. The capital costs are less than 10% of the total cost.

The hydrotreatment process was optimized by varying the feedstock composition. The uncertainty of the hydrogen price is studied for comparison with different treatment methods. Pyrolysis oil from waste plastic typically contains a high amount of olefins beside oxygenates and nitrogenates. Therefore hydrotreatment is an interesting technique for upgrading to applications in fuel industry. Unsaturated carbon chains are unstable and more toxic, hence, therefore less desirable in fuels such as gasoline. However, the high olefin content results in a high hydrogen demand and rises the cost of the process.

Comparison is made to alternative routes to obtain purified deoxygenated and denitrogenated pyrolysis oils which still contain unsaturated carbon chains and aromatics to be used in higher added value applications including plastics, detergents and adhesives. As there is to date no dedicated market for such purified pyrolysis oils, price uncertainty is high. The product price is assumed to be the same as for naphtha but could be higher. If new methods could purify pyrolysis oil without the loss of olefins at a lower cost than hydrotreatment, the demand for this product could increase. It is also taken into account that the price of hydrogen could decrease as a result of new technologies and thus the cost of hydrotreatment. These uncertainties are quantified and compared. The novelty of this work is the methodology combined with the approach for pyrolysis oil purification.

Conclusion: The hydrotreatment of pyrolysis oil has been techno-economically optimized and compared with alternative hydrogen-free purification processes. The composition of the feedstock has an impact on the cost of the purification. If more oxygenates and nitrogenates are present, the total cost of alternative methods could increase significantly. This is not the case for hydrotreatment. Both unsaturated molecules and oxy- & nitrogenates will be converted in the hydrotreatment process. As shown in Figure 1, pyrolysis oil with a 20% (mass basis) of oxygenates only decreases the hydrogen consumption with 3.6%. Therefore, the cost of hydrotreatment stays relatively stable in function of those impurities as it is mainly determined by the hydrogen consumption. The polynomial chaos expansion method has been implemented to account for the uncertainty on the composition of the pyrolysis oil entering the hydrotreater during the optimization, the product stream and the price of hydrogen (Bhonsale et al. (2019)). As such a robust process operation with respect to techno-economic performance and product purity is achieved. The techno-economic limitations of hydrotreatment for upgrading plastic waste pyrolysis oil have been quantified for a range of possible plastic waste pyrolysis oil compositions.

Keywords: Pyrolysis oil, Plastic waste recycling, Techno-economic assessment, Process optimization, Process flowsheet simulators.

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Process Systems Engineering prospects in Circular Economy implementation in industry

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Abstract

Many organizations, academics, companies and policy makers have acknowledged the circular economy as an enormous opportunity for more sustainable industrial models and strategies. According to this viewpoint, companies can make substantial cost savings and further revenues by adopting circular business models. Nowadays, these new business models are linked to the Industry 4.0 being transformed to an intelligent, connected, and decentralized production.

Industry 4.0 creates numerous opportunities for businesses to improve circular performance and can operate as a firm coordinator for optimizing the usage and utilization of resources as well as improving the monitoring of product lifecycle steps.

The present research is a part of a wide scope research activity with purpose to explore how rising technologies from Industry 4.0 can be integrated with circular economy (CE) practices to establish new methods, approaches and tools for the optimal use of resources in the industry in the whole life cycle of the materials and products, acknowledging the need in adopting circular economy principles in order to improve longevity of resources. The expected outcome of the study is the specific recommendation of circular (techno economic, optimization) prototypes and models for the process and manufacturing industry in order to make the optimal use of resources in the entire life cycle of materials and products including materials reuse, energy recovery, products remanufacturing, waste minimization, all relevant to minimizing resource consumption and negative environmental impacts. This will be implemented integrating industry 4.0 technologies, optimization models, feasibility studies and life cycle analysis to support CE practices.

Process Systems Engineering tools will play a very significant role in this novel area, by the development of relevant integrated models for the industry to use less resources and produce less waste when producing materials and products, enable circularity in the manufacturing and process industry focusing on the recovering and reprocessing of materials and products that will lead to the optimization of resources exploitation.

Process Systems Engineering (PSE) tools, able to integrate various production stages considering technical, economic and environmental considerations, will prove to be the most rational tools to approach these problems. Furthermore, Industry 4.0 technologies and tools will set the framework for the integration of the above and materialize the synergies leading to optimization of processes in a circular economy concept.

The work will highlight the potential of the PSE tools for the solution of the above problems. In parallel, the importance of a new field of PSE tools implementation and expansion will emerge as an outcome of the work providing very interesting and challenging perspectives in addition to their existing fields of application.

Keywords: PSE prospects, Industry 4.0, circular economy.

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Incremental financial analysis of black liquor upgraded gasification in integrated kraft pulp and ammonia production plants under uncertainty of the feedstock costs and carbon taxes

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Abstract

The pulp and paper sector is classified as an energy intensive activity and several efforts are being made to mitigate its atmospheric emissions, improve the recovery of residual heat and capitalize on its byproducts. The black liquor (BL) is a byproduct of the kraft pulping process, which contains more than half of the energy content in the total woody biomass. The BL can be gasified and the syngas can be used to generate electricity or produce chemicals and biofuels, through the broader biorefinery concept.

In this work, the conventional scenario of the BL use (i.e. concentration and combustion) is compared with the BL upgrading gasification process for ammonia production. The chemical processes synthesis, modeling and simulation are performed by using Aspen Plus® software, as reported in (Domingos et al., 2021). The determination of the heat recovery and the solution of the energy integration problem is handled by a mixed integer linear programming model. A sensitivity analysis of the variation of the INPV as a function of the carbon taxation (0-100 EUR/t_{CO2}) and the interest rate (0-21%) is performed. Firstly, it is assumed that the present values of the feedstock and the products are set as constant. Next, the incremental financial analysis incorporates the uncertainty related to the acquisition and selling costs of the feedstock and fuels produced, when embedded in a volatile market, by using the Monte Carlo method.

In anticipation of future carbon taxation scenarios, the incremental economic analysis found that only ammonia production route with partial electricity import may economically outperform the conventional kraft pulp mill for moderate carbon taxations (40-90 EUR/t_{CO2}), depending on the interest rate adopted. In this regard, middle-to-high carbon taxations (30-100 EUR/t_{CO2}) may render ammonia co-production attractive in the Brazilian context of a highly renewable electricity mix. This range is in agreement with that suggested by the High-Level Commission on Carbon Prices, which estimated that a global CO_2 price of 50-100 USD/t_{CO2} would be needed by 2030 (WBG, 2020) to achieve the goals of the Paris Agreement.

Keywords: Black liquor, Kraft process, Uncertainty, Ammonia, Decarbonization.

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A Capex Opex Simultaneous Robust Optimizer: Process Simulation-based Generalized Framework for Reliable Economic Estimations

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Abstract

During the design of a process, the most economically impactful choices are often taken with limited data and details available on the specifics of unit operations. Despite this fact, the effect some of these choices have on the final economic performance of the plant can be dramatic and far more influential than later decisions. The availability of fast and reliable preliminary cost estimations based on few key design parameters for the most common units can go a long way in improving flowsheet design. Due to the early design stage, these estimates don't need to be very accurate since errors in the range of 50% are admissible as long as the estimation requires few input data. Automating the costs computation process and making the interface with the most common simulation packages standardized and easily accessible for users not accustomed to programming languages is very important in speeding up the cost evaluation of the plant and reducing the human resources tied to this task. These concepts stand at the core design of the CAPEX OPEX Robust Optimizer (CORO) developed in this work. Aspen HYSYS serves as the commercial simulation package to estimate the input variable of the economic libraries. Excel is used both as a GUI and as a data extraction tool from Aspen HYSYS due to its widespread diffusion in industry and versatility provided by Visual Basic for Applications. The CORO code is detached both from Excel and HYSYS and interacts only with a standardized xml data sheet to allow for in-house expansions to other simulation packages. The long-term development goal is a generalized CAPEOPEN interface working with every commercial software that supports the interface. In the current CORO release, the interface can interact only with Aspen HYSYS. This paper will showcase the economic libraries implemented in CORO, the mathematical C++ optimization libraries, the overall structure of the tool, planned future expansions, and customization options.

Keywords: Economics, Aspen HYSYS, Simulation, Optimization

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A soybean supply chain model to analyze the greenhouse gas emissions of the transport sector

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Abstract

The study of agri-food supply chains is of great interest for agricultural producer countries due to its importance in the national economy and because of its participation in international markets. The supply chain modelling can become an important decision-support tool to improve resource management, the economy and environmental aspects involved in the operation. One of the main obstacles that prevent the use of this type of tool in the decision-making process, is that data collection and the representation of material flows at different scales is costly in terms of time and personnel required. Despite the large amount of information available from several public and private sources, there not exists a supply chain model that accurately represents its operation and the actors involved in the chain.

This article presents a mathematical model of the soybean´s supply chain for Argentina where the different stakeholders and the material flows among them are represented. The objective is to study the transport used in this sector: trucks, trains, and river ships. The use of diesel trucks involves millions of trips per year covering around 80% of the total transported, trains 15% and ships the 5% left. The objective is to analyze the greenhouse gas (GHG) emissions made by the transport in this sector by analyzing different scenarios where biodiesel and electrical trucks are used, and the share of trains and ships are increased.

The model generated is a mixed multi-period / multi-objective linear integer model, destined at minimizing operating costs and GHG emissions. To analyze the model behavior in terms of flows among the different levels of the supply chain and the transports used, the model results are compared to two statistical studies made by the Ministry of Transport of Argentina in years 2014 [1] and 2017 [2]. The results show a good fit with those reports. Then, an analysis of scenarios is carried out, where the transport costs of soybean and the number of emissions is optimized, according to the transport used. The results show the tradeoff between costs and reduction of emissions where it is possible to achieve a 30% GHG decrease with a reasonable cost.

Finally, it is concluded that the presented model is an important tool to improve the economic, social, and environmental aspects of the supply chain network. Some of those issues (the social aspect for example) will be included in future work.

Keywords: soybean, supply chain, emissions, transportation

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Ontology for Enhanced Industrial Process Control

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Abstract

The cyber-physical integration in the sense of industry 4.0, applied to industrial process control, needs to develop new methodologies. Both top-down hierarchies of commands for ERP, Optimization, Advanced Control, Local Control, and bottom-up flux of information from the plant floor to control system, optimization level, and planning strategy are dissolved, aiming to enhance the vertical and horizontal integration and flexible operability. Even though this is a requirement for Cyber-Physical Systems, it would be merely a coexistence of advanced optimization IoT technologies states of art. Therefore, there is a need for a new architecture of a functional system. Since it works essentially as an event-based system, ontology plays a key concept in the practical working of the new process control. First, an overview of the general ontologies framework applied in industry 4.0, and on the other hand, some ontologies published for chemical process design are discussed extensively here. Then the practical ontology and taxonomy needed for industrial process control are discussed. Here is presented how to recover the functional layers to each specific application of former traditional hierarchy top-down and bottom-up, now named as semantic layers. A description's language development for process control using this ontology is another challenging task, also proposed. A case based on the transition of the traditional batch reactor process to modern industry 4.0 application illustrates the change of the operation mode. Finally, the potential gains and technology limitations are analyzed as a critique as the enabling technologies (or pillars) of Industry 4.0 to show what concepts apply to this enhanced process control. It also compares and analyzes this modern approach in the manufacturing process and the difference with the industrial process control. The construction of a complete system based on ontology and description language ready for application is an impressive task to be developed further. The main objective of the work, for now, is to clarify the concepts and show the methodology with its practical application, discussing limitations.

Keywords: Cyber-Physical Integration, Industry 4.0, Ontology, Process Control

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Complementing Natural Gas Driven Syngas with Optimum Blends of Gasified Biomass Waste

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Abstract

The world strives to diversify the energy portfolio with a suitable alternative to fossil fuels whilst achieving the reduction in environmental impacts from released wastes. Co-conversion of biomass wastes and natural gas (NG) gained high-interest thanks to the potential improvement in downstream power and fuels production while minimizing greenhouse gas (GHG) emissions. This study explores the optimal blending of synthesis gas generated from biomass wastes and NG feeds. Aspen Plus is utilized to develop the models of biomass steam gasification, NG steam reforming and NG auto-thermal reforming considering Qatar's biomass and NG characteristics. Three types of biomass wastes; date pits, sludge and manure are gasified to generate the H_2-rich syngas which is blended later with NG-driven syngas. The simulated flowsheets have then been used to optimize the blending of downstream generated syngas by means of manipulating the biomass wastes and NG feeds. The optimization problem is constrained by the downstream quality of produced syngas to be utilized for the generation of power and fuels. Typically, the generation of syngas involves high-cost subsequent purification prior to the production of downstream value-added products. However, the optimization attained in this study has lowered the requirement of further syngas purification and waste removal through the blending of NG and biomass-driven syngas. This requirement can be further reduced by manipulating reaction agents and process conditions. The result of the optimization problem demonstrates an increase in biomass wastes utilization with the increase in syngas quality constraint. Dates pits biomass dominated the biomass utilization with a lower contribution from sludge and manure wastes. Moreover, optimum points of operation in terms of pressure, temperature and reaction agents have been drawn through different sensitivity analyses of key process parameters.

Keywords: Natural Gas, Biomass, Co-Conversion, Optimization, Syngas, Blending.

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How tools and technologies can help drive sustainability

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Abstract

The chemicals industry is facing a highly dynamic environment. Demand is continually fluctuating, and the pressure for new sustainable processes and products is rising. New environmental regulations are always expanding and becoming less harmonized globally, and customers are demanding sustainable products that are friendly to the environment. To follow all the market changes and remain competitive, companies need to invest to develop new processes and products. However, since it´s a capital-intensive industry, new investments need to be carefully managed.

Today, companies need to find ways to be more efficient in the execution of engineering projects. One way is to compress engineering cycles and adapt processes and products to comply with sustainable KPIs and new demands. The Unified Engineering methodology is one option enabled by the latest technologies and tools available. For decades, engineering to design and build industrial plants has been developed through projects with a complex and highly iterative workflow, using siloed solutions. The entire process is very time consuming, and the final deliverable to the owner/operator is a set of documents (P&IDs, datasheets, 3D model, etc.) with disperse data, with no guarantee of consistency.

To compress engineering cycles, a data-centric approach must be used. With this approach, documents and applications are always kept up to date with the latest validated data. The data-centric approach is the first step to apply the Unified Engineering methodology, which will evolve later to the plant Digital Twin. The Unified Engineering methodology uses a single source of information that is available for all the teams involved in the project. Drawings, process simulations, line lists, datasheets, 3D models, and isometrics, among others, are regularly updated with the data available in the unified source of information. Engineers become more efficient and work with reliable information as documents and models are updated in a controlled way as soon as any change is made. For even greater sustainability and effectiveness, the best way is to use the Unified Engineering methodology in the cloud. The cloud enables higher degrees of flexibility and collaboration among people working from different locations, which means that always the most appropriate resources can be allocated for each part of the project.

Unified Engineering reduces capital project costs, risks, and delays enabling shorter engineering cycles required to deliver new sustainable projects. By minimizing engineering errors and accelerating project execution, companies can get 5% reduction in Total Installed Cost.

Keywords: sustainability, compressed engineering cycles, unified engineering, process engineering

The use of game theory in the analysis of marine lubricant markets in ports

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Abstract

The supply of marine lubricants to vessels can be arranged by multinational companies (majors) or local suppliers (locals) who have interactions and contract agreements between them. This study concerns to the consumption of marine cylinder oil that is supplied in a port over a period of one year. The multinational companies have the biggest market share for the following reasons. They are established worldwide since many years and their brand is more recognized. From their international network of affiliates, they have access and long-term contracts with several shipping companies worldwide. They have strong R&D departments to continuously develop their products to diversify from competition. On the other hand, the lubricants of the local suppliers meet the specifications of the Engine Builders and ISO specifications and are suitable for the relative application. As the locals are more flexible and possible equally known in the local market, they can also obtain orders against the majors. It is considered that the quality of the lubricants of both suppliers is equal while the lubricants are not the same from each supplier. Furthermore, it is considered that shelling price of the lubricant is the same for both suppliers. The supply chains involve interactions between players as they produce lubricants under the same refinery of the local supplier. The lubricant cost for the local supplier is the production cost, while the major brand is charged with a premium. This premium is corresponding to the major supplier's specifications on the lubricant formulation and additives affecting the production cost. The market share can be significantly affected by the interactions between competitors. The challenge of the paper has been to use game theory to analyze how such a market share is connected to the level of interactions, the market constraints and how they can affect the overall profitability for each player. Straightforward application of the Stackelberg approach is not possible due to the strong interactions between players, the market nonlinear markets, and the fact that market conditions are different for each player. The paper presents the framework of players interactions that it formulates as a bilevel optimization problem with major (leader) and local players (followers) assigned to the outer and inner problems. Market constraints are used with different functions for each player and reformulations consider the impact of market conditions in defining market shares for each player. The model is used to assess threats and promises. The bilevel approach can be used to calculate parameter sensitivity and key aspects to retain market balance and profit share. The approach has been validated with real data in which the analysis achieved to predict the actual market and profit share using the model-based approach. Model extensions subsequently test parameters responsible for system stability and player options that address threatening moves from other players.

Keywords: marine lubricants, multinational companies, local suppliers, game theory, bilevel approach

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Plug Flow Reactor Analysis inspired by Entropy Generation Rate Minimization

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Abstract

Under constant stress in a highly competitive market, the industry has to reinvent itself with new methods and procedures for saving costs and energy in order to stay competitive. In the chemical industry, the reaction sector plays a strategic role in maximizing production, by saving energy and other costs and in providing a minimum of by-products. Tubular reactors, particularly the Plug Flow Reactor, are widely used in the chemical industry because they have a simple geometry, which reduces costs and facilitates maintenance. Thus, a well-established design for such reactors can lead to the best technical solution, being a decisive differential for industrial competitiveness.

To do this, mass and energy balances were considered, in addition to kinetic concepts to save energy. Having only the energy saving in mind, spontaneity can increase, which is desired, but at the expense of loosening the level of organization of the reactive system, that is, an increase in entropy, indicating that more by-products are being produced. Such a high by-production can generate negative impacts on the total energy saving. Although reversibility is an ideal transition between states, it plays an essential role, at least from a conceptual point of view, as maximum conversion, maximum work and maximum heat transfer occur in it (Bispo et al., 2013) Consequently, it is under reversible condition or in the condition closest to reversibility that the process must be carried out. First Principles on their own are not enough, because the First Law of Thermodynamics does not impose any restriction on the processes of heat transfer. Therefore, the Second Law of Thermodynamics should be used for imposing such restrictions, with a view to driving the system to the reversible state. To do this, the introduction of the entropy balance and the minimization of its production enables the system to be brought as close to reversibility as possible. Since some conditions and restrictions can be imposed on the system, then the set of Equations that governs the reactive system can be given by Eqs. (1) to (3). And, by rearranging such Equations, Eq. (3) can be modified to generate the Eq. (4).

$$\frac{\partial C_i}{\partial l} v_l = \pm r_i \tag{1}$$

$$\left[\left(\frac{\partial H}{\partial T}\right)_P \frac{dT}{dl}\right] v_l = \pm \dot{Q} + \Delta H_R(-rV) \tag{2}$$

$$\left[\left(\frac{\partial S}{\partial T}\right)_P \frac{dT}{dl}\right] v_l = \frac{\delta \dot{Q}}{T} + \delta \dot{\sigma} - \Delta S_R(-rV) \tag{3}$$

$$\dot{\sigma} = \frac{2\Delta H_R}{T}(-rV) \tag{4}$$

Such an Equation can be used to calculate the entropy production rate for a given process and any commercial software can solve the set of these easily, resulting in the concentration and temperature profiles and entropy production as well as the behavior of the Entropy Production rates.

It is often desirable to estimate the joint effects of conversion and entropy production both on the optimum operating conditions for the system, and on selecting the optimal size of a reactor. Graphical descriptions revealing the simultaneous behavior of conversion and the entropy production can provide a mean for cost/benefit and profitability analysis,

since conversion is related to profitability while the entropy production can be associated to cost, indicative of increased by-products. This study is based on the transesterification reaction for the production of biodiesel from supercritical methanol, based on the work of van Kasteren and Nisworo (2007), whose data has been reproduced and where Figure 1 shows the profiles obtained for conversion and temperature.

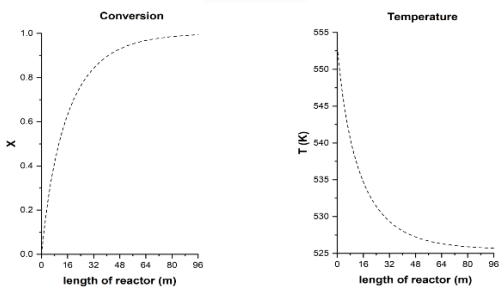

Figure 1: Profiles for Conversion and Temperature.

Figure 2A presents the entropy production rate, and the total entropy produced, represented by the shaded area. Where the shaded region indicates the net profit obtained after the optimization procedure, Figure 2B. The intersection point represents the optimal reactor size, which approximately corresponds to 18.8 m, 80.2% smaller than the base case developed by van Kasteren and Nisworo. Table 1 presents the technical and economic comparative analysis.

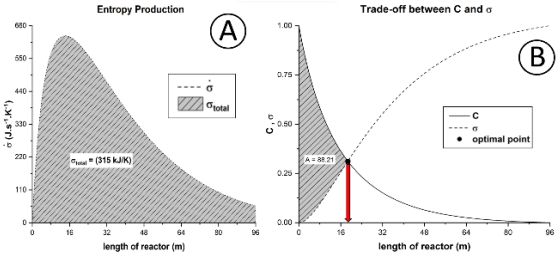

Figure 2: Entropy production rate profile and total entropy production and the trade-off between concentration (profit) and the entropy production (variable cost) normalized on a scale of 0 to1.

Table 1: Results obtained from technical and economic analysis.

Data	Base Case (van Kasteren et al.)	Optimized Case (Present Study)
Number of reactors	1	1
Length of a reactor (m)	96	18.77
Reactor cost $(US\$)$	3,790,024.04	1,446,915.82
Annual Producing Rate (ton/yr)	125,951.61	125,951.61
Annual Operating Cost $(US\$/yr)$	30,396,056.94	28,613,513.93
Production Cost $(US\$/ton)$	241.33	227.18

The conclusion to be drawn is that the economic analysis performed after the optimization procedures indicates that the cost of biodiesel production has been reduced by 5.86% for the same annual production, showing that the adopted strategy is potentially advantageous.

Keywords: Thermodynamic, Entropy Production, Optimization.

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An approach combining exergy and pinch analysis for the optimisation of a natural gas and recovered CO2 based methanol production process

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Background and motivation

Following the latest IPCC report (IPCC, 2022), fossil Carbon Capture and Utilisation (CCU) stands out as one major lever to enable Society's transition from a strongly fossil fuels dependent one to a fully decarbonated one. Nowadays, steam methane reforming, which is the main production path of syngas, generates about 11 $kgCO_2/kgH_2$ (ADEME, 2020). To lower these emissions, ground-breaking processes propose a valorisation of the produced carbon dioxide. The direct CO_2 integration within natural gas-based methanol production processes lies among these promising routes (Yang, 2018). In order to contribute to the development of such durable and sober techniques, innovative conceptual approaches must be implemented into the conception of already energetically outstanding processes. Over the last few years, exergy analysis has gained an ever-growing interest as to meet these objectives. Its ability to identify and characterise the process' thermodynamic inefficiencies makes exergy analysis especially able to bring the required assistance to the engineer in the development of innovative processes (Dincer, 2021). When it is combined with pinch analysis, it enables to build industrial processes both energy efficient and economically viable. In this paper, an approach developed in the Laboratoire de Génie Chimique of Toulouse (Gourmelon, 2015) is applied to the natural gas-based methanol production unit in which CO_2 was valued and utilised.

Study design

The case under study is a methanol production unit, in which the syngas is provided by a low carbon dioxide emitting methane reforming process (Yang, 2018). The reforming sector contains two reactors respectively performing steam reforming and dry reforming.

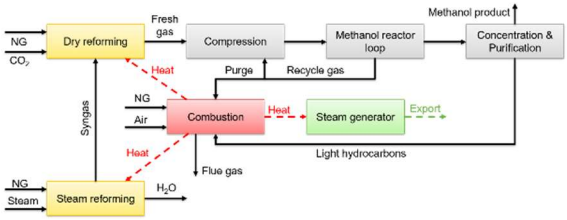

Figure 1: Process diagram for CO2 valuation in methanol production (Yang, 2018)

The latter are placed in a *parallel-series* configuration: each reactor is independently fed with reactants (*parallel* part). The syngas produced in the first reactor is then injected in the second (*series* part). This configuration type enhances carbon dioxide's conversion rate into methanol later on, hence low carbon emissions. However, energetic performances of the process have not been investigated under further exergy analysis. A study of the system's irreversibilities, beyond carbon emission reductions, consequently appears as a relevant contribution.

Methods

Based on a combined use of pinch and exergy analysis, the COOPERE approach (Gourmelon, 2015) relies on a model of the process (developed on ProSimPlus) to:

1. Perform an exergetic diagnosis of the process: the exergetic ternary chart, an original diagram, allows to characterise exergetic losses in each identified process area.
2. Carry out a case-based reasoning to build a process superstructure, which incorporates structural upgrades to cope with the inefficiencies detected on step 1. After this stage, multiple alternate processes are proposed, all minimising thermal and electrical energy consumption goals.
3. Execute a pinch analysis to build the final configuration out of all proposed alternatives of step 2, and design an efficient and viable heat exchanger network.

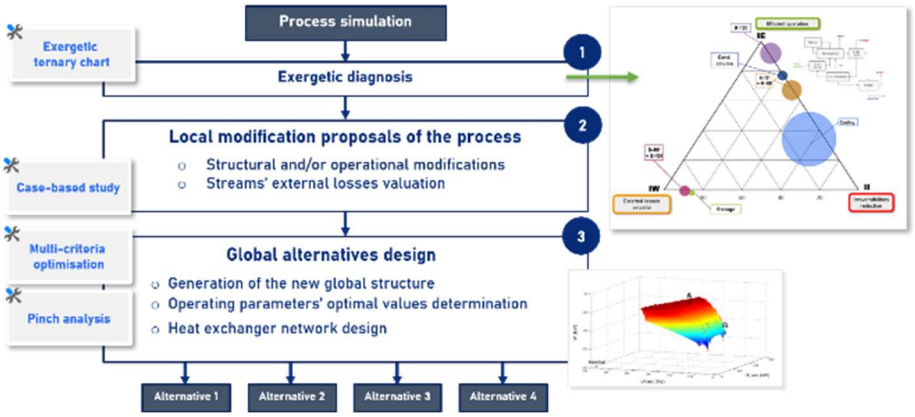

Figure 2: COOPERE approach

Conclusion

Thanks to its methodological dimension and its application to future processes, this contribution has the ambition to be a part of a global approach, aiming to promote a Future chemistry, which longs to be as energetically sober, as technically and economically viable.

Keywords: Exergy, Energy integration, Decarbonisation, Modeling, Simulation

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Multivariate metaheuristics in nonlinear energy systems modelling: application to the optimal hydrogen supply chain design

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Abstract

The pathway towards net-zero emissions requires substantial infrastructure changes to allow the current energy system to provide the same level of services as of today, but with limited impact to global warming.The greenfield design of complex energy infrastructures is typically tackled as an optimization problem solved with mathematical programming, based on a Linear Programming (LP) or a Mixed-Integer Linear Programming (MILP) formulation. The common approach to reduce the problem to LP or MILP often involves the linearization or piece-wise linearization of nonlinear functions and constraints. When nonlinearities are kept in the problem formulation (MINLP problem), the problem can be computationally challenging even for small scales of application, and no single algorithm emerges as a clear winner. Overall, the methods for the solution of a MINLP problem can be classified in two groups (Kochenderfer and Wheeler, 2020): (i) based on a single design point in the decision variables space, like descent direction methods, and (ii) population methods based on a collection of design points, like metaheuristic algorithms. Among the latter, a specific class has been proposed to allow an abstract representation of the optimisation problem, in analogy to the state-of-the-art solvers in mathematical programming: multivariate metaheuristics. Within the field of energy system design, in (Zhou et al., 2017) the authors apply a multivariate metaheuristic method in an economic dispatch problem for the operation of the electrical power system which includes a non-smooth and piece-wise function affected by the valve-point operation. For the optimization of the hydrogen supply chain design (HSCD), multiple works have already used metaheuristic algorithms, despite none is part of the class of multivariate metaheuristics (e.g., (Robles et al., 2020)).

This work is based on a two-stage hybrid optimisation algorithm integrating a multivariate metaheuristic with mathematical programming. The first stage computes the installed capacity of the production technologies, the output flows and the pressures of the network subject to the nonlinearities, while the second stage identifies the optimal flow and the installed capacities of the transport technologies. The comparison with a mixed-integer model solved with mathematical programming highlights the impact of the piece-wise approximations on the objective function and compares the respective computational costs for different sizes of the problem. The first part of the work focuses on the selection of one algorithm within the multivariate class, derived from different metaheuristics: Ant Colony Optimization (ACO-MV), Particle Swarm Optimization (PSO-MV), Differential Evolution (DE-MV), Adaptive Estimation Distribution Algorithm (AEDA-MV), and Genetic Algorithm (GA-MV). The second part of the work analyses the application of the selected algorithm to the optimization of the HSCD problem with nonlinearities. The analysis is based on

the comparison of the MINLP model with the respective MILP model in which the nonlinearities are linearized with a coarse (1 break-point) and a refined (101 breakpoints) piece-wise affine approximation. Four nonlinearities are considered: (i) capex and (ii) efficiency functions of the electrolyzer, (iii) cost of conditioning associated to the gas compression from the production node to the network input and (iv) the Weymouth equation which defines the pressure drops between two nodes of the transport network due to the friction of the pipelines. The case study is based on the estimated hydrogen demand and availability of electricity per geographical node with a spatial granularity at the NUTS2 level.

The comparison of the metaheuristics shows that all the algorithms, apart from GA-MV, achieve the global minimum with negligible scatter among the solutions. PSO-MV presents the highest increase in the quality of the solution in the first iterations, while DE-MV the smallest. However, the first metaheuristic achieving an approximation of the global optimum is ACO-MV, which was selected for the second part of the analysis. By taking the solution of the refined MILP model as reference case, the coarse piece-wise linearization introduces a negligible relative error in the total cost of the system of $1.37 \cdot 10^{-7}$, $2.82 \cdot 10^{-5}$ and $5.64 \cdot 10^{-4}$ for the case of 5, 14 and 25 nodes respectively. The MINLP model with nonlinear capex and efficiency leads instead to a relative error of $1.25 \cdot 10^{-3}$, $7.19 \cdot 10^{-4}$ and $8.50 \cdot 10^{-4}$ on the same number of nodes. The MINLP model with pressure drops and conditioning cannot be directly compared with the other models, but it leads to a further increase in the objective function of $2.50 \cdot 10^{-4}$, $7.78 \cdot 10^{-3}$ and $2.98 \cdot 10^{-2}$ relative to the MINLP model with only nonlinear capex and efficiency. The associated computational time is of different order of magnitudes when the metaheuristic is used and when not. The solution of the refined MILP model requires 0.16 s, 0.83 s and 1.88 s, while the solution of the MINLP problem with all the nonlinearities requires 16 min, 2 h 54 min and 9 h 42 min for the case of 5, 14 and 25 nodes respectively. In terms of impact on the system design, a comparison can be done by considering the largest capacity installed in each geographical scale. Compared to the refined MILP model, the coarse MILP model and the MINLP model lead to a smaller installed capacity with a maximum impact of 0.25% for 5, 14 and 25 nodes. The associated impact on the capex is negligible for the coarse MILP and around $33.5 \cdot 10^3$ EUR for the case of 14 and 25 nodes.

Overall, the comparison of the best performing multivariate metaheuristic ACO-MV for the solution of the MINLP version of the HSCD problem with the MILP approximations of the same problem reveals that the algorithm is capable of finding good approximations of the global optimum, while handling nonlinear constraints. The comparison of the associated computational cost reveals that the metaheuristic algorithm should only be used when the inclusion of nonlinearities is strictly necessary. In this work, it is the case of the Weymouth equation as nonlinear constraint, required to design the pressure levels of the transport network. Concerning the impact on the design variables of the problem, the introduction of the nonlinearities in the capex and in the efficiency only partially affects the capacity installed and the associated capex. In this case study, the maximum impact on the size of the installed capacities was found to be in the order of kW, limiting the relevance of considering the nonlinearities in capex and efficiency to case studies of small geographical scales of analysis.

Keywords: Multivariate Metaheuristics; Hybrid Optimisation; MINLP; Hydrogen supply chain.

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Generic exergy-based approach for the evaluation of emerging technologies: application to CO2 conversion pathways

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Abstract

Since the 20th century, there has been an increasing trend in the global annual average temperature. This phenomenon has increased since the 1980s due to the dramatic rise of CO_2 emissions mainly caused by human activity. To limit global warming, it becomes crucial to reduce the production of CO_2, methane and other GHG. An alternative solution could consist in valorizing the CO_2 already present in the atmosphere. Among the possible ways to valorize CO_2, the *Power To Liquid* principle consists in converting renewable electricity into a liquid energy vector. This vector, also known as synthetic fuel or e-fuels, is easier to transport and store (Schemme et al., 2017). Among the intermediates considered for e-fuel production, methanol appears as a key platform molecule (IRENA - International Renewable Energy Agency, 2021). As recently illustrated by ADEME, several CO_2 conversion routes exist but do not all report the same level of maturity (ADEME, 2014).
This work focuses on e-methanol, which is obtained from green hydrogen (hydrogen produced with renewable electricity) and captured CO_2 according to the following process steps (Figure 1).

1. Capture and purification of CO_2
2. Decarbonated hydrogen production (different means of production)
3. Conversion (direct or indirect, different reactor concepts) to e-fuel
4. Purification

This contribution aims at paving the way to the search of the development of the pathway that will meet the best compromise between technical feasibility, economic profitability, energy efficiency, representativeness and complexity of implementation. The preferred process will have to use the innovative technological building blocks that contribute to better energy efficiency and to the decarbonization of industrial systems. First, a state of the art related to the four pathways illustrated on Figure 1 will be summarized.

Then the methodological approach imagined to reach this goal will be sketched. Relying on a process system approach, the methodology will have to focus on a systematic study of the energy integration potential of the considered alternatives. To reach this goal, it will consist in systematically generating several process alternatives and then comparing them in a consistent way.

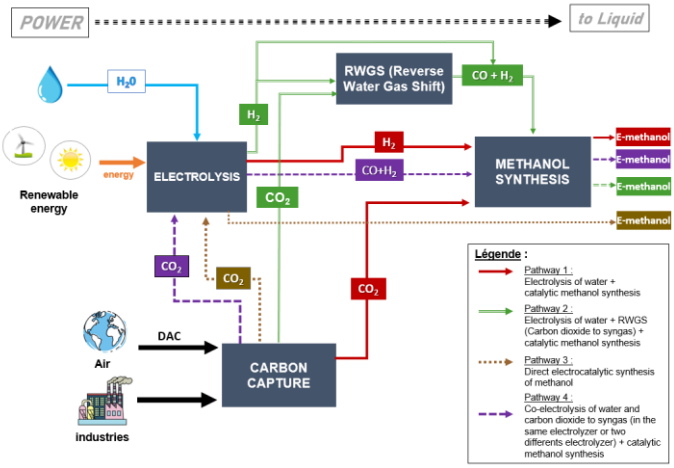

Figure 1: Scheme of four CO2 conversion pathways to e-methanol

Among the considered approaches, an iterative approach based on the construction of a superstructure as introduced by (Belletante, 2016) seems to be a good starting point. (Lee et al., 2020) applied a similar approach to direct CO_2 hydrogenation to methanol. This approach allows to scan a maximum of solutions and to evaluate them according to economic and energetic criteria. As energy efficiency appears as one of the most crucial criteria, special attention will be paid on the exergy efficiency indicator. A coupling of pinch and Exergy analysis as implemented by (Gourmelon, 2017), is a very efficient methodology to promote the development of processes that minimize the exergy losses and irreversibilities and optimize the heat recovery inside the process. Finally, one of the challenge is to integrate of uncertainties related to the considered technologies will be studied (Martín and Adams II, 2019).

Keywords: e-methanol, electrolysis, exergy, energy, generic approach

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Benchmarking Knowledge-based and Data-driven Molecular Fingerprints for QSPR Modelling

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Abstract

The properties of the molecules dictated whether they are suitable for any given application. These properties are highly dictated by its structure: the presence and absence of substructures and the relative positioning of these. Quantitative Structure-Property Relations (QSPR) are mathematical models that aim to relate the molecular structure in the form of a machine-readable molecular fingerprint to the property of interest (Gasteiger, 2016). These models are necessary to perform high throughput screening and exploring the chemical space beyond the available data. Deep neural networks (DNN) have been extensively applied as the model of choice for property prediction due to their capability of approximating any continuous function given a suitable choice of depth, width, and activation function. However, the choice of descriptor remains largely unanswered and is highly influenced by the background of the modeler. Chemical engineers have widely used the concept of groups and substructures to model properties as part of group-contribution models (Zhang et al., 2020). Pharmacologists and drug development scientists have used Extended-connectivity fingerprints (ECFP) as the "go-to" descriptor (Xiong et al., 2020). Recently, a new data-driven approach has caught the interest of both modeling groups and is capable of generating molecular fingerprints using graph convolutions on an attributed graph representation of the molecule.
In this work, we provide a proper benchmark of the molecular descriptors used to model QSPR. We benchmark three descriptors, the groups defined by Marrero-Gani, the extended fingerprints, and a recent graph convolutional network that has achieved the state of the art for many property data (Xiong et al., 2020). By unifying the preprocessing and training/evaluation procedures we aim to compare the performance and the ability to generalize to unseen data of these descriptors by applying them on three property data consisting of the flashpoint, the normal boiling point, and the critical temperature.

Keywords: Molecular property prediction, Deep learning, Thermophysical properties

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Data-driven, image-based flow regime classification for stirred aerated tanks

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Abstract

This article investigates the implementation of AI-based image processing algorithms for the identification of flow regimes in stirred aerated reactors widely used in the chemical and pharmaceutical industries. Monitoring and optimization of flow regimes is crucially important for the process efficiency and product quality. To date, manually generated flow maps and correlations are mostly used for this purpose. However, they all suffer from the strong rigidity. Among measurement-based in-line and on-line techniques such as probe-based ones, tomography and spectroscopy, image analysis is the only low-cost, non-invasive approach, which works with transparent media regardless of their physical properties. Great progress has been made recently in image analysis using in particular convolutional neural networks (CNN) and our aim is to evaluate the use of these technologies for optical data-driven detection of flow regimes in stirred aerated tanks. The experimental setup is built around the 30 l bioreactor of the industrial design with three flat blade turbine stirrers and a ring sparger. The camera is installed at the sight window of the reactor, allowing non-invasive observation of the flow pattern of bubbles inside the tank. For model training, around 10,000 labelled images of three flow regimes (flooded, loaded and completely dispersed) were collected under a wide range of process conditions, e.g. varied stirrer speed or gas inlet flow rate. To reduce the overfitting phenomena, light conditions and position of the camera were also regularly varied. Additionally, data augmentation techniques such as flip, zoom and rotate were applied. The process is modelled with CNNs of different architectures such as two custom shallow CNNs with 2 and 4 convolution layers, LeNet-5 with different sizes of the input layer as well as VGG16, MobileNet and DenseNet121. Afterwards, we evaluated several of the most promising pre-processing approaches on the best performing model for a possible additional increase in model accuracy. The best results were achieved after cropping, conversion to grayscale and applying the sharpening filter. For model validation, train/test/validate split was used. Testing data included also different liquid levels in tank. The class activation mapping technique was used for manual inspection and evaluation of the trained model to exclude the ”Clever Hans” effect. The results indicate that in contrast to more complex models, shallow CNNs and especially LeNet-5 can detect the flow regime with a higher accuracy (96%). The identification of the flooded regime is very reliable (F1 score of 99%). The other two regimes, which resemble each other visually, were more frequently misclassified, resulting in a lower recall for loaded regime (92%) and lower precision (94%) in completely dispersed regime.

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Keywords: stirred aerated tank, flow regime classification, computer vision, CNN.

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Data-driven modeling for physical property prediction of polypropylene composites using artificial neural network and principal component analysis

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Abstract

Recent research with artificial neural network (ANN)-based predictive model has emerged as a solution to reduce the number of trial and error effectively. However, it is still challenging to develop a high-performance model using a sparse dataset. Especially, the high-dimension and the small number of polypropylene composite's (PPC's) material data make it difficult to develop a predictive model. In this study, we proposed the ANN-based predictive model using principal component analysis (PCA) to predict the physical property of PPC with the high performance. The optimal dimension reduction of the raw dataset was suggested by the proposed framework to overcome incomplete dataset of PPC materials including the zero or missing values. The dimension reduced dataset was used to develop the ANN-based model for physical property prediction of PPC. As a result, the model accuracy based on the reduced dataset is 0.9061, and 4.6% higher than the model using the raw dataset. This result demonstrates that ANN-based model with dimension reduction improves the prediction performance by reducing the sparsity of PPC material data. Moreover, the proposed model is expected to reduce the number of trial and error in the PPC development process.

Keywords: polypropylene composite, principle component analysis, artificial neural network

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Optimization of the Wastewater Treatment Plant Aeration Using Artificial Neural Networks Models

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Abstract

Typically, the aeration energy is responsible for two thirds of the total energy spent at the Wastewater treatment plant (WWTP). This study aimed the optimization of the aeration-controlled system of the WWTP for minimizing the aeration energy, while maintaining the desired effluent quality. The optimization decision variables were the weighting factors associated to the air flowrates distributed along length of the aerated reactors. A municipal WWTP with an Anaerobic-Anoxic-Oxic configuration and with dedicated control loops for Dissolved Oxygen and for nitrates concentration was considered.

Although complex first-principle activated sludge models are available for the description of the WWTP processes, one of their major drawbacks is their need for high computation time and resources, aggravated when used for optimization. Artificial neural networks (ANNs) are capable of modeling complex non-linear processes in a much shorter time. ANNs were chosen in the present work for modelling and optimization. Different types of dynamic ANN models were considered, such as: time-delay neural networks, recurrent neural networks, generalized regression neural networks and radial basis neural networks. The data required for training the networks were obtained from simulations using the calibrated WWTP model and the Design of Experiments methodology. The topology of the neural networks was varied in order to find the most accurate ANN model. Time needed for training and mean absolute percentage error (MAPE) at the ANN models testing step were considered for selecting the best ANN.

The highest performing type of ANN was found to be the generalized regression neural network that showed fast simulation time, while maintaining the expected accuracy (MAPE < 5). The best of the trained ANNs was used for the optimization of the WWTP aeration. Advantages emerged from using the ANN based model in optimization, i.e. the computation time was about 5-8 times shorter and accuracy was good, when compared to the results obtained by optimization using the first-principle model. The investigated optimization algorithm (either gradient descend and genetic) with best results was also found. They revealed the incentives of the plant operation based on the optimal distribution of the air flowrate, aimed to improve the WWTP performance.

Keywords: Artificial Neural Networks, Wastewater Treatment Plant, Optimization.

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Root Cause Diagnosis of Process Disturbances Based on Edge-Group Sparse Principal Component Analysis and Transfer Entropy

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Abstract
In this work, an edge-group sparse principal component analysis (ESPCA) method was adopted for process chemometrics, which integrates process data and connectivity information. Then, transfer entropy was used to analyse causal relations between candidate process variables identified by ESPCA, the results of which indicate the root cause variables of process disturbances.
Keywords: root cause diagnosis, edge-group sparse principle components analysis, transfer entropy, process chemometrics, process monitoring

Introduction
Principal component analysis (PCA) has been a popular process chemometrics method for years. However, the lack of sparsity and ignorance of process physics often makes the PCA results difficult to interpret. In this work, an edge-group sparse PCA (ESPCA) method (Min et al., 2018) was adopted to overcome the shortcomings of PCA by considering the connectivity between process variables. ESPCA outperforms PCA in identifying critical-to-fault variable groups. Based on the results of ESPCA, transfer entropy (TE) (Schreiber, 2000) was used to analyse the inter- and intra-group causal relations between variables and reveal the root cause of process disturbance.

Methodologies
Different from the conventional PCA, ESPCA is based on both process data and a graph describing process variable connectivity. In the graph, each vertex denotes a process variable, while the edge between two vertices indicates a direct connection between the variable pair. The first loading of an ESPCA model can be estimated in the following way:

$$\underset{\|p\|_2\le 1,\|v\|_2\le 1}{\operatorname{argmax}} \; p^T X v, s.t. \; \|p\|_{\mathcal{G}} \le k \tag{1}$$

where $\|p\|_{\mathcal{G}} = \min|\mathcal{G}'|$, $\forall \mathcal{G}' \subseteq \mathcal{G}$, $\mathrm{support(p)} \subseteq \mathrm{V}(\mathcal{G}')$, p is the loading vector, X is the matrix of process data, v is the score vector, k is the adjusting parameter controlling the sparsity of p, $\mathcal{G}$ is an edge set of the graph, $\mathcal{G}'$ is a subset of $\mathcal{G}$, $V(\mathcal{G})$ is the vertex set induced from edge set $\mathcal{G}$, $support(p)$ denotes the set of indices of nonzero elements of p, and $|\mathcal{G}'|$ denotes the number of edges in $\mathcal{G}'$. The subsequent ESPCA loadings can be calculated in a similar manner after deflation. After modeling, process information can be explored by analyzing the loadings and scores, e.g. the groups of variables critical to process disturbances or faults.

Transfer entropy measures the information flow among stochastic processes, whose results often indicate whether causal relations exist. Denoting $x_i^{(l)} = x_i, \cdots, x_{i-l+1}$ and $y_i^{(k)} = y_i, \cdots, y_{i-k+1}$, the transfer entropy from time series X to Y is calculated as

$$T_{X\to Y} = \sum p(y_{i+1}, y_i^{(k)}, x_i^{(l)}) log_2 \frac{p(y_{i+1}|y_i^{(k)}, x_i^{(l)})}{p(y_{i+1}|y_i^{(k)})} \quad (2)$$

In causality analysis, a TE value significantly greater than zero indicates the existence of causality. The above calculation can be easily extended to two groups of time series. Herein, a hierarchical causality analysis procedure is proposed to analyse both the inter- and intra-group causal relations and reveal the root cause of process disturbance.

Case study

In this work, a case study was conducted on the benchmark Tennessee Eastman problem. 22 variables related to the reactor unit were chosen to be analysed for root cause diagnosis of disturbance IDV1 which was caused by a step change of A/C feed ratio in flow 4. The sensor closest to the root cause of disturbance is variable 23 which is the composition of component A in stream 6. This variable should be diagnosed as the root cause variable. For diagnosis, IDV1 data was used for ESPCA model building. The graph indicating variable connectivity is plotted in ***Fig. 1***, which was obtained from analysing the P&ID chart. The score plots are shown in ***Fig. 2***, which indicate that the disturbance significantly affects the first and second principal components (PCs). The loading plots are depicted in ***Fig. 3***. Thanks to the sparsity, it is easy to identify the variables contributed to the loading corresponding to each principal component (PC) as shown in ***Fig. 1***. The calculation of TE shows that the variables corresponding to PC1 form a cause group while the variables contributed to PC2 are the effect group. Further causality analysis within the cause group implies that variable 23 is the root cause variable.

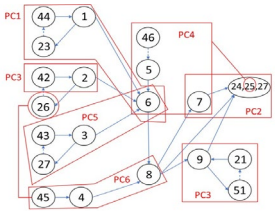

Fig. 1 Variable connectivity

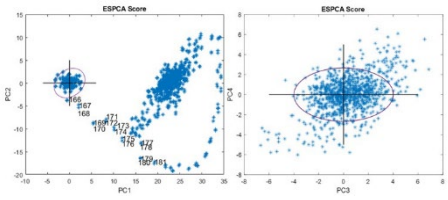

Fig. 2 ESPCA score plots

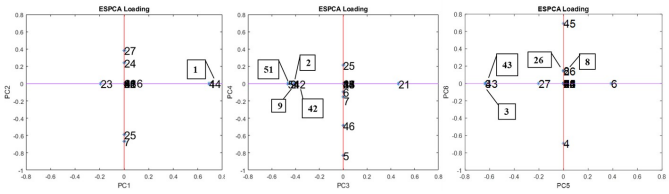

Fig. 3 ESPCA loading plots

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Advances in the SynGameZero Approach for Flowsheet Synthesis by Reinforcement Learning

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Abstract

Reinforcement learning (RL) is a novel machine learning technique which is trained from interactions with an environment (Sutton and Barto, 2018). We recently developed an RL method called SynGameZero (Göttl et al., 2021a), which trains an RL agent without prior chemical engineering knowledge to synthesize process flowsheets solely by interaction with a flowsheet simulator. The general idea in this approach is to transform the process synthesis into a turn-based two-player game. Both players synthesize a flowsheet by adding unit operations or recycles to their flowsheets. Each player can decide when its flowsheet is finished and the synthesis is terminated. The game's goal is to create a process flowsheet more valuable than the opponent. This is measured by the net present value after both players have finished their flowsheet (at a tied game, the first player to finish wins the game). The winner receives the reward 1, the loser the reward -1. This setup allows the usage of a modified version of an RL training algorithm initially proposed by Silver et al. (2018) for the board games Chess and Go. During training, the agent switches between the roles of both players and plays against itself. It consists of an artificial neural network (ANN) combined with a tree search for strategic planning. The ANN has an actor-critic structure and takes the stream tables of the flowsheets as input and outputs a suggestion for the following action and a prediction of the winning chances of the current player. Both outputs are used to guide the tree search, which explores future actions and the resulting flowsheets. Of course, it is not tractable to evaluate all possible actions in the tree due to limits in computational power. Therefore, only promising actions are explored, which are quantified by the outputs of the neural network. During the tree search, several statistics, for example, visit counts of the explored states, are stored. Those statistics are the basis for the final decision of the agent in the game. Additionally, these statistics train the ANN to output better suggestions for the following action in the future. Recently, we have improved the SynGameZero approach by structuring the agent's decisions hierarchically (Göttl et al., 2021b).

In the present contribution, we adopt the hierarchical structure and optimize it further. We have restructured the hierarchical decisions to eliminate unnecessary complexity. For example, we treat recycles and mixers in a common framework. We have added novel separation units besides distillation, e.g., membrane separations, and have added the possibility to add specifications to units, e.g., split ratios for distillation columns. The hierarchical method works as follows: First, the agent chooses an open stream or can terminate the synthesis. At the second level, a unit operation is selected. If the agent decides to admix or recycle some stream to another stream, it has to decide on the

destination at a third hierarchy level. As shown in Figure 1, the agent consists of three hierarchical actor-critic networks, which generate outputs for the subsequent tree search. The hierarchical structure avoids the combinatoric explosion when the problems require flowsheets with many process units.

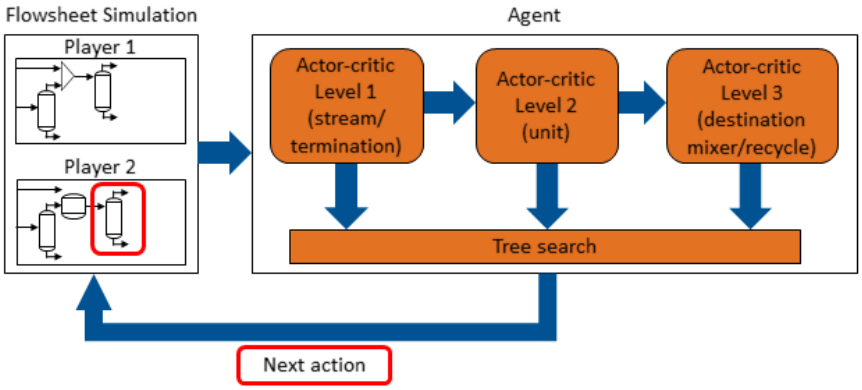

Figure 1. The agent's structure. Stream tables of both players are used as input to the hierarchical ANN. The next action in the game is determined in the tree search, guided by the ANN outputs.

Novel design problems were developed and presented to demonstrate the improved capabilities of the advanced hierarchical SynGameZero method. They include, e.g., a process to produce alternative fuels in a seven-component mixture. By studying the examples, the agents' training process and decisions are analyzed in detail, which leads to a better understanding of why the approach with a two-player game is successful and how the method can be further refined and improved.

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Keywords: Automated Flowsheet Synthesis; Artificial Intelligence; Reinforcement Learning.

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The truncated *Q* statistic for Statistical Process Monitoring of High-Dimensional Systems

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Abstract

Among the process monitoring methods for high-dimensional systems, the most widespread and researched are those belonging to the class of latent variable approaches (Jackson, 1959, Kourti et al., 1995). As more variables are continuously gathered, the existing latent variable methods start to experience difficulties in maintaining their properties. Of particular importance is the decreased sensitivity in detecting localized faults through the *Q* statistic (by localized, it is meant faults affecting one or a small number of sensors). In brief terms, the main reason for this behavior is the accumulation of residual contributions arising from a large number of variables, which effectively raise the basal level of the *Q* statistic during normal operation conditions. Thus, faults are only detectable if their signatures surpass not only the normal operation variation of the faulty variables, but also the sum of all irrelevant residuals, which may be considerably high for large systems. To overcome this limitation, we propose the use of the truncated *Q* statistic that screens for the relevant residuals before summing them. This is performed by comparing the residuals against a statistically motivated allowance threshold and only the residuals beyond the threshold are kept and used to compute the truncated *Q* statistic (this step is then repeated for each new observation). The performance of the proposed statistic was analyzed through Monte Carlo simulations of several latent variable processes with 5 000 to 20 000 variables. Process monitoring was performed by replacing the *Q* statistic in the standard combination of T^2 & *Q* of MSPC-PCA (Jackson, 1959), but other latent variables monitoring methods can also benefit from this proposal. The results obtained clearly show that MSPC-PCA with the truncated *Q* statistic becomes much more sensitive than the original formulation; for instance, it can detect faults with a magnitude of 2 standard deviations more than 90 % of the times, whereas MSPC-PCA with the standard *Q* statistic only detect faults with a magnitude of 4 standards deviations less than 40 % of the times. This methodology was also applied in a real world process to monitor more than 17 000 variables associated to printed circuit boards (PCB) produced by Bosch Car Multimedia Portugal. For this case, the proposed truncated *Q* statistic was able to identify 17 abnormal PCBs while the standard *Q* statistic only detected 5 PCBs.

Keywords: Statistical Process Monitoring; Latent variables; High-dimensional processes; Industry 4.0.

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Development of a predictive emission measurement system using hybrid models with real industrial data

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Abstract

The climate changes debate has promoted a growing collective awareness about the impacts of emissions on the quality of life in general population. Because of that, many governments have created legislation mechanisms in order to monitor, reduce or even prevent the accumulation of environmental pollutants gases in the atmosphere. In this context, stationary emission sources such as thermoelectric power plants are targeted and a rigorous monitoring methodology based on gas analyzers (CEMS) has been used on site. In order to mitigate those economic impacts, nowadays many countries have regulations for the implementation of predictive monitoring approaches such as the predictive emission measurement system (PEMS), a model-based software that can estimate emission levels using more common measured process variables, as a cheaper alternative to the CEMS technology. There has been already presented in literature many successful case studies of PEMS application, mostly using data-driven models. However, the major challenge that still persists is the model development using real industrial data. In many plants, for example, it is impossible to collect an ideal and rich data-set due to safety and operational constraints or even a flawed controlling system. In this paper we present a study for the development of hybrid models using thermodynamic equilibrium calculations and machine learning (ML) algorithms using real operation data of a gas turbine from the largest thermoelectric power plant in Brazil. The main goal of this study was to generate accurate NO_x prediction models from actual plant history data in order to replace the current CEMS in operation. A phenomenological equilibrium model based on the minimization of the Gibbs energy was coupled with several ML models such as artificial neural networks (ANN) with different architectures, supporting vector machines (SVM), gradient boosting, among others. In this framework, the data-driven models were used to estimate the error of the theoretical model, then, the prediction of pollutant levels was made by the sum of both results. An analysis was made with 6,513 samples split between training and validation sets. Three key performance indicators: (i) maximum absolute error (MAE), (ii) root mean squared error (RMSE) and (iii) the correlation coefficient were evaluated and the results have shown that the hybrid approach can be overall up to 50% more accurate than the single models alone, at least for the gas turbine in study.

Keywords: PEMS, Machine learning, Gas Turbine

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What Do Machine-Learning Algorithms Truly 'Learn'? On The Interpretability of Graph Neural Network in QSPR modelling

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Abstract

Recent surge in the development and applications of machine learning (ML) algorithms have paved the way for rapid advancements in many fields and noticeably the field of molecular property prediction. Graph Neural Networks (GNN) is considered a promising approach for property modeling compared to the use of traditional descriptor-based models due to their enhanced expressive ability compared to traditional descriptor-based models. However, most machine-learning approaches are 'black box' systems and lack the aspect of interpretability, which could hinder their wider acceptance and usage (Dobbelaere et al. (2021)). Two approaches have emerged to try and solve this issue: a model-agnostic(or post-hoc) approach such as GNNExplainer (Ying et al. (2019)) or a model-specific approach by providing access to the model internals e.g. contributions of the various input area (Coley et al. (2017)). The purpose of this work is to interpret the learnings of GNN-based models used in property modeling using both approaches and by illustrating the substructures influencing the target property. This is demonstrated by applying the attention-mechanism applied in models such as EGAT (Chen and Chen (2021)), FraGAT (Zhang et al. (2021)) and AttentiveFP (Xiong et al. (2020)). Several thermo-physical properties obtained from AIChE DIPPR® database including boiling point and flash point are used to investigate the interpretability.

Keywords: Molecular Property Prediction, Quantitative Sructure-Property Relations (QSPR), Machine-Learning (ML), Graph Neural Networks (GNN), Interpretability

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Predictive Maintenance in the Digital Era

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Abstract

Predictive maintenance is becoming increasingly popular as part of Industry 4.0. The implementation of predictive maintenance has the potential to improve manufacturing capabilities by identifying equipment faults and preventing the shutdown of the production process. The popularity has led to an abundance of research solely concentrating on developing new machine learning techniques that use historical data to predict when maintenance is required. Therefore, in this work, we focus on the application of machine learning for predictive maintenance by prioritising a robust comparison of methods to investigate the accuracy of readily available classification methods for predicting whether a failure has occurred in each machine. We then outline how predictive maintenance can be used as a promising application to develop robust maintenance scheduling in an industrial plant.

For the purposes of comparison, this study uses data provided by a cyber-physical production system that records sensor reading enriched with control commands enabling the opportunity to monitor and detect faults in machines (Klein and Bergmann, 2019). The large Fischertechnik (FT) model factory provides a realistic and challenging case study for detecting faults on 14 machines using 61 sensor readings indirectly related to each machine. Classification machine learning models are applied to the data providing an insight into the promising tools readily available to prevent failures in industry. Further, this study provides a rigorous approach to compare and evaluate the classification models, analysing various error metrics and ultimately choosing a machine learning method to provide further analysis.

Altogether, we evaluated the accuracy of five readily available machine learning methods. We found that the Quadratic Discriminant Analysis (QDA) performed the best with respect to the FT model factory dataset, achieving an F1 score of 0:877. Statistically, the significance of the results provided validation that the QDA was the best choice of method. Conclusively, the integration of machine learning and maintenance can significantly improve process safety and save money.

Results showed that the machine learning methods adopted were accurate enough to provide predictive maintenance and offer vital analytics. This provides a route for robust maintenance scheduling for many existing industrial plants.

Keywords: predictive maintenance, machine learning, process safety, classification models

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An evolutionary approach for techno-economic assessment

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Abstract

Increasing productivity is a key issue in Industry 4.0. From this perspective, methodologies to achieve operational excellence with further cost reductions have been gaining importance. Decision-making can be facilitated by merging both the production and market scenarios. In an Industry 4.0 environment, techno-economic assessment is crucial to achieve a competitive advantage. Then, it is challenging to enlarge the scope of derivative-free evolutionary strategies to be able to exploit them in this context. Evolutionary algorithms can efficiently be applied in broad practical issues by tailoring their operators to the specific combinatorial problem under study.

Based on Genetic Algorithms (GAs), a Master-Worker strategy for techno-economic assessment enhanced with an ad hoc chromosome redefinition is proposed. A dual structure of the phenotype, where boolean and real genes are combined in a single chromosome, was adopted so as to include a wide variety of decision-making variables. Since production usually involves temporal dependency among processes, crossover and mutation operators were properly adjusted. Rules were implemented so that the decision-maker places value on the economy of scale and the efficiency in logistics. A specialized crossover operator that uses specific information about the problem's constraints was designed to make sure that all ensuing individuals were feasible. Moreover, it was observed that the use of standard mutation operators was prone to create non-feasible individuals quite frequently. It should be noted that a single chromosome comprises time-ordered information corresponding to a rolling horizon, thus including the state variables for various points in time. Since annual information should not be freely swapped, a mutation operator that always performs permutations within the same year was incorporated. Besides, many scenarios should be solved as quickly as possible to give effective support to the decision-making. Therefore, parallel programming was adopted so that the Workers can simultaneously explore different instances.

In particular, the software was implemented in order to optimize value chains aiming at the maximization of the Net Present Value. The proposed methodology, where designing suitable operators led to a successful GA, simultaneously optimizes several realistic scenarios and manages to boost the space search. The test results have shown that the optimizer is useful to make satisfactory comprehensive financial decisions.

Keywords: Techno-economic assessment, Optimization, Genetic algorithm.

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Optimization of an artificial neural network structure for modeling carbon capture in spray columns

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Abstract

The anthropogenic CO_2 emissions reinforces the global warming. The most mature CO_2 capture technology is the absorption of CO_2 into monoethanolammine (MEA) in spray or packed columns. However, this process is not economically viable due to low mass transfer coefficients (kGa). Kuntz and Aroonwilas (2008) showed that spray columns increase the kGa compared to packed columns. The authors investigated experimentally several parameters such as gas and liquid flowrates, MEA concentration and CO_2 concentration. Because of the high intercorrelation between the parameters, the modeling of this process is a non-trivial task. Machine learning techniques have shown great accuracy in modeling this kind of systems using large amounts of data. Artificial neural network (ANN) is the most promising and modular technique in this field. The aim of this work is to find the best ANN structure to model the kGa for CO_2 absorption in spray columns using MEA. The data to train the model are extracted from literature sources. The ANN is trained using the back-propagation algorithm and its structure is searched by a Bayesian optimizer. Cross-validation and regularization techniques are employed to avoid overfitting. The trained model has a determination coefficient R^2=0.98 and a mean squared error MSE=7.89e-4 on the validation set with errors below 20%. The ANN structure optimizer found the best solution in an encoding-decoding shape. This shape has great feature importance extrapolation capabilities, this allows the ANN to have a high prediction accuracy. In conclusion, the usage of ANN has allowed to model the CO_2 capture in spray columns with a high accuracy. The trained model can be utilized to maximize the kGa in order to design and control spray columns that run in optimal process conditions. In addition, the prediction capabilities of the model can be expanded by adding new data to the training set. The proposed procedure can be applied also for other processes where the kGa needs to be estimated and optimized.

Keywords: CO_2 capture, machine learning, artificial neural networks, absorption, spray columns

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Hierarchical Statistical Process Monitoring based on a Functional Decomposition of the Causal Network

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Abstract

As industrial monitoring systems expand and more data collectors are installed in the process units and streams, more variables become available to be handled by the plethora of multivariate Statistical Process Monitoring (SPM) methods currently available (Reis et al., 2019, Qin, 2012, Ge et al., 2013). However, with the explosion of the monitoring dimensionality, even the state-of-the-art methods begin to experiment difficulties, especially when it comes to detecting localized faults, whose signatures easily pass unnoticed due to the large normal background noise associated to the many sensors under analysis; see for example (Reis et al., 2021) for a detailed description of the underlying problem and some solutions (including a real case study). In this work ~~article~~, we propose a new systematic approach based on a functional decomposition of the system's causal network. The methodology consists in finding the natural functional modules of the causal network, by exploring its graph topology and identifying the strongly linked "communities". Two hierarchical monitoring schemes are then applied to monitor the overall state (aggregating information from the modules and their interactions). In this way, as the dimensionality of the modules is smaller, the sensitivity of the distributed system to small or localized faults becomes, in principle, higher. Furthermore, the causal nature of the method facilitates fault diagnosis, especially for sensor faults. However, the overall false alarm rate of the methodology must be controlled, which may take away some of the sensitivity of the proposed method. We report results that demonstrate an increased sensitivity in fault detection of the proposed methodologies when compared to methods that monitor the complete causal network. The proposed approach also led to a more effective and unambiguous complementary fault diagnosis activity.

Keywords: Statistical Process Monitoring; Causal Network; Hierarchical Monitoring; Community Detection; Distributed Monitoring

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A Recurrent Neural Networks-Based Approach for Modeling and Control of a Crystallization Process

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Abstract

Crystallization is a separation and purification process applied in many industrial sectors. The goal of this unit operation is to achieve desired crystal size and shape distribution, making process control a key tool for its success. Despite the importance of controlling batch crystallization processes, there is still a lack of studies applying neural networks-based control strategies to them. Therefore, this work aims to model a crystallization process to predict the moments of the particle-size distribution with neural networks used as the internal model in the predictive controller. Four different neural networks paradigms were considered: a classic single Multilayer Perceptron (MLP) network, a set of four MLP networks in series, and two recurrent networks, the Echo State Network (ESN) and the Long Short-Term Memory (LSTM). The dataset used for training and testing applied a co-teaching learning algorithm [1], which utilizes simulated and experimental data. The 479 experimental values of concentration, and particle's number, length, area, and volume were obtained for several temperatures and ten different batch experiments of potassium sulfate (K_2SO_4) crystallization. The 9000 simulated data were generated using dynamic simulation of the population balance. First, the four network structures were trained to predict the moment's values one step ahead, using the current temperature and moment's values as feed. As a result, all strategies were successful, achieving values of R-squared of about 99% for the test samples. Then, the network's predictive performance was studied for larger prediction horizons. The ESN had the best performance, achieving values of R-squared above 90%, for eight out of 10 experiments and up to five steps ahead prediction. In comparison, the other strategies reached values below 90% for more than two experiments. Finally, a Nonlinear Model Predictive Controller (NMPC) based on the selected ESN was successfully applied to the batch crystallization process to maintain crystal size and shape distribution on their desired trajectories by manipulating the operating temperature. The controller behavior was studied for four reference trajectories: constant, 1st order, 2nd order, and adaptative 1st order. As a result, the ESN-based NMPC presented better results, both in terms of performance and computational demand, than an NMPC based on the classic MLP, evidencing the potential of the proposed strategy.

Keywords: Crystallization, Neural Networks, Echo State Network, LSTM, NMPC.

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SYSTEM IDENTIFICATION WITH PHYSICS INFORMED NEURAL NETWORK

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Abstract

System identification is a typical problem in a control system. In this work, a physics informed neural network (PINN) is applied, which is capable to solve nonlinear ordinary differential equations (ODEs). We believe that PINN is potentially promising in data-driven system identification, because ODEs can describe the dynamic behaviors of many different physical systems. By using PINN, the parameters of the active magnetic bearing system can be automatically identified during the process of model training.
Keywords:
Keywords: system identification, deep learning, active magnetic bearings system, physics-informed neural network

Methodology

In this work, we demonstrated the capability of physics-informed neural network (PINN) (Raissi et al., 2019) in system identification using an active magnetic bearing (AMB) system (Huang, 2020). PINN is a neural network that takes physics information into model training. Usually, two losses are optimized in PINN through back-propagation, which are the prediction loss and ordinary differential equations (ODEs) loss, respectively. In doing this, both the neural network parameters and the system parameters can be obtained during model training at the same time. The losses can be expressed as

$$\mathrm{MSE} = \mathrm{MSE}_{\mathrm{pre}} + \mathrm{MSE}_{\mathrm{ode}} \tag{1}$$

$$\mathrm{MSE}_{\mathrm{pre}} = \frac{1}{N}\sum_{i=0}^{N}(f(\mathbf{x}_i, \mathbf{u}_i, t_i) - \mathbf{x}_{i+1})^2 \tag{2}$$

$$\mathrm{MSE}_{\mathrm{ode}} = \frac{1}{N}\sum_{i=0}^{N}\big(f(\mathbf{x}_i, \mathbf{u}_i, t_i) - r(\mathbf{x}_i, \mathbf{u}_i, t_i)\big)^2 \tag{3}$$

where i is the index of time interval, $\mathbf{u}_i$ is the input vector of the system, $\mathbf{x}_i$ is the state vector, t_i represents the time value, $f(\mathbf{x}_i, \mathbf{u}_i, t_i)$ is the prediction value of $\mathbf{x}_{i+1}$ provided by the neural network, and $r(\mathbf{x}_i, \mathbf{u}_i, t_i)$ is the theoretical value of $\mathbf{x}_{i+1}$ derived using the Runge-Kutta method. The structure of the PINN is shown in ***Fig. 1.***

Case study

The system considered in this work is an AMB system which uses two currents i_{x1} and i_{x2} to control the rotor's displacement and tilt angle. The system can be described as

$$M\,\ddot{x}_c = 2k_x x_c + k_i i_{x1} + k_i i_{x2} + k_i k \theta_c \tag{4}$$

$$I\,\ddot{\theta}_c = k_x(l_1^2 + l_2^2)\theta_c + k_i l_1 i_{x1} - k_i l_2 i_{x2} + k_i k x_c \tag{5}$$

where M is the mass of rotor, I is the transverse moment of inertia, x_c is the displacement of the rotor's center of mass, θ_c is the tilt angle of the rotor, i_{x1} and i_{x2} are the currents, l_1 and l_2 denote the distances between the bearings and the rotor's canter of mass, and k_i and k_x are the the current stiffness and unstable displacement stiffness, respectively. The

coefficient k is composed of $\frac{k_x}{k_i}(l_1 - l_2)$. In the open-loop identification, the system inputs are i_{x1} and i_{x2}, while the state variables are x_c and θ_c. Denoting $y_1 = x_c$, $y_2 = \theta_c$, $y_3 = \dot{x}_c$ and $y_4 = \dot{\theta}_c$, the ODE system can be transformed to

$$\dot{y}_1 = y_3 \quad (6)$$

$$\dot{y}_2 = y_4 \quad (7)$$

$$\dot{y}_3 = ay_1 + bi_{x1} + bi_{x2} + cy_2 \quad (8)$$

$$\dot{y}_4 = dy_2 + ei_{x1} - fi_{x2} + gy_1 \quad (9)$$

where the symbols a to g denote the system parameters to identify. ***Table. 1*** shows the identification results achieved by PINN. Herein, the model training was repeated ten times to calculate the means and standard deviations of the estimated parameters.

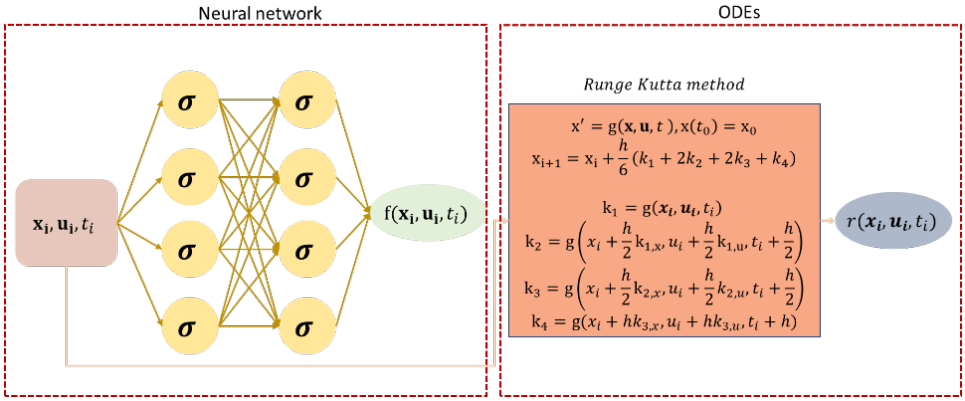

Fig. 1 Network Structure of PINN

	a	b	c	d	e	f	g
Real	2.978	49.64	-0.088	3.791	392.2	680.5	-8.649
Mean	2.941	49.64	-0.064	3.944	393.2	680.8	-8.700
STD	0.044	0.079	0.032	0.235	0.432	0.958	0.101
STD/Mean	0.015	0.002	0.502	0.060	0.001	0.001	0.011
Relative error	-0.012	0.000	-0.276	0.040	0.003	0.000	0.006

Table. 1 System identification results achieved by PINN

Conclusions

The preliminary case study results show that PINN successfully estimate the open-loop dynamics of an AMB system. In the next step, a proportional–integral–derivative controller will be added to the system. The more challenging closed-loop identification (Forssell, 1999) will be studied on the AMB system under feedback control.

Acknowledgments

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Battery materials identification using SciBERT word embeddings

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Abstract

Natural language processing (NLP) is an area of machine learning that deals with extracting information form text and converting it into a form which could be analyzed by machine learning algorithms and statistical analysis. At present there is an overwhelming amount of literature available across all research domains. We need tools to effectively identify connections between different concepts available in literature. Materials design for functional applications carried out using conventional trial and error methodologies is expensive and time consuming. Machine learning techniques can be used to discover materials for functional applications from existing literature. This article demonstrates an NLP based methodology using which suitable alternate electrode materials for rechargeable lithium-ion batteries could be identified. We have used the BERT framework [1] in this study since it takes context of words into consideration while computing word embeddings. Therefore, the word embeddings obtained could be much more informative than context-free language models like Word2vec [2].
SciBERT [3], which is a language model developed based on BERT framework is pretrained on scientific literature across multiple domains. This model was developed to improve performance of BERT framework on downstream scientific NLP tasks. Since the model has been trained on scientific literature it's vocabulary is rich with words used in scientific research and hence the improved performance. However, the SciBERT model is not trained in the field of *materials science* or *rechargeable batteries*. To get over this hurdle, the model was retrained in these domains using abstracts form Springer. 197,000 abstracts were obtained by querying the keyword '*battery*' directly. Abstracts were also obtained in the subject areas of '*Materials science*' and '*Inorganic chemistry*'. The corpus prepared from the abstracts was preprocessed to remove Chinese texts and subsequently the model was trained. Downstream tasks were devised to extract materials suitable for usage in lithium-ion batteries. Word embeddings were obtained from the trained SciBERT model. The obtained word embeddings would be used to identify materials that are similar to the already existing lithium-ion battery materials using cosine similarities between the embeddings. These materials can be seen as candidates to replace existing materials. The materials obtained could be studied for their viability to be used in lithium-ion batteries. Here we have demonstrated a method that identifies materials for batteries using an algorithm that operates in a completely unsupervised manner. These techniques could be used to select materials and set future research directions in the field of materials discovery.
Keywords: Natural language processing, Materials discovery, BERT model, Battery, Text mining

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A digital twin-based approach to automatic design space identification in smart process equipment assemblies

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Abstract

Modular plants (MPs) built from process equipment assemblies (PEAs) provide a promising solution to increasing requirements to time-to-market and flexibility in the pharma industry. While process design and engineering have been discussed before (cf. Schindel et al., 2021), support and acceleration of process validation in MPs remains an open research topic. In contrast to conventional plants, highly specialized PEA manufacturers are expected to cause a shift in knowledge distribution. Both, PEA manufacturers and owner/operators (O/O), will hold valuable prior knowledge in form of partial models and data for the design space characterization. This knowledge will be partially protected by intellectual property (IP) restrictions.

This paper presents a digital twin-based concept and framework for automatic identification of the design space in smart PEAs, which considers the distribution of knowledge between PEA manufacturer and O/O. According to the concept, PEA manufacturers will deliver smart PEAs with customizable digital twins (DTs) containing knowledge gained during PEA design and engineering as well as from similar PEAs. These DTs are a combination of behavioral models in form of DAE systems and information models providing further information on equipment like operation ranges of actors and sensors (cf. Boschert et al., 2018). O/Os can customize the DTs based on their prior knowledge e.g. regarding kinetics. Afterwards, automatic identification (Waldron et al., 2019) and dynamic feasibility analysis (Dimitriadis and Pistikopoulos, 1995) are used to identify the design space while automatically considering the prior knowledge. We implemented the framework in MATLAB and tested it utilizing virtual PEAs in several fed-batch process scenarios. We found that the tight integration of knowledge, algorithms, and equipment in a cyber-physical system can reduce the manual effort of the O/O. E.g., equipment related model parts are available to O/Os instantly and control parameters including ranges are available for design of experiments and feasibility analysis in machine readable form.

Keywords: Smart equipment, modular plants, digital twin, design space

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A Quality by Digital Design framework for pharmaceuticals and biopharmaceuticals

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Abstract

The pharmaceutical and biopharmaceutical industries are subject to stringent regulatory requirements to ensure quality, safety, and efficacy of the drug products. It is therefore paramount to intelligently design and operate the pharmaceutical and biopharmaceutical processes to deliver quality assurance over the product lifecycle. The introduction of the science and risk-based approach, Quality-by-Design (QbD), has addressed some of these objectives and significantly contributed to the adoption of more effective quality systems. As a result, QbD is increasingly seen as the most reliable regulatory standard in the Pharmaceutical and Biotechnology sectors. However, QbD still requires extensive experimental efforts despite the advantages offered by the traditional model-free design of experiments (DoE) commonly associated with QbD. Most importantly, QbD misses the opportunity to leverage effective model-based methodologies, and more broadly process systems engineering tools, to effectively minimize the experimental efforts, maximise reliability of the design space and achieve robust and fault-free operation. With the emergence of pharma 4.0 and digital transformation, there is an urgent need to develop a digital quality ecosystem which integrates more flexible and effective regulatory standards and advanced digital tools.

To reduce the cost of quality and reduce reliance on Quality-by-Testing, a novel Quality by Digital Design framework is suggested. Firstly, a mathematical model is developed based on the prior knowledge followed by the structural identifiability analysis to determine whether unique model parameter values can be estimated from input-output data. After addressing any structural non-identifiabilities, the prediction capability and reliability of the mathematical model are then refined based on the estimability approach combined with an effective model-based DoE (e.g. D-optimal, A-optimal). The objective is to identify the most influential and least correlated model parameters and minimize the cost of experimentation to help ensure information rich data and optimal estimates of the model parameters (Fysikopoulos et al., 2019). After validation, the mathematical model is firstly used to perform uncertainty and sensitivity analysis to help identify the Critical Process Parameters (CPP) and Critical Material Attributes (CMA). This process characterization step is considered as one of the most important challenges in the implementation of traditional Quality-by-Design which is commonly addressed by combining human expertise and expensive designs of experiments (e.g. factorial DoE). It also common to combine this approach with the risk assessment. A model-based method (e.g. Bayesian inference) is used to identify the design space (DS) and robust design space (Peterson, 2008). The approach allows effective incorporation of measurement noise and prior knowledge. The next step, model-based risk assessment, can be implemented after the development of the DS but may also be considered or duplicated after the

development of process control. The objective of risk assessment is to identify the most likely hazards and evaluate or quantify inherent risks. The approach is also used to confirm the set of the CPP identified earlier. After validation of the design space, the next challenge is to identify optimal normal operating range (NOR), an operating box within the robust DS space, which translates into finding the set points and flexibility margins (e.g. quality and safety margins) for process control. It also possible to consider dynamic operating ranges (i.e. a normal operating tube) for dynamic systems such as batch processes. Process control is the ultimate step and aims at selecting and demonstrating that the control strategy (e.g. MPC, PID) is robust and reliable enough to keep the CQA within the robust operating ranges despite noisy measurements, process-model mismatch and possible process upsets. The control strategy may also allow optimal trajectory tracking in the case of batch processes or dynamic transitions in continuous processes (e.g. start-up an shutdown). The suggested framework also allows continuous improvement that may be triggered by the availability of new data, new models, or new process characterization information such as new CPP and/or CMA. To validate the QbDD framework, the antisolvent cooling continuous crystallization of Aspirin (acetylsalicylic acid) is used as a case study (Liu and Benyahia, 2022).

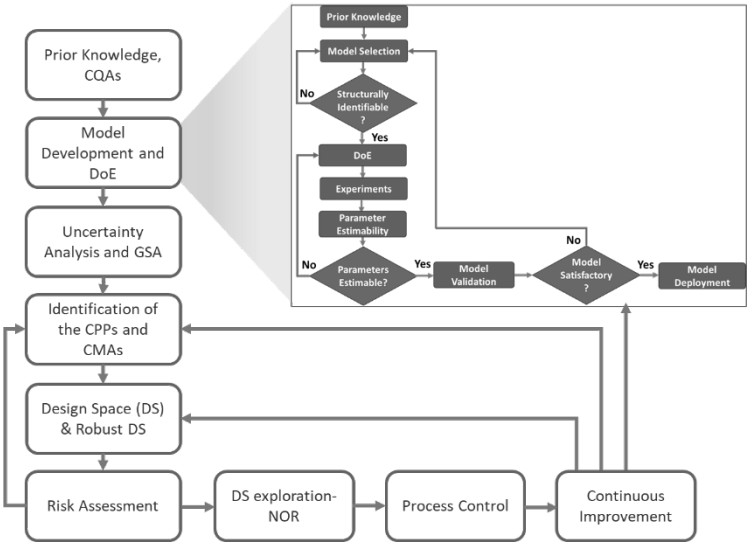

Figure 1. Framework for Quality by Digital Design

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Online state of charge estimation of lithium-ion battery using surrogate model based on electrochemical model

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Abstract

As electric vehicles (EVs) become popular, the use of lithium-ion batteries is increasing. However, it is difficult to ensure the reliable use of the battery because the state of charge (SoC) of a lithium-ion battery cannot be measured directly. SoC estimation is necessary to ensure the safety of battery systems by preventing over-charge and discharge of the battery and to extend battery life through efficient use. The optimal battery balancing strategy, estimation of the remaining driving range of EV, and Vehicle to Grid strategy can be developed through accurate SoC estimation. Therefore, it is necessary to study how to estimate the SoC of the battery in real-time. As methods for estimating SoC, equivalent circuit model, electrochemical model, and recently artificial neural network-based model are being studied. The electrochemical model is not suitable for real-time use due to its high computational complexity. Artificial neural network-based models require a large amount of data for learning, but most of the data is collected in the lab, which can lead to a lack of data and is difficult to ensure accuracy in such cases.
In this study, a surrogate model based on electrochemical models for SoC estimation is developed to solve computational complexity problems of electrochemical models and the accuracy problems of data-driven models due to data dependence. Based on the 1C discharge experimental data, parameter identification of the electrochemical model was performed using a Genetic Algorithm. Output variables such as Li-ion amount in the negative electrode and voltage for various drive cycle loads are derived from this model to create a sufficient amount of data for model training. The surrogate model is trained using these output variables and compared with data-driven models in terms of accuracy and computational complexity. Based on the Long Short Term Memory (LSTM) architecture, the artificial neural network-based model was trained gradually with 1C discharge data, Hybrid Pulse Power Characterization (HPPC) data, and driving cycle data, and then compared with the surrogate model at each step. As a result, the surrogate model based on an electrochemical model using fewer data showed feasible computational complexity and high accuracy. Through the proposed method, it is expected to accurately estimate battery SoC in real-time and make the battery use efficiently.

Keywords: Lithium-ion battery, Battery modelling, State-of-Charge

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Machine-learning based prediction of infinite-dilution activity coefficients of ionic liquids using physiochemical properties

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Abstract

Ionic liquids (ILs) is an organic salt in the liquid state, which have an excellent property as a favorable solvation for a range of polar and non-polar compounds. Recently, a number of ILs have been already used in a separation process, e.g., extraction of aromatic and aliphatic compounds from hydrocarbon mixtures, due to its high-energy efficiency compared to conventional separation processes that requires a considerable thermal energy or electricity. One of critical properties forward a wide application of ILs is the infinite dilution activity coefficient (IDACs) of solutes (45 types of organic solutes) and the equation of state (EoS) parameters. However, the discovery of a perplexing principle of ILs behaviors requires highly-sophisticated experiments on a number of solutes.
Moreover, the validity of conventional property models such as UNIFAC, Abraham and COSMO-RS for predicting IDACs show some limits in that only few solutes are applicable within a certain range of operating temperature. Therefore, in this work, we aimed to propose the machine learning (ML) based IDAC prediction model to rapidly provide precise properties and parameters of ILs separation process. First, ILs experimental data and their physicochemical features are collected from the literature. We then developed an IDACs prediction model using artificial neural networks (ANNs) and validated the model with accuracy metrics such as coefficient of determination (R2) and root mean square error (RMSE). Finally, the capability (accuracy and quantity) of the ML-based prediction model are discussed by comparing conventional models. As a result, it was revealed that the ML-based approach shows higher accuracy (approximately 50~10%) of a larger number of solutes (approximately 10 times) compared to conventional property models. A database of predicted properties based on data-driven strategy could lead to wide applications of ionic liquids in separation technique. From proposing a strategy for ILs utilization, the ML-based approach was able to provide the essential information on the ILs design and promote the future environmental-friendly separation processes.

Keywords: Ionic Liquids; Infinite-dilution activity coefficients; Machine-Learning;.

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The Impact of Reward Shaping in Reinforcement Learning for Agent-based Microgrid Control

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Abstract

In order to reduce CO2 emissions, electricity networks must increasingly integrate renewable energies. Microgrids are distributed electrical networks with their own generation and load, often supported by an electrical storage system. It can be connected to the external electrical network or isolated. Since electricity consumption, price and renewable production are stochastic phenomena, the control of microgrids must adapt to uncertainties. The complete physical model-based approach for high level control is thus unsuitable considering these uncertainties. However, with the increasing use of sensors, data-driven models and in particular reinforcement learning (RL) have become efficient algorithms in high-level microgrid control. RL are agent-based algorithms, which interact with their environment and learn with a numerical reward signal. A good control policy is a sequence of choices that maximizes rewards. A certain behavior can implicitly be expected when the reward system is formulated. For example, a reward system that encourages the agent to interact as little as possible with the external network will explicitly increase the autonomy of the microgrid. Implicitly, it can be expected to schedule the battery to maximize the ratio of renewable energy used to the amount producible. The objective of this study is to identify if there is a link between the most common reward function found in literature and the effective behavior of the agent. The simulated case studies concern a simple microgrid coupled to the main external electrical network, with photovoltaic panels (PV), electro-chemical batteries with a sufficient power density to accommodate the instantaneous power supply of the microgrid, and a load profile corresponding to residential power consumption. For the RL agent training phase and simulations, yearly real consumption and PV generation data profiles are used. The first year's data are used for the training and the other data for the validation phase. The RL algorithm is based on deep reinforcement learning with a neural network computing Q-values for each action from the microgrid states (inputs). Q-learning algorithm has been used due to its performance in discrete action space, which simplified the benchmark complexity. An agent is trained with different reward functions commonly found in the literature related to data-driven microgrid control algorithms. The agent parameters do not vary from one case study to another. Indicators are set up to evaluate the agent behavior. They are based on implicit behavioral criteria in the definition of the reward system such as the ratio of renewable energy used, the amount of energy stored during peak hours, etc. This study enables to find a way to rationalize the choice of a reward system to control in a near-optimal way microgrid while meeting implicit secondary objectives. It could lead to a choice on weighting coefficient in a combination of reward functions.

Keywords: Microgrid, Reinforcement Learning, Control, Reward

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Knowledge mining from scientific literature for acute aquatic toxicity: classification for hybrid predictive modelling

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Abstract

Properties of molecules lie in the heart of any sustainability assessment method. Predictive models, developed via typical statistical regression or advanced machine learning (ML) approaches, reduce the amount of experimental testing but strongly depend on availability of pre-existing data. Limitations on data often hinder the development of robust models, leading often to overfitting of model parameters and decreasing their applicability domain. This can be, for instance, of great importance during computer-aided design of novel materials. An approach combining ML methods with knowledge existing in the field might be one of the solutions to this problem, typically called hybrid modelling. The amount of work required to process the enormous volumes of information might hinder the utilization of the existing knowledge. Moreover, systematic methods of knowledge extraction from the vast amount of scientific literature are lacking. Thus, fast and to the extent possible automated procedures are needed to process the ever increasingly number of publications in any specific domain.

This work proposes a systematic, iterative method consisting of state-of-the-art text processing approaches, and human-machine interaction for the extraction of useful sentences and data in tabular, graphical, and numerical form for the development of a classification structure, containing information particularly relevant for hybrid modelling. It is applied to the domain of acute aquatic toxicity of chemicals, which is particularly relevant for the safety, health, and environmental hazard assessment of chemicals. Nearly 400 papers from 2000-2021 were identified and processed with the proposed method. The results indicated that the vast amount of knowledge can be efficiently processed in orders of magnitude faster than conventional methods without any loss of detail and interpretation depth. The classification scheme comprises more than 600 QSAR models and molecular descriptors, 200 alerts, 700 patterns and trends, and general statements, and around 50 chemical classes. Knowledge update mechanisms based on complementation, competition, and new classification categories addition was systematically applied to demonstrate the expected update of the proposed classification structure over a 5-years period. The information is in a form that can be useful in hybrid modelling with respect to model and predictor selection, prioritization, and constraints, addressing data gaps, and validating and interpreting model performance.

Keywords: machine learning, text mining, sustainability

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Machine Learning for the prediction of the thermochemical properties (enthalpy and entropy of formation) of a molecule from its molecular descriptors

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Abstract

This work investigates the use of machine learning (ML) methods for the prediction of thermochemical properties (i.e. enthalpy and entropy of formation) of a molecule from its molecular descriptors. Although quantum chemistry (QC) or group contribution (GC) methods have been commonly employed to calculate these properties, they have shown limitations in terms of applicability to more complex or larger chemicals and/or computational costs (Dral (2020); Dobbelaere et al. (2021); Yalamanchi et al. (2020)). Inversely, ML methods, based solely on data, already demonstrated their ability to tackle complex problems in other fields when classical approaches fail or are inefficient. Additionally, the use of diverse approaches (QC, GC, ML...) can help to confirm the reliability of the obtained thermochemical properties when the different methods provide similar values. In this work, public data from DIPPR (Design Institute for Physical Properties) database, containing 2230 molecules classified in different families and subfamilies, were used to train different ML prediction models.

Any ML approach requires a well-curated data set. In this sense, the first step of this study consisted in identifying and extracting relevant molecular descriptors (i.e., features influencing the targeted thermochemical properties) for the different molecules. The enthalpy and entropy of formation depend highly on molecular geometry, being expressed via the moments of inertia. The latter were therefore identified as relevant molecular descriptors. Different software for descriptors extraction were compared and the investigation of the effect of different descriptors on the accuracy of the trained ML models was assessed. This procedure was repeated for different groups of molecules. The predictions of enthalpy/entropy of formation obtained so far with moments of inertia descriptors (7 descriptors) are more accurate for the "alkanes" family, this being improved when considering a subfamily of "alkanes" such as "n-alkanes" as demonstrated by the following average RMSE values:

Average RMSE (kJ/mol)	**Alkanes**	**n-alkanes**
Enthalpy of formation of ideal gas	60.94 (validation) 46.43 (test)	7.99 (validation) 5.57 (test)
Entropy of formation of ideal gas	38.91 (validation) 30.95 (test)	17.02 (validation) 11.43 (test)

This work is part of a bigger project aiming at designing reactive working fluids for power cycles. The next step of this work will be to identify the most suitable ML methods and descriptors, and to fine-tune these methods, according to each family of molecules. The developed models will eventually serve in discovering new molecules that meet specific requirements for use in combined heat and power cycles.

Keywords: machine learning, enthalpy of formation, entropy of formation, molecular descriptors.

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A Novel Machine Learning-Based Optimization Approach for the Molecular Design of Solvents

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Abstract

The choice of suitable solvents is of central importance in separation processes, such as gas purification and extractive distillation, for achieving a high product purity and reducing the energy consumption. In the past decades, the computer-aided molecular design (CAMD) method has been widely used for solvent design where group contribution (GC) methods are usually employed for property prediction. Standard GC models sometimes cannot accurately predict certain properties, and moreover they cannot well distinguish between structural isomers.

For overcoming these limitations, we propose a new CAMD approach for solvent design by combining machine learning (ML) with deterministic optimization techniques. As powerful generative ML method, the variational autoencoder (VAE) is introduced. The VAE consists of an encoder that transfers a molecular structure into a continuous latent vector and a decoder converting the latent vector back to a molecular structure. Solvent properties of interest are estimated by another ML model (e.g., feed-forward neural network) using the continuous latent vector as input. By jointly training the VAE and property model with collected data, a continuous latent design space can be constructed for the optimization-based molecular design. Specifically, firstly the deterministic nonlinear optimization is performed to identify optimal latent variables featuring desirable solvent properties based on the established property prediction model. Secondly, knowing the optimal latent vector, the corresponding target solvent molecule is generated by the pre-trained decoder. Notably, an improved SMILES-based one-hot molecular encoding strategy is developed to ensure the structural feasibility and uniqueness of generated molecules during molecular design.

The solvent-based extractive separation of 1-butene and 1,3-butadiene is considered as industrially relevant example to investigate the reliability and efficiency of the proposed CAMD method. A set of solvent candidates showing superior separation performance are generated. To filter suitable solvent candidates for industrial application out of this set, additional aspects, such as cost and synthesizability, are analyzed.

Keywords: molecular design, solvent design, machine learning, nonlinear optimization

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A methodology for gray-box modeling of nonlinear ODE systems

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Abstract

In process modeling a gray-box model describes the extension of a purely mechanistic model with a data based or machine learning (ML) method. There exists a multitude of approaches to setup a gray-box model, an overview over different ideas can be found in Willard et al. (2020). Here, the focus lies on setting up models, that are posed as a set of ordinary differential equations (ODE) derived from physical understanding, where some model variables are described using ML approaches. Finding a suitable model structure along with parameter values is challenging. The intuitive approach to find an ML model structure together with a set of parameters is to guess the structure, and to initialize the values of the parameters randomly. Using standard parameter estimation techniques the set of parameters can be optimized.
This approach comes with two issues. Firstly, solving the ODE system can be numerically challenging, when the MLmodel parameters are randomly initialized, as both signs and magnitudes of their output can vary strongly. This can lead to unstable systems, for which the parameter optimization is challenging. Secondly, the fact that the ML model structure can only be guessed and iteratively adapted leads to a high effort in applications.
To address this problem we suggest a generalization of the methodology proposed by Hebing et al. (2020) for a special situation. We here include nonlinearity of the model regarding the ML model parts. The key idea is to decompose the problem into different steps. In a first step, an input-output data set for the ML model is constructed. In related work, Scheffold et al. (2021) use an unscented Kalman filter to estimate the quantity which is then modeled with an ML model.
In our method the ML model parts are substituted by explicit functions of time, which allows for generating an input-output data set that can be used find a suitable ML model structure and simplifies solving the full scale parameter estimation problem. We demonstrate the approach for a fermentation model. Our results show, that using this methodology an accurate gray-box model of the fermentation process can be obtained efficiently.
Keywords: process modeling, gray-box modeling, machine-learning

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Optimal aeration of wastewater treatment plants based on recurrent neural networks and real plant data

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Abstract

The aeration of a wastewater treatment plant is a highly relevant aspect of complying with environmental regulations for effluent concentrations as the dissolved oxygen is required for the aerobic decomposition of organic components and other pollutants. In addition, the power consumption of the air compressors is a major cost driver, which makes optimal control of these compressors desirable. However, wastewater treatment plants pose severe challenges for online model-based dynamic optimization strategies because the underlying nonlinear biological and biochemical reactions are hard to model and inlet concentrations are difficult to measure due to the particulate system. This makes the application of reference models, such as the well-known ASM family by Henze et al., to online applications much more difficult. Data-driven models can be a viable alternative to these classical first-principle models. In this approach, all relevant output variables, e.g., concentrations, are predicted by a data-driven model.

To this end, recurrent neural networks (RNNs) within Tensorflow2 with and without long short-term memory and a self-implemented RNN based on a multi-layer perceptron from Scikit-learn are trained with real data from a plant in Germany. Here, the feedback of outputs allows previous regressors to have an impact on the current prediction. Inputs of the trained RNNs are the volume flow of the influent, the levels of the four rainwater basins, and the compressor power of the four aeration compressors. The trained outputs are pH value and the concentrations of phosphate and ammonium ions, dissolved oxygen, and solids. Instead of choosing the hyperparameters of the RNNs by trial-and-error, a hyperparameter tuning is carried out for optimal performance.This results in RNNs with a maximum mean squared error between the predicted outputs and the testing (scaled to unit variance) of less than $1x10^{-3}$. Given this small prediction error for the outputs, the optimal aeration trajectory for the compressors can be determined online every 15 minutes to minimize their energy consumption while keeping the effluent concentrations within the legal limits. In the full contribution, the investigated part of the wastewater treatment plant is explained in more detail. Then, the training, tuning, and testing of the RNNs using real plant data is discussed. Finally, a comparison between the optimal and the actually applied aeration trajectory is presented. This allows a quantitative analysis of the economic benefit of our approach. As data from the colder winter season has not been available yet for training because of recent modifications to the plant, the predictions will likely be less reliable during this time as reaction rates during winter are significantly lower. This missing data will be added to the training as soon as possible.

Keywords: Machine learning, Recurrent neural networks, Wastewater treatment, Optimal control, Dynamic real-time optimization

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Soft Sensor of key components for Recirculating Aquaculture Systems, using Artificial Neural Networks

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Abstract

Recirculating Aquaculture Systems (RAS) have two dynamic sub-systems: fish metabolism and water treatment. The water treatment system is responsible by keeping the water quality at high standards, reducing water consumption, and reducing contact with external pathogens (European Market Observatory for Fisheries and Aquaculture Products, 2021).

Regarding the water quality, some components are important to be monitored due to toxicity, but are hard or not able to be measured in real-time, such as dissolved carbon dioxide and ammonia. One way of using information of the process to estimate the concentration of these toxic components is by using soft sensors (Fortuna et al., 2007). The soft sensor technique is a combination of data, for parameter estimation, and process knowledge, with feature selection. The development of the data-driven models can be, for example, using machine learning models, such as Artificial Neural Networks (ANN).

In this work, the main objective is to apply artificial neural networks (ANN) as a soft sensor for land-based aquaculture of Atlantic salmon (*Salmo salar*). The data is acquired from a steady-state model of the water treatment process with uncertainties, using extent of reactions. The uncertainties were changed using latin hypercube sampling (LHS) so it could contain the operating region, which gives optimal growth and where the model is valid. After addition of noise, the data is used to train different ANN for predictions of carbon dioxide and ammonia concentrations.

As ammonia concentration is really low and its range is quite narrow, the ANN was not able to predict it, giving flat predictions. The way we bypassed this problem was by developing a soft sensor for ammonium instead. The ANN were able to predict the concentrations of ammonium and dissolved carbon dioxide. The ANN that gave the best performance in the validation phase were tested with industrial data to evaluate accuracy of its estimation skill.

Keywords: Soft sensor, Recirculating aquaculture systems (RAS), Artificial neural networks, Atlantic salmon

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Sensitivity Enhancement of Optical Signals for Plasma Etching Processes Endpoint Detection with Machine Learning Methods

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Abstract

The plasma processes in the semiconductor manufacturing industry become more complicated to control due to the reduction of critical dimension and introduction of 3-dimensional structure in the integrated circuit. In the plasma etching process, etching endpoint detection (EPD) is conducted to stop the process at the appropriate moment to prevent device failure and yield reduction. Optical emission spectroscopy (OES) is generally used for EPD with non-invasive characteristics. However, as the open area gets smaller and processing pressure lowers, conventional EPD using a single spectra signal becomes difficult. In this work, machine learning methods are modified and applied to OES data to enhance the sensitivity of optical signals.

EPD experiments were performed in an inductively coupled plasma etching chamber. An RF source power of 13.56 MHz was delivered through the inductive coil, and an RF bias power of 12.56 MHz was supplied to the electrodes. Both source power and bias power were set at 250 W. CF_4, Ar and O_2 were injected into the chamber at flow rates of 40, 40, and 10sccm, respectively. The chamber pressure was maintained at 50mTorr. A SiO_2 coupon wafer for the etching target was placed on a bare Si wafer, and plasma etching was performed. The area ratio of the SiO_2 coupon wafers varied as 8.0, 4.0, and 1.0% for 4-inch Si bare wafers. An optical spectrometer with 6144 channels was installed, and peaks between 194.1 and 885.51 nm were collected every 500ms.

In this work, k-means cluster analysis (KMC), gaussian mixture model (GMM), and spectral clustering (SC) were applied to enhance the sensitivity of optical signals of EPD and compared with signal-to-noise ratio (SNR) value. KMC, GMM, and SC are clustering methods that divide data into groups according to similarity indicators of each method. KMC performs clustering based on distance from centroids of clusters, GMM performs clustering based on probability of belonging to the cluster, and SC performs clustering based on the value of similarity of each data in graph dimension. Each clustering method was modified for multivariate and time series characteristics of optical signal data. At each point in time, OES data collected for the last 5s are normalized, and the normalized data are divided into two clusters by clustering analysis. The degree of clustering was evaluated with the clustering validity factor (V factor). The validity factor that is much

smaller than 1 indicates that the data are classified into two groups: before endpoint and after endpoint. In addition, wavelengths correlated to reactants and by-products of chemical reactions in the plasma process were selected to enhance the performance of modified clustering methods.

All the modified clustering methods showed the improvement in EPD compared with single spectra signal for relative areas of 8.0, 4.0, and 1.0 %. The sensitivity of the OES signal was improved about two times improved using modified KMC and improved about three times and 2.5 times by the modified GMM and modified SC, respectively. The selected wavelengths enhanced the performance of modified clustering methods about three times on average. Therefore, modified machine learning methods are effective for EPD with optical signals, and a chemical engineering-based approach to endpoint detection is expected to increase the effects of the machine learning methods.

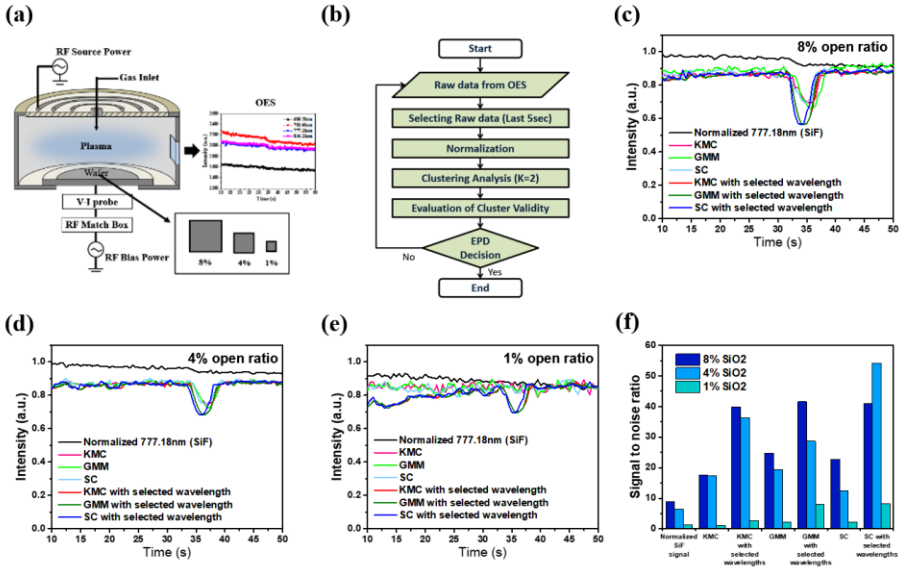

Figure 1. (a) Plasma etching endpoint detection with OES signals, (b) Real-time EPD algorithm by clustering analysis, and endpoint detection with etching of different relative area of SiO_2: (c) Result of EPD in 8% area SiO_2 etching, (d) Result of EPD in 4% area SiO_2 etching, (e) Result of EPD in 1% area SiO_2 etching, (f) The comparison of the sensitivity factor: Normalized single spectra signal, KMC, GMM, SC.

Keywords: Plasma process, Optical Emission Spectroscopy (OES), Machine Learning

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Digitalization in sustainability assessment for supporting agri-food waste circularity

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Abstract

In January 2020, the European Commission (2019)presented the European Green Deal including the main action plan named “Circular Economy Action Plan” which encourages industries to move towards a clean and circular economy. To achieve these objectives, industries must take into account the entire life cycle of their products and processes. The last decades have seen the development of life cycle thinking in the field of agriculture and in particular through the creation of recycling processes of agricultural waste to make biofuels, biomaterials or biomolecules. Since these processes must be economically viable and environmentally responsible, researchers and R&D engineers use environmental and economic analyses - called here sustainability analyses - when designing them (Sammons et al., 2009). However, these sustainability analyses require many processes data – also called foreground data. These data are difficult to access and process. They can actually be extracted from scientific articles and the public web.

The paper suggests a digitalization of sustainability analysis taking benefit from artificial intelligence (AI) and data science technologies (DS). The digitalization approach couples sustainability analyses and IA/DS to assist in the selection of biomasses and/or biomass pretreatment technologies to produce glucose. Five steps characterize this proposed approach: (1) goal and scope, (2) data architecture, (3) sustainability assessment (4) data visualization and analysis of results and (5) decision. The first step, *goal and scope of the study*, comes from Life Cycle Assessment (LCA) ISO approach (ISO 14040:2006, 2006). Life cycle thinking is recommended. This thinking encourages a "cradle-to-grave" or "cradle-to-gate" approach if the logistics of a value chain are difficult to get. The *data architecture* is directly inspired by the construction of big data architecture and consists of five sub-steps: (i) data collection and extraction from Knowledge Engineering, (ii) data enrichment and storage thanks to Process Engineering, and thanks to Machine Learning (ML), (iii) data cleaning, (iv) (raw) data analysis, and (v) (raw) data visualization. The third step, *environmental and economic impacts* are calculated thanks to Life Cycle Impact Assessment (LCIA) and Life Cycle Cost (LCC). In the forth step, the use of ML tools for *analysis and visualization of results*. At the end of the previous step, the result obtained is a matrix with the processes, biomasses, environmental and economic impacts, which is difficult to analyse for a non-expert in LCA. From the statistical literature, this step combines traditional techniques for dimension reduction and unsupervised clustering to extract knowledge about LCIA and LCC. In final, the visualization of data clusters from the previous step can help the researcher with his decision-making. This *decision* can be made by the researcher himself or by a group composed of different engineers/researchers from different fields.

The case study is the selection of biomasses and/or biomass pretreatment technologies to produce glucose. In this abstract, we detail the raw data analysis step. The others step are detailed in Prioux (2021). An ontology to semi-automatically extract and collect pretreatment processes data from 30 published scientific articles which represents

more than 23K data (numeric or not). After this step, we clean the data and we will study the partial dependence plot (PDP) (Friedman, 2001) which allows us to characterize, in a certain way that we will try to delimit, the influence of a variable in a model. We are working on the prediction of glucose yield by neural networks. The PDP shows the marginal effect of a variable on the prediction of a classifier or regression. It identifies both the direction (positive or negative) and the form (linear, non-linear, stepwise) of the relationship. Figure 1 shows the PDP and Individual Conditional Expectation (ICE). The PDP shows the marginal effect one or two features have on the predicted glycose yield (GY) of a neural network (MLP). It indicates whether the relationship between the GY and input variables is non-linear, monotonic, or more complex. An ICE curve is calculated by maintaining the input variable of interest x_i at a value x_{ip}, where x_{ip} is the value of x_i in the p row of the dataset, and varying all other inputs across their values in the dataset. A bar plot demonstrates how the value of the input variables affects the sensitivity of the output variable. Two variables have a more significant impact on glucose yield: the maximum temperature used and the quantity of water.

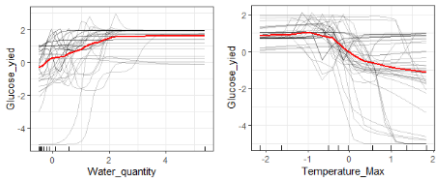

Figure 1 PDP (red) and ICE plots (black). The PDP is mean of ICE curve.

This raw data analysis provides first learning to the data for the researcher who can adapt his research. After, we can continue the approach with the calculation of economic and environmental impacts and the analysis of the result with another ML tool. A general approach coupling DS/IA and LCA/LCC was proposed. Composed of five steps, this approach is presented as a decision aid for the researcher in a pre-study. The life cycle analysis is therefore carried out at a research TRL scale (TRL scale 1/2) which can lead to a change of scale if we want to switch to an industrial pilot. Another limitation in the data concerning the abundance and quality, which can be very low for some innovative and new processes such as biomass pre-treatment processes. It would be interesting for future studies to change the functional unit and broaden the boundaries of the study to take into account the overall logistical scale or to consider effluent recycling. A final limitation comes from the main input, which is biomass, a waste product from agriculture. Furthermore, it is necessary to evaluate its durability and supply, which could also vary over time.

Keywords: Machine Learning, Data visualization, Life Cycle Thinking, Knowledge Engineering, Waste Valorization

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Interpretability of neural networks predictions using Accumulated Local Effects (ALE) and sensitivity measures.

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Abstract

Recently, Machine Learning (ML) techniques, especially deep neural networks models, have become a crucial tool for various engineering applications such as chemical engineering. These techniques have achieved high predictive accuracy and are mostly owed to their ability to model complex nonlinear interactions between predictors and model outcomes. However, most accurate predictions remain in the black box frameworks, meaning that interpretation of the model's parameters and explanation is partially (or entirely) hidden to the experts. Understanding the reasons behind predictions is very important to one plan to act based on these predictions. In this paper, in order to enhance the interpretability of machine learning, Model-Agnostic methods are used and applied to real complex data and prediction problems (Molnar, C.,2020).

One of the interesting model-agnostic methods available is Accumulated Local Effects (ALE) Plots (Molnar, C.,2020). Our previous work dived into other model-agnostic methods and discussed the main effect dependence of $f(x_1, x_2, \dots, x_n)$ on each predictor $x_1, x_2, \dots, x_n$ (Danesh et al., 2021). This study will work on ALE Plots to detect the lower order interaction effects among different predictors and compare with other visualization tools for interpretability purposes. Multilayer Perceptron (MLP) prediction model has been used to test ML-sensitivity measures. We also studied the influence of the network architecture on the sensitivity measures of the model.

Model-Agnostic methods were performed on real data from a Combined Cycle Power Plant (CCPP) for six years (9568 data points) (Tüfekci, P., 2014). The system considered ambient temperature (AT), vacuum (V), atmospheric pressure (AP), and relative humidity (RH) as input parameters; and electrical power output (PE) as system's output.

The significant advantage of model-agnostic methods is their flexibility. These methods can be applied to any ML model (regression and classification). The visualization provided by these tools is an important model diagnostic technique.

Keywords: Machine learning, Neural Network, model-agnostic, Sensitivity analysis

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Hybrid Models in Chemical Engineering – A Purpose driven Perspective

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Abstract

Models are mathematical abstractions of real-life systems, often attempting to predict future states, or even gain insights of said systems. As opposed to tasks in computer vision or text classification, chemical engineering systems are guided by fundamental laws comprising of but not limited to conservation equations and constitutive laws. These, if correctly obtained, completely describe the system. However, as the complexity of systems increases, obtaining these first-principles models becomes exceedingly difficult. At the other end of the spectrum, are models developed solely on the basis of data. These techniques are rooted in statistical approaches, often estimating parameters, uncertainties, predictive accuracy etc. While they provide little to some insight of the underlying mechanism that drives the system, they manage to perform well in industrial settings. This however, comes at the cost of not being able to provide detailed reasoning for the model's performance. Further, interpretability issues arise which could lead to a well-performing model not being accepted by end-users. Such models are termed 'black-box' models, since there is no under-the-hood information available. As a result, hybrid models are developed, while combining the available first-principles' knowledge, with techniques developed for black-box modeling. These attempt to exacerbate the drawbacks of both approaches involved, and provide insights of the system. Hybrid models are developed for different end-user purposes – interpretability, mechanistically-driven, performance (execution speed and accuracy), guaranteed adherence to constraints, interoperability (including extrapolation), and enhanced predictive modeling. This review article describes these disparate but linked approaches, and provides a summary of notable progress in this field. Further, it provides a perspective for potential future research in this domain.

Keywords: mechanistic models, hybrid models, data-driven model, reduced-order model

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A data driven model for prediction of adsorption energies on metallic surfaces

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Abstract

Processes based on electro-catalytic reactions on metallic surfaces comprise promising low carbon pathways for the production of chemicals. As examples, recent works from Fan et al. (2020); de Arquer et al. (2020) have shown that is possible to reduce captured CO2 into methanol, ethylene, formic acid and others, in renewable-electricity-powered electrochemical reactors. However, these reactions are highly non-selective and it is not yet clear which conditions favor some products over other ones. Understanding this, is key for proper reactor and process design.

Given the reactants and a set of reaction rules, softwares such as RING (Rangarajan et al. (2012)) can be used to generate the chemical reaction network and assess which products should be expected. Models to predict network energetics are needed to identify those routes that are thermodynamically feasible.

This work presents a data-driven model for prediction of adsorption energies of reaction intermediates on metallic surfaces. First, a database of adsorption energies for different adsorbate/surface pairs is built taking data from Chowdhury et al. (2018); Schmidt and Thygesen (2018). Then, in order to determine the features that best describe the metallic surface, a principal components analysis followed by Varimax rotation is applied to the database. PCA-Varimax is chosen over plain PCA as it allows a greater degree of simplification. Finally, these PCA-Varimax derived features, together with bond information of the adsorbate are used as inputs to learn a model for adsorption energies. After testing several regression techniques, it is found that by using Kernel Ridge Regression it is possible to train a model that provides a mean square error MSE of 0:01 on training data and 0:1 on test data.

Keywords: Machine Learning, Electrocatalysis, PCA Varimax, Kernel Ridge Regression

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Probabilistic graphical models for reaction pathway identification and analyses in water treatment

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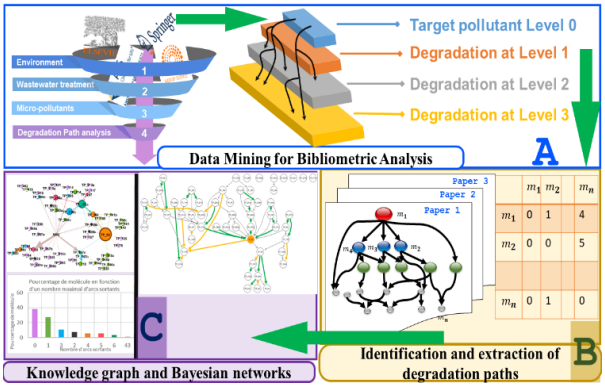
Abstract

Water is a scarce resource, the ultimate receptacle of anthropogenic pollution. Its preservation and treatment are the subject of new paradigms in terms of analytical development, processes and even data management. In the last decades, the scientific community has pointed out the presence of new synthetic molecules in all aquatic compartments. Several studies proposed a degradation pathway of a targeted micro-pollutant, which could be different depending on study objectives, analytical methodology, etc. Often these studies are oriented on the formation of Transformation Products (TPs), in controlled conditions and with a singular process. The methodology was applied to Sulfamethoxazole (SMX).



In this study, we proposed a hybrid approach based on Knowledge Engineering for process data extraction (data mining for bibliometric analysis) and probabilistic graphical models (Pearl, 2014; Heckerman et al.,1995) for identification and analyses of reaction pathway of molecule degradation in water treatment (Figure). The bibliometric analysis gathered more than 45 articles for more than 140 molecules and 177 reactions pathways. The Bayesian Network have shed new light on the interaction between the TPs in water treatment. Among all tested algorithms for learning structures, the obtained structure based on a Bayesian Dirichlet likelihood-equivalence (BDe) score gives a good compromise between the graph structure and its interpretation.

Keywords: Knowledge Engineering, Bayesian Networks, Graphical Models, Reaction Pathway.

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Integrating autoencoder and heteroscedastic noise neural networks for industrial data analysis and soft-sensor design

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Abstract

Viscosity represents a key indicator of product quality but has traditionally been difficult to measure in-process in real-time. This is particularly true if the process involves complex mixing phenomena operated at dynamic conditions. To address this challenge, a promising solution to monitoring product viscosity is to design soft-sensors which correlate viscosity with easily measured process variables. In this study, we developed an innovative machine learning based soft-sensor construction framework by integrating different types of advanced artificial neural networks. The framework first employs a deep learning autoencoder to generate information-rich statistic latent variables by compressing high-dimensional industrial data, and then adopts a heteroscedastic noise neural network to simultaneously predict product viscosity and process variance based on the extracted latent features. To evaluate its accuracy and robustness, the data-driven soft-sensor was used to predict product viscosity for a number of industrial batches operated over different seasons. It is found that the soft-sensor has both high accuracy (prediction error <12%) and high robustness in most of the cases, indicating its great potential for industrial batch process monitoring and quality control.

Keywords: Machine learning, data analytics, dimensionality reduction, quality control, uncertainty estimation.

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How digital twin solutions can drive the hydrogen economy?

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Abstract

Hydrogen is an emerging energy vector that has been identified as a key driver for achieving sustainable development goals. Its inclusion in the energy grid allows managing the intermittency of renewable energy sources (i.e., solar and wind), offers low-carbon fuel supply, and enables the integration of gas and electricity grids. However, some challenges must be overcome. The future of the hydrogen economy depends primarily on the development of (i) new technologies that operate optimally using available resources, (ii) radically lowering the costs and risks associated with the value chain, (iii) optimal management of distribution networks, and (iv) clear certification and traceability schemes. Digital Twin solutions and Artificial Intelligence (AI) could help to address these challenges. This work presents a synthesis of a return of experiences from different industrial and R&D projects linked to renewable energy and green hydrogen production, which allows identify some opportunities and perspectives for the development of Digital Twin technology applied in this sector. Digital Twins, along with the Internet of Things (IoT) and based on AI technologies, offer the possibility of transforming today's manufacturing paradigms towards intelligent manufacturing (Y. Wang et al., 2020). Through a permanent exchange between the physical hydrogen value chain and the virtual model, it would be possible to: (i) offer R&D prospects for system improvement and integration to achieve higher Technology Readiness Levels (TRLs) (B. Wang et al., 2020), (ii) decrease the uncertainty associated with investment costs and risks (Corlu et al., 2020), (iii) optimize the operation and maintenance of systems on a real time basis, (iv) dynamically adapt to a changing markets and environment, and (v) carry out certification and traceability. Therefore, Digital Twin solutions can contribute to ensure a robust and profitable hydrogen economy in line with the energy transition ambitions.

Keywords: Digital Twins, IoT, Artificial Intelligence, green hydrogen, renewable energy.

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Predicting the density of natural deep eutectic solvents by the combination of a group-contribution method and artificial neural networks

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Abstract

Background: Natural deep eutectic solvents are gaining attention in the chemical society as sustainable designer solvents due to their lower volatility, flammability and toxicity and better biodegradation compared to common organic solvents or ionic liquids (Paiva et al. (2014)). NADES are the mixture of two or more naturally derived organic compounds (usually a quaternary ammonium salt and a hydrogen bond donating component, like urea or a polyol) which form a strong intermolecular hydrogen-bonding network. This network gives outstanding stability to the system and significantly decreases the melting point of the mixture compared to the initial compounds. The properties of NADES can be fine-tuned through the alteration of the compounds and their molar ratio, facilitating the application of NADES as designer solvents for various chemical reactions and applications (Zhang et al. (2012)). However, the large number of possible solvent systems would require the prediction of their properties in a prior screening step, but currently no practical and versatile model is available for this.
Methods: To tackle this issue, we developed a density prediction model for NADES. We composed a database with 1387 instances, based on earlier reported density values between 0.928 and 1.342 g/cm^3. Using a group-contribution method, we translated the compounds of NADES into functional groups. The number of these groups, together with the molar ratio of the compounds in NADES and temperature were the input variables of our model. The data was split into training/validation/test subsets in 70/15/15 ratio. To predict the density of the NADES system we trained a multi-layer perceptron regressor (Adayemi et al. (2018)). The final number of hidden layers (6) and nodes per layer (30) were determined in an optimization step, based on the MSE and R^2 values of the trained model's predictions on the validation set. The model used hyperbolic tangent activation function, adaptive learning rate and momentum of 0.9.
Results: The regression coefficient (R^2) of 0.86 and an absolute relative percentage error of 2.5% on the test dataset indicate that our model quantitatively predicts the density. Although these metrics are worse than some earlier published models (Shahbaz et al. (2011)), the use of functional groups as features provides more versatility to our approach, as these variables can be calculated to any novel compound without an additional computational or experimental step. Our method uses a larger feature space, which requires a complex model. On the other hand, these variables can be calculated for any compound based on the chemical structure. Therefore, the incorporation of novel systems is simple, in both training and prediction. The same approach can be applied for other properties (viscosity, refractive index) if the appropriate database is available.

Our current model shows lower accuracy for some functional groups. This is related to the imbalances in our dataset: while some functional groups are well represented (methyl, hydroxyl and carboxyl group occur in 1678, 2242 and 411 cases, respectively) some functional groups are scarcely available in the literature (e.g., amides in 28 cases). Additional data on these groups would increase prediction accuracy and the robustness of our model.

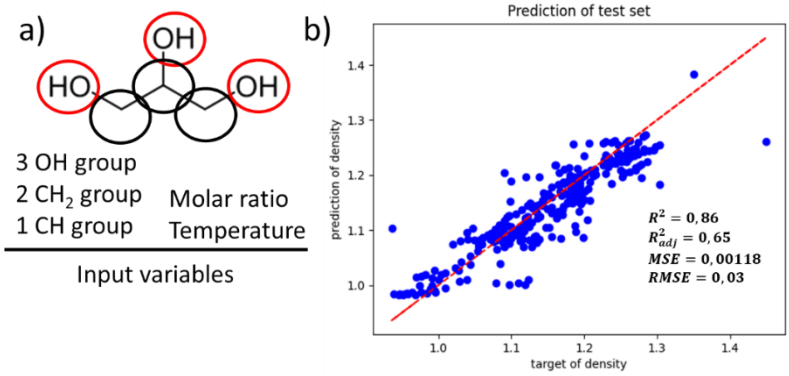

Figure 1: a) Input variables: number of functional groups in compounds, molar ratio of compounds and temperature. b) Performance of trained model on test set

Conclusion: The proposed approach is suitable for the quantitative prediction of NADES' physicochemical properties. Our study demonstrated this on density. The described modeling approach provides versatility and flexibility as novel mixtures and compounds can be included easily due to the use of functional groups as descriptors. However, the current model has multiple limitations. Firstly, we included only NADES with two components, while ternary and quaternary systems occur frequently in practice. Secondly, the water content of the NADES was neglected in our model, while in reality this plays key role in the physicochemical properties of NADES. Thirdly, the predictions of novel systems will be accurate only if their functional groups are properly incorporated in our model. We intend to address these issues in our further work. In addition, the same approach will be applied on viscosity. We also consider the application of interpretable machine learning models on this dataset to study the structure-property relationship of NADES.

Keywords: artificial neural network, deep eutectic systems, density prediction, group-contribution method, machine learning.

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Machine Learning-Based Surrogate Models and Transfer Learning for Derivate Free Optimization of HTPEM Fuel Cells

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Abstract

The discovery of new materials like catalysts, polymeric films, and biomolecules, is driven by industrial needs such as improving reaction or separation selectivity, enhancing therapeutic effects on medical treatments, or reducing costs of replacement. However, deployment of these advances in industrial applications is often hindered by the lack of models needed for design and optimization. Due to the novelty of the materials and devices, experimental data and first principles knowledge is scarce, making it hard to build models either via data-driven or knowledge based approaches. In this context, a way to efficiently combine domain knowledge with data could provide a pathway to streamline new materials discovery for industrial applications. Transfer Learning (TL) is an extension of Machine Learning (ML) in which knowledge learned for a particular task can be leveraged to ease the training for a new task. In terms of modeling for electrochemical systems, models developed for a given device or material can be leveraged to reduce the amount of data needed to accurately predict how new materials, operating parameters, and device configurations affect system performance. When the data for the initial training stage comes from a simulation, domain knowledge can be easily incorporated into the data-driven model, while at the same time reducing the number of experiments to be conducted – which can be timely and costly. This approach generates surrogate models that approximate the real behavior of the systems with adequate accuracy at a reasonable cost. In this work, a TL framework for the development of ML-based surrogate models to be used with a derivate free optimization algorithm is presented. Simulations from a compositional knowledge-based model validated using experimental data was used to generate training examples for a ML-based surrogate model. Then, TL learning was used to improve the performance of the ML-based surrogate model by using experimental data as training examples. Finally, an implementation of Particle Swarm Optimization (PSO) was used as demonstration of the applicability of this approach for optimization. Results show that knowledge from the simulated training data is effectively preserved and transferred to the new model whilst the information contained in the real experimental data can be incorporated to produce a new improved and robust surrogate model. PSO reached a physically consistent solution after 15 iterations.

Keywords: Surrogate modeling, machine learning, transfer learning, high temperature polymer electrolyte fuel cells.

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A Methodology for The Optimal Surrogate Modelling of Digital Twins Using Machine Learning

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Abstract

Process simulation and digital twins are of paramount importance to design new processes or optimizing already existing plants and equipment. The main drawback with current process simulation software is the computational time required to obtain a solution convergence towards a new steady-state. Especially when the input or the output to a system are perturbated. This procedure may take up to minutes in large systems or with strong non-linear recycles. A typical optimization strategy, may it be, e.g., for energy minimization or product maximization, requires many iterations at different input-output conditions to be successful. This number of iterations is not fixed and may range from an order of thousands up to millions and eventually more depending on the tolerance of the solution. In typical systems, the number of iterations and the convergence time are strictly positively related, when the first one increases the second follows through and vice versa. In sum, performing a simple optimization using a process simulation that is already slow to converge is too much time-consuming and consequently impossible to debug.
The solution proposed in this work is a framework that automates the surrogate modelling of process simulations using the best-fit machine learning algorithms for each process variable. The framework has been developed around a real case study of an amine washing process for acid gas removal inside the Itelyum exhausted oil regeneration refinery of Pieve Fissiraga, Lodi (Italy). The process is composed of three sections, a low-pressure absorber, a high-pressure absorber, and a regenerator. The data used to train the machine learning framework is taken directly from the process simulator, in this case, Aspen HYSYS V10 using the Excel Visual Basic programming language. For each stream or unit operation inside a flowsheet, all the properties needed to identify their thermodynamic state are extracted. The data extraction is performed for a fixed number of desired points inside a domain chosen by the user where each variable may have a minimum and maximum value. Many permutations of the input variables to the streams and units are created and the simulator tries to find a convergence for each point. After all the simulation data is collected the machine learning step takes place and the framework tests many different algorithms (polynomial fit, ada-boost, random forest, neural networks, etc.) to find the best-fit-lowest-complexity model.
In conclusion, the framework is able to find the less complicated algorithm that fits successfully each process variable and thus it is possible to recreate the behaviour of the real process simulation. Using the machine learning models thus constructed is way faster and does not require a convergence procedure since it is a direct calculation. One of the main usages of this tool is the possibility to approximate the actual process and perform optimization strategies with less time consumption.

Keywords: surrogate model, machine learning, digital twin, amine washing

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Bayesian Neural Network Calibration for Urban Air Quality Sensors

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Abstract

With the growing urbanization process in several cities around the world, air pollution mitigation has become one of the main environmental challenges of present time. Recently, low-cost and small size sensors have become a current trend in the air quality control area, since they are an affordable alternative for deployment of massive multiple point networks for air quality monitoring with high spatial resolution. However, these devices, normally based on MOS (metal oxide sensors) and ECS (electrochemical sensors), suffer interference from external conditions such as temperature, humidity and other pollutants, reducing their accuracy. Besides that, they generally cannot maintain a stable measurement accuracy over a long time due to drift sensor problems. Therefore, periodical calibration of these sensors is essential to maintain the quality of their measurements. Calibration methods based on machine learning recently emerged the excellent alternatives for in-field sensor calibration, since they are based on multivariate learning models that account external factors and time series data non-linearity to calibrate sensor raw data. Hence, this work presents a novel machine learning calibration method based on a Bayesian neural network model. All steps of calibration including the pre-processing of the raw data, model training, and model testing are presented. The proposed method is trained and assessed using a real public available dataset. The results of the test experiments show that the method has a good accuracy performance, with a lower mean absolute error compared to other machine learning methods applied to the same dataset. In addition, the method presents the advantage of directly providing estimations of the uncertainty of the calibrated measurements, which is an important metric used to assess the quality of data provided by air pollution sensors and that most of other calibration methods usually cannot provide.

Keywords: air quality evaluation, sensor calibration, machine learning, Bayesian neural network

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Ensemble machine learning for predicting the microbial growth

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Abstract

In biochemical engineering, the exponential phase in the growth microbial is very important, because the kinetic parameters are obtained, these one are used in the design and control for biological reactor. However, the kinetic microbial reported in the literature are obtained under specific growth conditions, which limit their possible application in dynamic models. For this reason, in this paper we propose employed machine learning for predict growth microbial, which provides information on the effect that variations of pH (5, 7, 9) and concentration of the culture media (10, 20, 40, 60, 80, 100% v/v) have on the growth rate. The case study biological reaction and sets of experimental exploratory data is for Pseudomonas aeruginosa (P. aeruginosa). The versatile and robust metabolism of P. aeruginosa are responsible of its ability of growth in different environment conditions even at low nutrient and oxygen levels, in an ample range of temperatures (4-42º C) and polluted sites. We propose a technique for obtained experimental data that consist in the measurement the optical density (growth microbial) in Multiskan™ FC Microplate Photometer, Thermo Scientific. The experimental data obtained, are processing in black box model based in artificial intelligence. Our contribution suggest using Hyperconic Multilayer Perceptron (HCMLP) as tool computational approaches to predict microbial growth, out the set conditions in the experimental design. The HCMLP includes the estimation of a conic. The neurons included in the hidden layer are named Hyperconic Neurons (HCN). The HCN uses a transfer function that defines decision boundaries using hyperboloids, paraboloids, spheres and ellipsoids. The computational model obtained from this tool allows us to obtain both the response surface and make predictions of growth before pH and concentration values that were not evaluated experimentally but these one are into the range experimental variable values. According to results, our mathematical and computational model HCMLP is robust and capable to predict the dynamic growth of bacteria P. aeruginosa when tuning two main operation conditions: pH and concentration culture media. In conclusion, we have proposed the first model to predict the growth of the native bacterial strain P. aeruginosa based on hyperconic networks and conformal algebra. We have developed a mathematical and computational method to systematically select the structure of kinetic models and partially automatize the laboratory process. We have collected experimental data of our bacterial strain and statistically validated our approach to predict the microbial growth under operation conditions.

Keywords: microbial growth, machine learning, fitting experimental data, Hyperconic Multilayer Perceptron

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Data Driven Economic Nonlinear MPC for Gas Lifted Oil-Well Network

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Abstract

Reinforcement learning (RL) is of growing interest among the control community. The primary advantage of RL is the ability to provide an optimal policy with the explicit assumption of process uncertainty. There have been some studies in recent, showcasing RL in process control such as for Real Time Optimization (RTO), Powell et al. (2020) and for chemical process, Hubbs et al. (2020). However, much of this work relies on validating the proposed method with offline simulations of the same model which was used to train RL policy. This leads to an assumption that the underlying model is the perfect description of the process whereas in practice, the real process is never perfectly described by the available model.

In a typical process industry, the control hierarchy is often divided into multiple decision making layers. The bottom layers consists of RTO and supervisory control (MPC and/or PID). These layers rely on the plant model for daily production optimization (DPO) and controlling the process at the desired setpoint. Most of the times, these models may have parametric uncertainty or structural mismatch, which in turn may divert the process from optimality. Furthermore, the optimal solution provided by the RTO layer to the supervisory layer may not always be feasible and/or violate constraints.

In this work we combine both the layers, RTO and MPC since both of them rely on the same process model. By converting RTO into a dynamic optimization problem, RL is used to update the parameters in the ENMPC scheme along with the RTO layer to gain an optimal policy of the real system. The idea of using RL to achieve optimal policy while accounting for the model mismatch by modifying the model itself, cost and constraint function was first proposed by Gros and Zanon (2019). In the context of RTO, to combat model mismatch modifier adaptation methods utilizing steady-state updates have been proposed, Marchetti et al. (2009). However, the approaches to tackle model mismatch such as RL and modifier adaptation do not differ quite a lot from each other. Through this work, we attempt to bridge the gap between the process community and motivate to use powerful tools such as RL by showcasing its benefits.

The proposed approach was implemented on a simulation model of gas lifted oil-well network. Contrary to the popular usage of Deep Neural Networks (DNN) as appropriator for the RL, we suggest to use NMPC instead. The results were promising and the method is able to compensate for the structural mismatch and parameter uncertainties bu updating the required parameters.

Keywords: Nonlinear process control, reinforcement learning, economic NMPC (ENMPC)

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Digitalization Boosts Decarbonization: Accelerating net zero from the perspective of carbon capture and utilization

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Abstract

Net zero requires an accelerated transition from fossil fuels to renewables. Carbon capture and utilization (CCU) is reported to decarbonize fossil fuels, and thus CCU may be an intermediate solution before the ultimate solution – an energy system fully relying on renewables. However, many CCU research works contain renewables, which may mislead stakeholders regarding the hotspots of CCU systems. Herein, this work creates a hypothetical industrial park, where power plants are integrated with CCU, but no renewables are involved.

This industrial park contains several options for both capture and utilization pathways: amine scrubbing and pressure swing adsorption are modelled to capture CO_2 from gas power plants; following this, the concentrated CO_2 is reformed to syngas, which is further converted to fuels *via* Fischer-Tropsch and methanol synthesis. As such, this industrial park leads to a large energy system in the process level. To pursue the best system performance, we establish a digitalization method for the fast evaluation of sub-systems [1], and a three-level approach to the optimization of the overall CCU system [2], as shown in Figure 1.

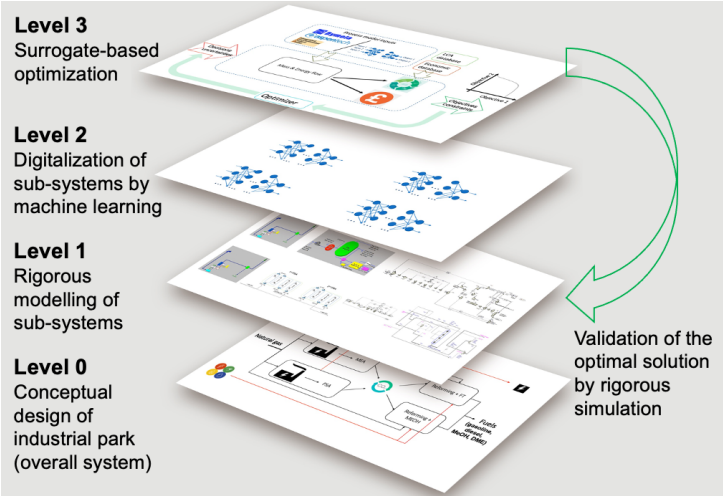

Figure 1. Three-level approach for the optimization of an integrated industrial park.

The optimized CCU can reduce GHG emissions by 13% compared with the conventional process. Heating is identified as the most significant contributor to GHG emissions, accounting for 60%. Electrifying heating fully using low-carbon electricity can further reduce GHG emissions by 47%, but such extreme conditions will significantly sacrifice the economic benefit. By contrast, the multi-objective optimization can show how the decisions can affect the balance between GHG emissions and profit.

Keywords: carbon capture and utilization, digitalization, life cycle assessment, multi-objective optimization.

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Hybrid modelling of industrial scale fermentation process

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Abstract

The biotechnological industry increasingly applies mechanistic models because it has realized their significance. These models are preferred as they contain relevant scientific knowledge needed to describe the system behavior. Mathematical models are the ideal tool for process optimization and intensification. However, biological systems are notoriously complex, developing such a model can be a massive time and resource investment. To simplify things, first principles models most often utilize an empirical approach to describe growth of the cell culture, the list of appropriate equations to choose from is large Muloiwa (2020) and that is only accounts for cell growth, further modeling is needed to account for production of products, substrate uptakes, gas evolution and more.

The production of pharmaceuticals has always had a strong focus on quality. A common method for producing Active Pharmaceutical Ingredients (API) is via biological processes or fermentation of high producing bacteria or fungal strains. These processes have been subject to mechanistic modeling for use in batch optimization, monitoring and control Gernaey (2010). However, the metabolic pathways responsible for the main product can lead to accumulation of related substances in the batch that hamper the final product quality and may be impossible to remove in the downstream process. Mechanistic models rarely take batch quality into account and most model development is focused on main product only.

Due to the complexity of the biological systems a hybrid model approach is used as an alternative. The concept of hybrid modelling in this context is the combination of a first principles mechanistic model and machine learning models into single model. Machine learning and Artificial Intelligence algorithms such as Artificial Neural Networks (ANN), have seen an increase in popularity in various research fields and the use of Hybrid modelling has seen success in chemical engineering such as in particle processes Nielsen (2020).

This study focuses on the application of a hybrid modelling framework on the fermentation of a filamentous fungi that produces Fusidic Acid. A first principles biochemical model is built influenced by existing literature based on penicillin fermentation models Birol (2002). Sophisticated ANN models are subsequently trained to predict the kinetic expressions for the evolution of products and consumption of substrate. The fully integrated hybrid model is subsequentially used for predicting productivity and quality of industrial scale batches currently in production to facilitate further process optimization to maximize the yield of the batch process without compromising the quality of the final product.

Data is collected by regularly sampling tanks located at the LEO Pharma production site in Ballerup, Denmark. The samples are analyzed by measuring the dry weight for biomass concentration. Main product and related substances are measured using an HPLC on the collected samples. PAT package records all other relevant critical process parameters such as pH, dissolved oxygen, temperature and more. Five industrial scale batches were sampled frequently to create the data set for training the model. A hybrid model is set up to simulate a production batch using a first principles approach. A feed-forward neural network is set up to predict the specific rate of change of all batch components based on the current batch state and any external inputs to the batch. The ANN consists of three hidden layers to take advantage of automatic feature selection. The amount of nodes in each layer is decided based on validation performance. The output of the neural networks is then fed to a set of ordinary differential equations that describe the overall change in the batch state. Fed-batch concentration balance is utilized as the first principle model with modifications to account for water evaporation. The entire setup is built and solved with MATLAB R2021b.

While the model is trained on a few selected batches, the model really only needs information about external inputs and initial conditions when simulating a new batch. This information is recorded on all production and lab batches; thus, the model can be validated by running it on an entire year's worth of production data. The performance indicator of interest is how well the models can predict yield of main product and concentration of related substances during the harvest. When predicting the main product, the mean absolute percentage error (MAPE) of all batches was 9.2% with an R^2 value of 0.94, a good performance indication for biological processes. Predicting related substances turned out a bit more difficult as expected but the hybrid model still achieved a respectable performance with an R^2 of 0.89 and a MAPE value of 11.3%.

Over the course of this work, we have successfully developed a hybrid model to work as a digital twin of an established industrial pharmaceutical process. This work was started because a mathematical model was needed to facilitate process optimization and intensification. However, traditional modeling methods failed to explain the growth of related substances and thus could not predict the quality of the batches due to lack of knowledge regarding system dynamics. The collected data was used to train a Neural Network to predict the relevant biochemical kinetics which was then coupled to a first principles model. The established model predicts the quality of the batches extremely well while also able to be competitive to traditional model when predicting the main product. Hybrid models have major potential in the bioprocess industry as they can facilitate key engineering decisions when relevant scientific information is still lacking.

Keywords: Hybrid-modelling, Pharmaceuticals, Bioprocess, Industry, Neural Networks

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Optimal Contract Selection for Contract Manufacturing Organisations in the Pharmaceutical Industry Under Uncertainty

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Abstract

Over the past few years, large R&D pharmaceutical companies have increasingly outsourced non-core activities, such as manufacturing, to Contract Manufacturing Organisations (CMOs), which are companies without their own product portfolio. This policy enables R&D multinationals to reduce costs and emphasise on drug discovery and marketing, which are the key parts for their value chain. Typically, drug development is a time-consuming process, as it takes at least 10 years on average for a new medicine to be in the marketplace. Additionally, demand of newly developed pharmaceutical products is usually highly uncertain. Lower drug efficacy can affect the demand and total sales, while in the worst case, it can lead to the suspension or even the withdrawal of the drug. Under this dynamic and uncertain environment, a CMO must decide the best contract combination to accept, so as to maximize its profits (Marques et al., 2020).

This work presents an integrated planning and scheduling framework for the optimal contract selection problem of Contract Manufacturing Organisations under uncertainty. Considering a multistage, multiproduct batch facility of a secondary pharmaceutical process industry, an aggregated MILP planning model is firstly proposed including material balances and allocation constraints. Utilizing a rolling horizon approach, the production targets are provided to a precedence-based MILP scheduling model to define batch-sizing and sequencing decisions in detail. A feedback loop is incorporated to converge production targets among the planning and scheduling decision levels. To model product demand uncertainty, a scenario-based approach is proposed, considering the Conditional Value-at-risk measure. Since large number of scenarios creates significant challenge to computations, a scenario reduction framework is integrated to reduce the total solution time when considering large-scale problem instances (Li and Floudas, 2014). The proposed methodology increases the profitability of CMOs by selecting the optimal contract combinations depending on their risk tolerance while taking into account the availability and optimal utilization of underlying production resources.

Keywords: Contract Manufacturing Organizations, Conditional Value-at-Risk, MILP

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A framework for economic optimization of carbon capture and sequestration from Italian industrial sources under seismic risk constraints

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Abstract

Cement plants, steel mills and refineries in Italy are responsible for a significant share of carbon dioxide (CO_2) emissions (EEA, 2020), which are among the greenhouse gases responsible for the global threat of climate change (IPCC, 2021). The implementation of carbon capture and storage (CCS) technologies is key to reduce a significant portion of CO_2 emissions from these hard-to-abate sectors (Bui et al., 2018), and the optimization of such complex and multi-stage supply chains (SCs) proves fundamental to achieve a substantial level of decarbonization (d'Amore et al., 2018; 2021). Additionally, when focusing on the Italian peninsula, widespread seismic activity poses an additional requirement during the planning, installation, and operation of a CCS system, particularly with regards to pipelining (Psyrras and Sextos, 2018).

This contribution provides a techno-economic assessment and optimization of a comprehensive CCS SC from Italian industrial stationary sources (i.e., cement, steel and refinery sectors) by aim of a multi-objective mixed-integer linear programming (MILP) modeling framework. In particular, the model is conceived to simultaneously optimize the economic (i.e., minimum cost) and seismic (i.e., minimum risk) performance of a CCS system in the geographic setting of Italy. The seismicity-related parameters are obtained through a dataset containing the coordinates of polling points over the entire Italian peninsula, which are then averaged into seismic areas and implemented to calculate the risk specific to each pipeline in the transport stage of the CCS system (Gehl et al., 2014).

Different case studies are presented and discussed, depending on the carbon reduction target that it is chosen to pursue. The minimum specific CO_2 avoidance cost resulting from the economic optimization is 59 €/t (20% capture target), 64.8 €/t (50% capture target) and 80.7 €/t (80% capture target), while the risk optimization produces an increase in costs in all analyzed scenarios, varying from a minimum of 97.0 €/t (20% capture target, i.e. +64.4%), to 79.4 €/t (50% capture target, i.e. +22.5%), up to 81.3 €/t (80% capture target, i.e. +0.74%). The Pareto curve resulting from the bi-objective optimization allows determining some trade-off configurations between the two objectives.

Keywords: Cement, steel, oil refining; Carbon capture and storage; Seismic risk; Multi-objective optimization; Mixed integer linear programming.

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Drug sorption to medical devices : experiments versus molecular simulations

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Abstract

Polymer materials such as polyethylene (PE) and polyvinyl-chloride (PVC) are widely used in medical devices as artificial nutrition tubings, intubation, catheters (Bernard et al., 2014). Nevertheless, these polymers have been shown to interact with medications leading to drug sorption (adsorption or absorption) and a loss of the active pharmaceutical ingredient (API). This impacts then on the effectiveness and success of the therapy (Treleano et al., 2009). Another phenomenon can occur with plasticized PVCs: the migration of the plasticizer (Tokhadze et al., 2019) into the drug solution impacting then the product's safety. A number of experimental procedures focusing on material analyses have been carried out without completely describing the phenomena involved in drug sorption to medical devices.

We take the route of investigating the adsorption of drugs (paracetamol, diazepam and insulin) onto polymer surfaces (PE, plasticized PVCs) by experiments and molecular simulations. In a first step, we used the HPLC method after static contact to investigate any drug loss by sorption. Experiments showed no diazepam loss by sorption with a pure PVC surface and an important drug loss just after filling that fell under 2% of the initial concentration after 4 days. In addition, a diazepam loss of 56% of the initial concentration at 14 days (Sahnoune et al., 2021) was established with PE tubings. For insulin, experiments showed a loss in the range of 8-15% for PE and PVC tubings, respectively.

In a second step, we propose to interpret the results of these experiments at the energetic and molecular levels. We used molecular simulations and the approach of the potential of mean force (PMF) to provide thermodynamic properties of adsorption. By using this approach, it is possible to model the interaction between the drug and the polymeric surface as a function of the separation distance between the centers of mass of both species. Some PMF curves often called Gibbs free energy profiles are given in Figure 1 along with a typical configuration of an adsorbed onto a plasticized PVC surface. All these PMF curves show a negative minimum of $\Delta G(z)$ close to the surface indicating that the adsorption is thermodynamically favored. The values of the free energy minimum fall into a range of -40 to -15 kJ mol^{-1}. This is in line with a pure physical adsorption of drug via van der Waals interactions. In addition, the PMF calculation gives a free energy of adsorption of -40 kJ mol^{-1} for the adsorption of diazepam on a plasticized PVC whereas it is of -20 kJ mol^{-1} for the adsorption of this drug on a pure PVC surface. The PMF calculation also confirms a stronger adsorption of diazepam onto a PE surface.

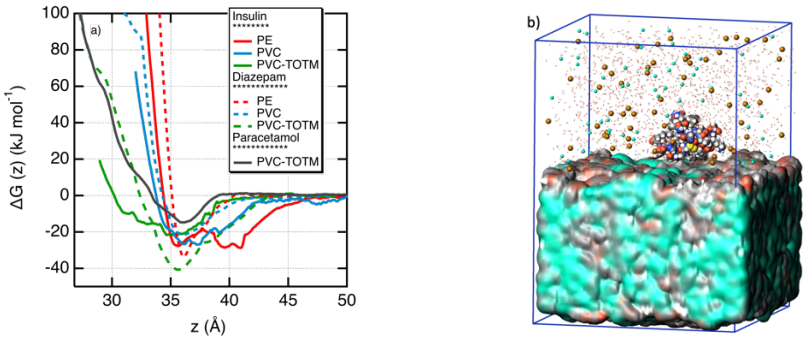

Figure 1: a) Gibbs free energy profiles ΔG(z) of drug molecules interacting with PE, PVC and plasticized PVC-TOTM surfaces and b) a typical configuration of aspart-insulin adsorbed onto a PVC-TOTM surface. The PVC chains are colored into green and the plasticizer TOTM molecules in gray and red for the oxygen atoms.

The comparison between experiments and simulations allowed to conclude that no drug loss was observed when Gibbs free energy was comprised between 0 and -20 kJ mol^{-1}. The results of the PMF calculations are in line with the experiments on diazepam and paracetamol drugs. We also propose to show the results of a more challenging system : the adsorption of insulin onto a plasticized PVC. Indeed, this kind of simulation is very time consuming due to the system-size (surface area, number of water molecules and insulin) and at the limit we can do with molecular models. However, the results of Figure 1 are very interesting and support the analysis of the experiments. The different local arrangements of drug molecules at the polymer-water interface will be discussed in a spirit of better understanding the adsorption of these drugs.

As a conclusion, the combination of experiments and molecular simulations proves to be efficient to rationalize the results of experiments in terms of energetics and should make it possible in the near future to design medical devices which do not present any drug sorption.

Keywords: adsorption, molecular simulations, drug-material interactions, medical devices.

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Energy-water Scheduling Decisions for Agricultural Scenario Planning

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Abstract

Food, energy and water resources are heavily interconnected in many process systems and therefore need to be taken into consideration holistically for sustainable decision-making, as summarized in the food-energy-water nexus (FEWN) framework (M. Di Martino et al.). The FEWN represents a promising decision-making support for regions characterized by scarce water resources, abundant renewable energy resources and significant population growth, as it tackles these different challenges simultaneously while taking into account the effect of each solution strategy on the resource systems. The current literature usually focuses on region or country wide solutions for an agricultural sector based on energy-water systems rather than focusing on a greenhouse farming scale decision framework (S.-H. Lee et al. 2020). This work investigates the implementation of an energy-water nexus decision-making tool in agricultural activities. Varying water demands in agricultural systems are evaluated on the basis of renewable, and non-renewable based energy sources, along with varying water sources. To this end, a greenhouse connected to a reverse osmosis desalination plant is modeled as a mixed-integer non-linear optimization program and optimized for an array of objectives to enable a cost-comparison on the basis of water scarcity. The decision-making tool is then extended towards energy-water scheduling decisions for the optimization of agricultural scenario planning.

Keywords: food-energy-water nexus, irrigation planning, energy-water scheduling, mixed-integer optimization.

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Optimizing the allocation of resources for the security of the water-energy-food nexus

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Abstract

Water, energy, and food are essential resources for meeting basic human needs and for economic development. In the last years, growing resources demand and limited access and availability of resources have caused increasing concern about water, energy, and food security. It has been highlighted that a driving factor to achieve long-term sustainability is the security of the water-energy-food nexus (Hoff, 2011), and its improvement implies optimal planning and management of resources, as well as a proper allocation or distribution of resources. The allocation of resources is one of the main concerns in social planning and, typically, is guided by the maximization of the stakeholder's utilities, which may lead to non-unique solutions since different allocations of resources can give the same total utility of the system (Sampat and Zavala, 2019). Considering this, different allocation or distribution schemes have been developed to capture the scales of the stakeholders, generate unique solutions, and provide fairness measures for the resource distribution. Allocation schemes in integrated water-energy-food nexus systems have not been addressed. Therefore, the novelty of this work is the development of a mathematical formulation for the optimal design and management of resources to enhance the water-energy-food nexus security. Resource security is measured through indicators related to the availability, access, and sustainability of water, energy, and food. Furthermore, the problem was analyzed under different allocation schemes (social welfare, Rawlsian, Nash, and Rawlsian-Nash) to maximize resource security and obtain the optimal design of the system. To show the applicability of the model, a Mexican state evaluated by regions was selected as a case study. Results show that through this approach, it is possible to increase 14%, 44%, and 15% the security of the water, energy, and food sectors respectively, and 25% the security of the water-energy-food nexus in the addressed case study. The proposed water-energy-food nexus framework can be applied to any region with the corresponding data.

Keywords: Resource security; Allocation schemes; Sustainability; Optimization; Water-energy-food nexus.

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Application of CAPE Tools into Prospective Life Cycle Assessment: A Case Study in Recycling Systems Design of Lithium-Ion Battery

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Abstract

In this study, we are tackling systems design with assessments for emerging technologies. Because of the data limitation on the systems and processes adopting emerging technologies, computer-aided process engineering (CAPE) tools such as process design heuristics, process simulation, optimization, parametric analysis for characterizing sensitivity and alternative generation, and decision making with uncertainties have huge potential to compensate such data limitation and jump up to the deep technology assessments with quantified results. In this paper, we examine the applicability of CAPE tools for systems design and assessment adopting emerging technologies with a case study of recycling systems design of Lithium-ion battery (LiB).

The recycling of cathode particles and aluminum (Al) foil from positive electrode sheet (PE sheet) dismantled from spent LiBs was experimentally demonstrated by applying a high-voltage pulsed discharge. This separation of LIB components by pulsed discharge was examined by means of prospective LCA (Kikuchi et al., 2021). The indicators selected were life cycle greenhouse gas (LC-GHG) emissions and life cycle resource consumption potential (LC-RCP). Through this case study, it was demonstrated that the application of CAPE tools into prospective LCA enables the strategic technology assessments for systems design. Especially in the proof of concept on technology implementation can be verified and validated with the ranged values of uncertainties in emerging technology under development.

Keywords: Spent lithium-ion batteries, Recycling, Positive electrode active materials.

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A Fair-Sustainable Approach for the Optimization of an Integrated Fuel Production System

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Abstract

To achieve sustainable development, certain objectives must be considered. A fair allocation of resources is key for long-term sustainability. Therefore, these objectives can include attaining environmental fairness and sustainability metrics. Besides considering the fair allocation of resources, equity in policies, implementation, and equality in outcomes need to be addressed. Recently, several fairness schemes have been applied as measures to allocate resources in multi-stakeholder systems. These schemes have been analyzed in different sectors, such as an agricultural system and an integrated residential complex. These studies have verified the deficiencies of certain approaches and highlighted the importance of comparing different allocation schemes. On the other hand, an economic approach to include sustainability in process integration projects has been reported recently. Here, a new sustainability metric is proposed. This metric is denominated as the Sustainability Weighted Return on Investment metric (SWROIM). The metric is based on the economic return on investment but also evaluates the contribution to sustainability. Extended forms of the metric have been proposed to include safety and resilience. In this work, we propose a fair-sustainable approach that involves applying fairness schemes along with the sustainability metric SWROIM for the optimal income allocation of an integrated system to produce fuels and simultaneously capture emissions. The analyzed schemes are the social welfare, Rawlsian welfare, and Nash approaches. The involved stakeholders in the integrated system include refineries, biorefineries, and eco-industries. To foster the reduction of emissions, we include economic compensations for the eco-industries. Furthermore, we analyze the avoided emissions (environmental function) and the generated jobs (social function) obtained through the different schemes and the sustainability metric. To demonstrate the applicability of the optimization approach, a case study for the future planning of the energy system in Mexico was presented. In the results, important differences are observed for the stakeholders' income allocation, as well as for the environmental and social functions under the schemes and the sustainability metric. These differences highlight the importance of exploring these different allocations since they can be key for decision-makers. The results also show that the Nash scheme can provide fair trade-offs among the stakeholders' income and the environmental and social functions.

Keywords: Optimization, Fairness schemes, Sustainability metric.

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The advancement of zero- and near-zero-emission natural gas power plants and their role in the future energy supply

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Abstract

Global warming has become one of the most pressing scientific and technological challenges to overcome in this century. Reducing the CO2 emission from the power sector is one of the effective ways to achieve the goal to keep global warming to less than 2°C. In traditional gas power plants, huge amounts of CO2 is generated, which has to be captured to achieve the near-zero emissions target. Carbon capture in power industry is technically and economically challenging due to the energy penalty and high capital cost. Generally, carbon capture on a natural gas power plant is not economic due to the high operating and capital cost. However, CO2 taxation will accelerate the progress of zero-emission power plants.

The concept of zero- and near-zero-emission natural gas power plants combines advanced power cycles and carbon capture technologies. Recently, many advanced power cycles have been proposed in the context of zero-emission natural gas power plants, such as the Allam cycle, S-GRAZ cycle. Carbon capture and storage (CCS) is a direct and practical way to reduce greenhouse gas emissions. There are four categories of CCS technologies for natural gas power plants: pre-combustion carbon capture, post-combustion carbon capture, oxy-combustion carbon capture, and chemical looping combustion (Hossain and de Lasa 2008). Therefore, novel systems combining carbon capture technologies and advanced power cycles are reviewed in this paper. Due to the different regulations and the status towards carbon-neutral society, each country has its own roadmap and timeline to achieve the zero-emission target in power sector. Therefore, the role of the zero-emission natural gas power plants depends heavily on the country. In this paper, the USA, China, Denmark will be taken as examples to illustrate the prospect of the zero-emission natural gas power plants in the future energy supply.

Keywords: zero-emission, natural gas, power plant, prospect

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Optimal Decarbonisation Policymaking Software Inspired by Process Integration

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Abstract

While many decarbonisation software tools exist for rigorous energy planning, these tools often rely on the a priori definition of many scenarios, require highly detailed insights into specific technologies, and are often tailored to specific (mostly European and North American) regions and technologies. This work seeks to develop a decision support software framework, based on rigorous mathematical optimisation models and interpretable results, for planning decarbonisation, in line with commitments made while signing the Paris Agreement, with an emphasis on supporting ASEAN (Association of South East Asian Nations) economies. The planning framework relies on a combination of proven, mature technologies such as the Carbon Emission Pinch Analysis (Tan and Foo, 2007) and deterministic optimisation, and is inspired by process integration techniques developed within the systems engineering community over the past 50 years. These tools provide easily interpretable results that can show what is feasibly achievable at a high level, providing an accessible lens through which policymakers can view. Additionally, the developed software also utilises novel mathematical optimisation formulations that provide rigorous guarantees on the qualities of the solution, subject to constraints such as budget, technology readiness levels etc. The optimal decarbonisation software developed in this work, in collaboration with Malaysian government stakeholders, is based on a multiperiod energy planning framework. The satisfaction of the CO2 emission limit is achieved using a combination of new technologies to replace older infrastructure, negative emission technologies (NETs) and carbon capture and storage (CCS) employed on existing infrastructure. The energy planning is subjected to constraints surrounding the decommissioning of existing infrastructure, times of commissioning new infrastructure, and the potential future costs of promising new technologies for CCS and NETs. We demonstrate the software's utility by optimising over several objectives, such as minimal emissions and investment, and also show the influence of considering cumulative emissions. The software is open-source, well-documented, and developed in Python, requiring only spreadsheets as inputs for users. We hope that the software can, in future, provide clear guidelines on the necessary actions to be undertaken by countries/industries achieving the net-zero carbon goal by 2050.
Keywords: Energy planning, negative emission technology, process integration

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Interplaying of industry 4.0 and circular economy in cyber-physical systems towards the mines of the future

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Abstract

Today's Industry 4.0 (I4) is redesigning industrial activities and reshaping communities into the so-called Society 5.0 (S5), enabling the creation of a new industry-society-environment nexus. Novel technologies for pervasive sensing, widespread internet of the things (IoT), in-depth artificial intelligence (AI), and robotics, aim to sense, calculate, and actuate by employing data-driven architectures and automated decisions.

In this work we address the digital transformation and the introduction of cyber-physical systems (CPS) towards smarter operations within the mining industry. Decision-making in mining operations is often done by human inspections and computer algorithms, with an increasing use of autonomous machines (e.g., trucks, drills, drones, conveyor belts). High-performance computing (HPC) with advanced modelling and solving algorithms (MSA) are necessary for the autonomous handling of hazard and harsh environments, where no or reduced manpower is required. For that, information and communication technologies facilitate innovative solutions to re-shape and re-design production systems. The interplaying of advanced technologies of the I4 mandate and CE ideology towards the mines of the future creates a smart connected mining industry that transforms vast amounts of data into predictive and fully integrated intelligent systems.

In the mining system, improved stockpiling operations can be achieved by employing better processes for separating and transporting ore, preventing evaporation, and producing drier tailings through a hybrid dynamic control application. Thus, additional safety, stability, and predictability can be achieved to maximize the ratio of metal to ore output while minimising the environmental impacts and the operating and capital costs. In addition, this creates sustainable communities to identify socio-economic development opportunities. This paper argues on how advances in technology towards the I4 age drive opportunities to redesign and re-execute operations in the process level (stockpiling) into improved states for applications in the mining industry towards technologies over the CE ideologies based on the environmental, economic, and social pillars. In this context, CE theories within I4-S5 introduces novel sustainable industry principles for innovative processes that are driven by safer, more efficient, and more accurate mining.

Keywords: Industry 4.0, circular economy, mines of the future.

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Environmental Impacts of Rice Husk-Derived Silica under Uncertainty: Is ”Bio” better?

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Abstract

140 million tonnes of rice husk (RH) are produced annually as an agricultural waste Lim et al. (2012). An area of interest for RH valorisation is to use rice husk ash (RHA, a by-product of RH combustion) as a replacement in products currently using mineral-derived silica. However, most studies focus on using RHA as-is, rather than recovering RH-derived silica as an intermediate. Also, little information is available on the environmental benefit of producing RH-derived Silica.

This study provides the first evaluation of the environmental benefit of recovering silica from RH. The functional unit considered is one kilogram of silica. Using Life Cycle Assessment (LCA), a model has been developed to quantify the global warming potential (GWP) of mineral-derived silica based on inventories reported for European Synthetic Amorphous Silica (SAS) industry. A second LCA model has also been developed to quantify the GWP of silica derived from the combustion of RH (including co-recovery of bioenergy) and subsequent processing of RHA. To assist the RH-derived LCA model, a third model has also been developed to quantify the effect of RH feedstock quality and the efficiency of silica recovery on the bioenergy recoverable and RH demand associated with producing one kilogram of RH-derived silica.

To produce robust research findings, the effect of uncertainty on the outcomes of LCA models are quantified using the data quality matrix method Weidema (1998). Literature values have been used to account for uncertainty in RH quality and the efficiency of recovering silica from RHA. The effect of these uncertainties on overall GWP predictions simulated using Monte-Carlo methods.

Findings demonstrate that the contribution of mineral feedstocks to the GWP of mineral-derived SAS is low. Therefore the recovery of silica from RHA alone is not of a large benefit to SAS manufacture. However, if bioenergy co-recovery is used to substitute for regional grid electricity use during production then a net reduction in the carbon footprint of SAS is possible. Asia-Pacific is used as a case study to demonstrate the affect that this reduction could have on the annual GWP of SAS industry. Finally, uncertainty in RH feedstock quality and silica recovery efficiencies are used to visualise the design space in which a RH-derived process may operate with regards to the bio-energy recoverable and RH demand per kilogram of RH-derived silica produced.

Keywords: Silica, Rice Husk, Life Cycle Assessment, Uncertainty, Global Warming Potential

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Economic analysis of novel pathways for recovery of lithium battery waste

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Abstract

Landfill and incineration are highly unsustainable remedies for waste management as they use large areas of land. This results in the release of greenhouse gases, such as carbon dioxide (CO_2) and methane (CH_4), as the waste dissociates thereby causing health and environmental threats to developing countries. The recent energy transition to renewable energy sources has resulted in an increase in the demand of high value metals for production of lithium ion batteries (LIB) for energy storage used mainly in electric vehicles. Ore mining of the component metals (nickel, lithium, cobalt, manganese, etc.) has contributed to high environmental impact as well as the pollution of groundwater and adjoining ecosystems due to disposal of the LIBs at landfills after their use. Furthermore, the mineral deposits of the ores are also distributed across few countries around the world, thereby creating economic over dependency on these countries for their supply. This has led to the need for effective management and recovery strategies.

Due to a variety of factors such as technological challenges, implausible economic burdens, high environmental impact, complex chemical reactions, and so on, the optimum nature of the LIB recovery process and technologies has yet to be determined (Azpagic, 1999). Creating a circular economy (CE) by recycling after their use could lower manufacturing costs, increase revenue streams, provide tax advantages, and reduce resource dependency, while also protecting the environment. The CE is a regenerative strategy to waste reduction that aims to ensure the environmental sustainability of post-use items (Yun et al. 2018). Using the Umicore process, a current state of the art recycling process flow in the metal recovery industry for LIBs (Georgi-Maschler et al. 2012) as a baseline, this paper examines economic and environmental friendly solutions for effective metal recovery from spent LIBs. At the same time, possible synergies between existing resource use from other manufacturing and waste treatment industries (e.g., wastewater treatment, energy intensive industries, etc.) are considered as a valuable input to metal recycling, while also reducing the amount of atmospheric carbon. This further presents a case for possible integration of various waste management approaches as a single business unit for economic incentive and profitability for possible investment.

Keywords: lithium ion battery, waste recovery, e-waste, circular economy.

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Transition Paths Towards a CO_2-Based Chemical Industry Within a Sector-Coupled Energy System

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Abstract

The chemical industry uses 10% of the global fossil resource demand today (IEA, 2017). Due to increased demand for chemicals, the chemical industry is expected to account for more than a third of the growth in oil consumption by 2030 (IEA, 2018). The defossilization of the chemical industry is particularly challenging since 58% of its fossil demand comes from carbon-based feedstock. This carbon is eventually released to the environment during the chemicals use and end-of-life.

One way to reduce the industry's reliance on fossil feedstocks is via carbon capture and utilization (CCU). In CCU, CO_2 is captured from point sources or directly from the air and converted to chemicals, contributing to a circular industry. However, CCU is highly energy-intensive and requires an abundance of clean electricity. Kätelhön et al. (2019) showed that a CCU-based chemical industry would require 126% of the projected global renewable electricity production in 2030. Thus, a transition to a CCU-based chemical industry needs to be aligned with developments in the overall energy system. Other sectors that rely on increasing amounts of clean electricity, (i.e. mobilility and heating) need to be considered when evaluating the chemical industry's transition.

In this work, we present an integrated model of a sector-coupled energy system and chemical industry. The integrated model allows us to evaluate the potential of CCU for the chemical industry's low-carbon transition. We couple the transition of the chemical industry with the transition of the energy system and thereby include other electricity-requiring sectors (Baumgärtner et al., 2021). We model the transition pathway for a one-node system as a linear optimization problem with hourly temporal resolution and a rolling horizon strategy. The optimization problem minimizes costs subject to greenhouse gas (GHG) emissions constraints. The model of the chemical industry includes the major bulk chemicals ammonia, methanol, ethylene, and propylene and considers both fossil-based and CCU pathways for chemicals production.

We apply the integrated model to the case of the German sector-coupled energy system consisting of the electricity, mobility, and heating sectors. We optimize the transition pathway until 2045 with a net-zero emissions target. We exclude the option for negative-emission technologies to focus on the CCU-enabled transition of the chemical industry. We prohibit electricity imports and consider hydrogen imports as a last-resort option to prioritize the use of domestic resources.

Our analysis shows that without imports, domestic clean electricity availability is expected to be insufficient for achieving net-zero emissions within the sector-coupled energy system and chemical industry. We see a deficit of 40% of clean electricity availability even when considering only the stoichiometric CO_2 and hydrogen requirements for the chemical industry and for heat-generating e-fuels. When allowing

for hydrogen imports, domestic clean electricity is sufficient for the maximal decarbonization of all sectors. However, hydrogen imports help to balance the intermittency of the clean electricity supply. The transition pathway to a net-zero system requires 13M tons of hydrogen imports in 2045. 68% of imports go to e-methane mostly for high-temperature heat and the remainder go to CCU.

Our results show that net-zero emission targets cannot be reached without including negative-emission technologies. Residual emissions amount to 11M tons CO_2-eq, equal to 10% of overall emissions in 2045. Thus, negative-emission technologies will play a role in reaching net-zero targets.

The cost-optimal transition of the sector-coupled energy system and chemical industry prioritizes technologies and sectors that most efficiently reduce overall system emissions. The chemical industry is among the last to transition to minimal emissions along with the heating sector (Figure 1). The chemical industry begins to transition in 2040. However, most of the industry's transformation occurs in 2045 along with that of high-temperature heat, which is assumed to require e-fuel technologies.

Figure 2 shows the detailed evolution of the chemical industry. At minimal system emissions in 2045, all chemicals are produced via CCU. Ammonia is produced directly from hydrogen rather than from methane. Methanol transitions from being produced via syngas to its CCU pathway and becomes a key molecule in the production of other chemicals. Both ethylene and propylene are produced from methanol rather than via their respective CCU pathways. The methanol route is preferred because methane is a by-product, which benefits the overall sector-coupled system.

Concluding, the analysis shows that imports as well as negative-emission technologies will play a key role in the decarbonization of the German sector-coupled energy system and chemical industry. The chemical industry along with the heating sector are decarbonized last. In the decarbonization of the chemical industry, methanol plays a large role. The presented model thus identifies opportunities and challenges for the transition of the chemical industry as part of the overall energy transition.

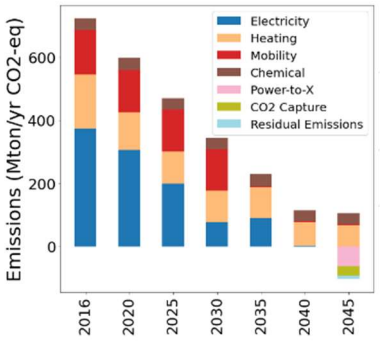

Figure 1: Operational emissions transition by sector

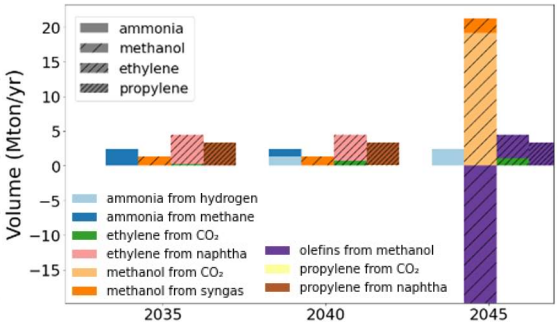

Figure 2: Chemical industry transition by product

Keywords: carbon capture and utilization, CCU, greenhouse gas emissions, net-zero

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How can PSE approaches can help to design Water-Energy-Food Nexus systems?

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Abstract

Global demand of water, energy, and food has grown in the last decade, and is predicted to continue for the year 2030 (National Intelligence Council, 2012). The increment in the demand is attributable to climate change and rapid population growth, expected to rise by 50% for the year 2050 (Ferroukhi et al, 2015). The connection of these resources has been called the Water Energy Food Nexus (WEFN) and, since its conception in 2011 (Hoff, 2011), the number of studies about it has been increasing (Wichelns, 2017).

Various review articles have been carried regarding the WEFN from a wide range of aspects, including simulation tools and methods, bibliometric analyses, and policy making, etc. Furthermore, many optimization models have been formulated with the aim of WEFN management. However, to the best of our knowledge, there is no literature review that collects optimization models for WEFN management in a single article.

In this study, we provide an analysis of the optimization models elaborated and implemented for WEFN management in the literature. The search was conducted using Google Scholar and Web of Science databases with the following terms: “water food nexus optimization”, “water in agriculture optimization”, “food waste for water treatment”, “water energy nexus optimization”, “heat integration system optimization”, food energy nexus optimization”, and “water energy food nexus optimization”, searching them separately. A total of 68 articles concerning optimization of WEFN systems were reviewed and characterized according to a variety of properties including: nexus type, geographic and temporal scale of the case studies, and the type of optimization problem.

Regarding the nexus type, five different nexuses were identified within the 68 selected articles for this study: water-energy nexus (WEN), water-food nexus (WFN), energy-food nexus (EFN), WEFN, and extended WEFN (E-WEFN). The WEN had more studies than any other nexus, accounting for 26 of the 68 studies. Most of the optimization problems in this nexus were non-linear, due to the consideration of heat transfer equations as constraints. Uncertainty treatment was present in 19 of the 68 selected articles. Different authors listed as future directions of their research the inclusion of stochastic elements (Galan-Martin, et al. 2017). In the WEFN and E-WEFN, multi-objective optimization problems were more numerous than single-objective, given by the opposition of agents in the three sectors. Multi-agent systems were under-investigated, with only two articles addressing it via Nash-based formulations (Guo et al., 2020, Memarzadeh et al., 2020).

Six spatial scales were identified from the reviewed articles: household, processing plant, city, region, nation, and transboundary scales. Only one article was found to address the household scale, where a WEFN system for a family of four was optimized (Karan et al., 2018). Different authors have stated that the household scale is under-investigated; noting also that for future research, this must be a core component of policies and strategies

development (Garcia & You, 2016). The most numerous scale was the regional, with 25 out of the 68 selected articles, addressing mainly water irrigation schemes for agriculture in river basins. At the processing plant scale, most of the optimization models were non-linear, because of the physical-chemical phenomena equations, and single-objective optimization problems, due to the presence of only one agent in most of the case studies.

Concerning the temporal scale of the reviewed studies, five different time scales were identified: daily scale, monthly scale, 1 to 9 years, 10 to 19 years, and >20 years. Most of the articles considered the time scale of 1 to 9 years, and the articles within this scale addressed all spatial scales, resulting in a similar distribution to the one of all the articles. Less articles addressed the daily scale and >20 years scale, indicating a correlation with the spatial scale where the studies also tend to group in the middle scales.

This study reveals different research gaps where process system engineering (PSE) approaches could be helpful in order to design and manage WEFN systems. Household scale studies should be addressed in future research and, in conjunction with studies at the process plant scale, scaled up to city scale studies. Uncertainty treatment was recurrent as future directions for different studies. Stochastic programming by means of different approaches, such as chance constrained programming or fuzzy numbers, can be a supportive manner to address this topic. Multi-agent systems analysis was highly under-studied, considering the complex interactions and opposing goals present between different agents in the nexus. Nash-based formulations and multi-stakeholders decision models can be a useful way to tackle this particular issue of the nexus.

Keywords: water-energy-food nexus, multi-agent analysis, process system optimization, literature review.

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Assessment of the Techno-Economic and Sustainability Potential of Engineered Cell Factories in a Xylitol Biorefinery

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Abstract

Integrated biorefineries harbor eminent potential as a critical concept for transitioning towards a bio-based and ultimately more sustainable economy. Despite being investigated in research for decades, second-generation biorefineries with lignocellulosic biomass as feedstock have scarcely been implemented into full-scale operation. This is mainly relatable to economic hurdles in biomass pretreatment and downstream processing (Chandel et al., 2018). This is contrasted by the significant advances in synthetic biology, which allow for targeted engineering of pathways in cell factories to increase yields of existing pathways or introduce novel pathways (Straathof et al., 2019).

In this study, we investigate the potential of using such engineered cell factories in a case study of a xylitol biorefinery, which has been conceptually designed based on mechanistic models in an optimization-based framework under the objective of high economic feasibility (Vollmer et al., 2021). These mechanistic fermentation models are used as a basis for adapting the cell factory's performance according to results in other studies on the fermentation performance for the products xylitol and succinic acid in this biorefinery. The processes with the engineered cell factory are equally subjected to the optimization-based framework. With the resulting consolidated process design, both techno-economic analyses and life-cycle analyses are performed and benchmarked. The results of this study provide a guideline on the successful utilization of novel synthetic biology tools to strategically design biorefineries, which are both economically viable and sustainable to promote more sustainable production patterns in a bioeconomy.

Keywords: Biorefinery, Techno-Economic Analysis, Life-Cycle Analysis, Optimization, Cell Factory Design

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Optimal design and planning of supply chains for viral vectors and RNA vaccines

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Abstract

COVID-19 pandemic has accelerated the research and development of new platform technologies for the production of vaccines against infectious diseases, including the novel corona virus, aka Severe Acute Respiratory Syndrome Corona Virus 2 (SARS-CoV-2). Platform technologies such as viral vectors and RNA have been used to develop vaccine candidates to combat COVID-19. However, these vaccine types pose a new logistics and distribution challenges, for example, unlike conventional vaccines, RNA-based vaccines require ultra-low temperature throughout the distribution network to avoid loss of potency.

This work develops a new multi-product MILP supply chain model that supports the planning and distribution of viral vectors and RNA-based COVID-19 vaccines, from manufacturing plants to vaccination centres where vaccines are administered to high-risks and vulnerable individuals. Unlike previous work, the proposed optimisation-based supply chain model comprises of five echelons, including manufacturing plants and/or imports, fill-finish plants, central warehouses, regional stores, and administration points. A recycle loop for vaccine thermal shippers from warehouses to administration points and back to warehouses is implemented to ensure efficient management of vaccine thermal shippers. Including these features within the supply chain model allows cost-effective distribution of viral vectors and RNA-based vaccines, in addition to setting production targets at manufacturing and fill-finish plants. The performance of candidate supply chains is assessed using relevant key performance indicators such as vaccine availability, logistics cost, logistics cost per fully immunised patients, etc.

The capabilities of the proposed vaccine supply chain model are illustrated using a real-world case study on vaccination against COVID-19 in the UK, where both viral vectors (e.g., AZD1222 developed by University of Oxford and AstraZeneca) and RNA vaccines (e.g., BNT162b2 developed by Pfizer and BioNTech) are applied. Outcomes from this study compare the resources required and logistics costs when viral vectors and RNA-based vaccines are used during the COVID-19 vaccination campaign. Analysis of results shows that the logistics cost for RNA vaccines is slightly greater than that of viral vectors, and also transportation cost dominates logistics cost of RNA vaccines compared to viral vectors.

Keywords: COVID-19 vaccines, Vaccination campaign, Mathematical programming, Economic analysis, Vaccine availability.

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Different approaches to epidemic modeling – The Covid-19 case study

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Abstract

The Covid-19 pandemic changed our lives worldwide. Its impact is still vast at several levels, to cite a few: health, economy, formation, freedom, relationships. By far, the most important issue refers to health and hospital allocation to cope with critical patient conditions. Hospitals are also directly interested in the other non-Covid activities that suffer significant reductions and even inhibitions when pandemic outbreaks periodically occur. At present, most countries in the world are suffering from the fourth pandemic wave, and further waves are expected in the coming months.
The paper focuses on three different modeling approaches that can describe the dynamic evolution of a pandemic and that have been extensively tested in the field and applied to Italy, one of the countries that most suffered from the pandemic. The first category of models allows following dynamically the most important health variables (e.g., new positives, hospitalizations, intensive care units (ICU) allocation, and deaths) over short- and medium-term periods (Manca et al., 2020). These models can be used to predict the allocation of hospital resources (i.e. beds but also medical doctors and nurses) that being limited must switch from non-Covid to Covid policies (and vice-versa when the pandemic waves shrink and return to minimum operating conditions before a new outbreak possibly occurs).
The second category is based on compartmental models such as SIR/SIRD and describes the dynamic evolution of a population of individuals who are Susceptible, Infected, Recovered, and Death. We added a further compartment that accounts for the vaccinated individuals (i.e. SIRDV model), which measures the effect of different vaccination policies on the pandemic diffusion. These models are ground on a few parameters that allow assessing the effect of different political decisions such as start, duration and rigorousness of lockdowns, and compartmentation of age ranges. SIRDV models are used for medium- and long-term predictions and may be of real support for decision-makers.
The third category focuses on quantifying the impact of different vaccination politics and the efficacy of prioritizing certain age and fragile categories of individuals. These three types of models allow forecasting the evolution of future outbreaks and following the different waves of either recurring waves or new epidemics. Being able to anticipate the critical dynamics of epidemics allows increasing the efficacy of making decisions at the right time. The knowledge of the role played by different decision variables on the evolution of a pandemic and its impact on the society and the health system allows planning the switch of ordinary resources to emergency ones and anticipate how new supplies should be implemented and allocated.
Keywords: Covid-19, pandemic, modeling, early-warning, politics.

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Multi-objective Optimization to Design a Cogeneration District Heating using PCM Thermal Storage

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Abstract

District heating (DH) is an established way to provide heating to dwellings. DH is a subset of decentralized energy systems (DES), which has a better fuel utilization compared to traditional individual boilers and are promising to regions that have not yet adopted them. DES is constantly evolving, including electricity generation and new strategies. In this study, we consider a 4th generation of DES [1] with short-term thermal storage (TS) that includes phase changing materials (PCMs) and compare it with a similar system with traditional hot water tank (HW-TS). In comparison to HW-TS, phase changing materials (PCMs) use solid-liquid phase change to store heat, reducing storage size. However, PCMs have a lower thermal conductivity.

In this work, 4th gen cogeneration DES operates at around 80°C internally to improve heat transfer from PCM-TS. PCM-TS DES is more compact, which provides more flexibility in installation and space for future modifications compared to a system with HW-TS (HW-DES). Both these systems include a natural gas (NG) combined heat and power (CHP) unit, NG-boiler, TS, and heat exchanger to interface with the ultra-low temperature distribution loop [1]. They are modelled using a software that simulates dynamic systems using first principles models. A naive controller is implemented that responds to inputs, which proved to be satisfactory for this study without incurring the complexities of a model predictive control.

Given the different tradeoffs between choosing PCMs or HW-TS to incorporate into DES, we use a multi-objective optimization approach to determine how each technology is best incorporated into the DES and their associated optimal operational trajectories profiles. This can help us determine the circumstances in which one technology may be preferred to the other, as well as determine both technical and economic valuations of each. The optimization uses a Pareto-front-finding genetic algorithm with the objective to maximize thermal demand met, minimize equipment cost, and minimize fuel consumption. The multi-nature of the optimization creates a Pareto surface from which the best design points are shown in Table 1.

The table shows the resulting design for non-islanded DES under a fixed demand profile without considering the extra heat and electricity required to meet all the thermal and electrical demands. The community is estimated to be around 10,000 people and it is supplied by status quo (SQ), in which heat is generated by domestic boilers and electricity is drawn from the grid.

Some of the limitations of this work are: (i) the price of grid and DES produced electricity is static, meaning it does not change according to the time of the day (ii) these designs were selected based on their position in the Pareto front. Other candidate designs

are not shown for brevity but would have performed comparable to the results shown herein.

Table 1 - Resulting designs of HW-DES and PCM-DES

	HW-DES	PCM-DES
CHP (kW_{el})	600	352
Boiler (kW_{th})	945	1390
Tank volume (m^3)	8	2
Tank energy capacity (MJ)	33	180
Thermal demand met[2]	82%	81%
Electrical demand met[2]	40%	35%
Equipment cost (Thousand USD)	749	638

[1]Maximum capacity [2]Demands met by DES without considering makeup from grid and domestic NG boilers

For this analysis, both thermal and electrical demands are deemed important. Therefore, the LCOE in this case represents levelized cost of energy, including both the thermal and electrical generation with equal weights based on energy content. Considering a lifetime of 30 years for the systems, electricity cost of 0.11 USD/kWh, and a yearly turnaround for PCM, the LCOE for HW-DES was 0.066 USD/kWh and for PCM-DES was 0.063 USD/kWh, a difference of 0.003 USD/kWh.

For a similar thermal satisfaction, PCM-DES capital cost is inferior to HW-DES due to the reduced tank volume and CHP capacity despite the increased boiler capacity, as shown in the table. The tank volume is four times smaller in the PCM-DES than in the HW-DES. Even with this decreased volume, the PCM-DES tank has a five times higher energy capacity making it very energy dense. The bigger boiler capacity in the PCM-DES can be attributed to the low thermal conductivity of the PCM, that drives the optimization in the direction of higher capacity. With that said, it is very efficient and cheap to scale-up boilers.

It must be noted that HW-DES meets 40% of the electrical demand, while the PCM-DES meets 35% of the total demand. The remaining demand for the community is imported from the grid – 60% for HW-DES and 65% for PCM-DES. Therefore, a grid with a high carbon intensity is going to favour HW-DES over PCM-DES, albeit a very small gap. LCOE is very close for both the DES systems, such that we cannot conclusively ascertain one system to be better than the other purely based on it. This is despite the conservative PCM cycling consideration - PCM lose efficiency as they charge and discharge and must be replaced periodically to guarantee efficiency.

Despite the lower energy transfer rate, its energy storage capacity creates unique advantages due to its energy density like transportability and modularity. This study demonstrates that PCM-DES can be an economically feasible system to be implemented in high density communities. Future work will include a sensitivity analysis of the economic parameters.

Citation appears as: Monteiro, Adams, and Cotton (2021)

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An integrated and sustainable Ethanol-Hydrogen-Ammonia-Urea plant.

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Abstract

Considering the growing need for alternative fuels to replace the ones base on fossil fuels, and to reduce the environmental impacts associated, this work aims to present an alternative process that replaces natural gas (NG) as a source of H2 in the production of produce ammonia. The generated CO2 is fed to the urea synthesis section, which reduces greenhouse gas emissions through an integrated ethanol-ammonia-hydrogen-urea plant. To achieve these goals, an integrated plant was designed where the hydrogen from NG was replaced by hydrogen from the ethanol reform ("moss hydrogen") and electrolysis process (green hydrogen) where receives electricity from the co-generation ethanol system. The carbon capture process is carried out through sugar cane photosynthesis, and all CO2 emitted during the ethanol and ammonia production process is separated in the fermentation step to minimize ethanol inhibition and ethanol steam reforming, which was recovered and fed into the urea plant, supplying all the demand for the urea production from the outputs of the process itself and minimizing carbon emission to the atmosphere. Finally, after an evaluation performed in the Aspen Plus process simulator and based on metrics used in green chemistry associated with sustainability, it is concluded that the proposed plant can be considered sustainable with great potential, especially in regions rich in biomass, raw material for the alternative sources of hydrogen presented.

Keywords: Ammonia, Ethanol, Urea, Green hydrogen, CO2 emission.

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A methodology based on social life cycle assessment for social hotspots identification

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Abstract

Managing supply chains taking into account economic, environmental and social aspects has become an increasing concern for businesses. However, in the field of sustainable supply chain management (SSCM), social aspects are usually addressed in a very simplified manner (Seuring, 2013). Hence, the main goal of this study is to advance the field of SSCM by proposing a methodology for assessing the social performance of a supply chain and identifying the processes and regions within the supply chain responsible for the most critical social issues (i.e. social hotspots). As a step towards standardizing the way in which the environmental and social performance of supply chains are assessed, this methodology is based on the life cycle assessment (LCA) approach since LCA form the backbone of the environmental debate in the SSCM literature (Seuring, 2013).

The proposed methodology consists of six different steps including establishing the goal and scope of the study (Step 1); modelling the supply chain under analysis using specific and generic data (Step 2); collecting different social inventory indicators (Step 3); converting this inventory into potential social impacts (Step 4); identifying the most critical potential social impacts (Step 5); and the social hotspots (Step 6).

The developed methodology was applied to the supply chain of Portuguese natural cork stoppers to illustrate how this methodology can be used to support SSCM. The most relevant impact subcategories identified are Injuries and Fatalities, Occupational Toxics and Hazards, Corruption, Migrant Labor, and Children Out of School. The social hotspot recognized for these five critical impact subcategories is "Cork harvest in Portugal". Due to the use of generic data when modelling the natural cork stoppers' supply chain and the use of data on national or sector levels to quantify the social inventory indicators, site-specific data regarding Portuguese cork suppliers should be collected to determine if the results of the social assessment represent real social issues. If the social issues are confirmed, these supply chain partners can modify their activities/behaviors to improve their social performance, and consequently, the social performance of their supply chain. To assist in this task, a set of recommendations for companies dealing with one or more of the five relevant social issues identified is also provided in this work. If implemented, these recommendations will contribute to three Sustainable Development Goals, namely *Goal 4 – Quality Education*, *Goal 8 – Decent Work and Economic Growth*, and *Goal 16 – Peace, Justice and Strong Institutions* (United Nations, 2021).

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Modelling, optimisation and control of the continuous production of succinic acid from glycerol using a continuous packed bed bioreactor with immobilised cells

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Abstract

Succinic acid is a dicarboxylic acid with a vast range of applications ranging from the classic chemical to the pharmaceutical industry. Traditionally it is produced by the hydrogenation of the maleic anhydrite, a derivative of the petrochemical industry, but in recent years there is a growing interest for the shift to more sustainable ways of production. Biochemically it is produced using batch bioprocessing (Vlysidis et al., 2011), however for it, to be competitive with petroleum-derived succinic acid, novel bioprocessing approaches, with improved productivity have to be established. Continuous biochemical processes, offer the greatest potential and of those the ones involving immobilised bacterial cultures, are of particular interest. These processes are more productive than traditional free-culture processes and the subsequent downstream processing is less cumbersome and costly (Pateraki et al. (2016)). Moreover, the construction of accurate models that can describe the bioprocess is key for quick and reliable experimental development as well as for the construction of efficient optimisation and control strategies (Theodoropoulos and Sun (2019)). In this work we have developed a novel continuous packed-bed bioreactor for the efficient bioproduction of succinic acid. Moreover, we have developed a new predictive model of our continuous bioprocess and we have used it to develop an efficient model-based optimal control strategy. Our continuous reactor is 20-40cm long, packed with spherical alginate beads, 0.3cm in diameter, within which the bacterial cultures are immobilized. The substrate is glycerol, while the necessary CO2 input iss provided by MgCO3 in the feed. Here we propose a new kinetic model to describe the fermentation of A. succinogenes to produce succinic acid from glycerol our continuous packed-bed bioreactor. For this process a heterogeneous 2-phase, 2-dimensional partial differential equation- (PDE) based model of the packed bed-bioreactor was developed. The model takes into consideration the concentration profiles, both in the bulk of the reactor as well as inside the individual alginate beads, where the biomass is immobilised. A steady state behaviour is assumed inside the alginate, therefore the reaction rate throughout the radius of the particle is represented by second order ordinary differential equations (ODEs). The model assumptions were validated by experimental results and therefore it is safe to assume that immobilised cells follow the same intrinsic kinetics, as the free-cell culture. For the system to be simplified the reactor is considered axisymmetric, thus only 2 dimensions, are considered. Moreover, since the Peclet (Pe) number is greater than one, throughout the process, the diffusion term is dropped for the bulk equations. The system was solved numerically using a first order upwind scheme in MATLAB(ODE113) for the bulk phase

and backward finite difference method for the alginate beads. The model was validated against experimental data obtained by operating the packed bed bioreactor system with different initial substrate conditions and different bioreactor retention times. The model can confidently predict the concentration dynamics of glycerol, succinic, acetic and formic acid, with the error between the experimental data and the predicted values from the model ranging between 2% and 4%. Moreover, the model is used to develop a robust nonlinear model predictive control (NMPC) (Bonis et al. (2013), Mesbah (2016)) strategy for the optimal control of the process. As our 2-D 2-phase PDE-based model is too complex to use for online applications, model reduction is required to provide a computationally amenable model. Here we employ a double model reduction step combining Proper Orthogonal Decomposition (POD) and artificial neural networks (ANNs) (Xie et al. (2015)) to handle the high dimensionality of our bioprocess model, in conjunction with polynomial chaos expansion (PCE) (Xiu and Karniadakis (2002)) to address model uncertainty. Here, the process uncertainty arises from the substrate glycerol concentration and the diffusion coefficients in the alginate beads phase. The constructed POD-ANN surrogate models could accurately predict the high-dimensional dynamics of stochastic moments and bounds computed through the second order PCE method. The computed low-order models were then employed within a close-loop control scheme to generate a robust optimal control policy to improve the expected concentration of succinic acid at the exit of the bioreactor while satisfying the time-space upper bound constraints of byproducts acetic and formic acid. We also implemented robustness verifications for the bio-production process under 40 uncertain realisations and the computed optimal control policy. Computational results show that all random cases and the predicted upper bounds could rigorously satisfy the requirements of product quality (time-space byproduct constraints), implying the high robustness of the computed optimal control policy. Meanwhile, all the random trajectories of succinic acid concentration surrounded the predicted dynamics of the expected values while all the random time space dynamic trajectories of byproducts concentrations were below the calculated upper bounds, indicating the accuracy of the constructed surrogate models for MPC applications. In the future, less conservative control strategies will be exploited to further enhance the process performance.

Keywords: Succinic acid, Continuous bioprocess, Dynamic modeling, Nonlinear model predictive control, Stochastic partial differential equations

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A game-theoretical approach for the analysis of waste treatment and circular economy networks

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Abstract

Circular economy is emerging as a sustainable alternative to clean and waste management technologies in that waste is upgraded as a resource with a purpose to further use it as feedstock either to the same or to other industries. Major drivers include consumer needs, resource shortages, and technological breakthroughs. Other than materials and energy though, circular economy involves different stakeholders who have similar or different roles and entertain a different level of interactions with each other; the state, as government or municipality, is a major stakeholder and a player assigned with a role to incentivize or manipulate interactions. To understand the development of interactions, the use of game theory can be both insightful and powerful. Traditional applications in game theory typically follow Stackelberg formulations that feature players in open markets, with identical or similar roles. They compete each other on how they can access markets, by means of cost or market functions that dictate their profits. Approaches involve mathematical formulations produced as bilevel optimization problems optimized to determine the profit share of each player. Quite often, mathematical models take the form of multi-objective optimization approaches in which one optimization function balances trade-offs with another competitive function. Game theory can be applied to address interactions and roles in emerging and circular economy networks. However, the markets are not ideal while profits are primarily made at the purchase of raw materials (waste) rather than the production of marketable products. As the ownership of value chains involves many actors, partner payoffs depend not only on the choices of a single actor but on the choices of others. Drivers other than competitive advantage include a better management of threats, social and environmental benefits, and policies to establish a fair share of profits. Nash equilibria rather than Pareto optimal constitute more attractive and sensible objectives. Both in waste management and circular economy networks, there are two profit lines to consider: one at the receiving end and, potentially, a second one at the production as based on the valorization path that is selected. While in the context of a classical Stackelberg approach the competition relates to the product, in circular economy networks the competition is mainly for the feedstock; products may diversify with the players' choice to valorize feedstock. Moreover, while the profit share is important to study, it is equally important to study the equilibrium of the overall system in the context
of Nash as the network are subjected to several threats and opportunities from the players involved. The paper presents a game-theoretical approach for the analysis of waste management and circular economy networks. Players include waste producers, competitive technologies, and the governing authorities. The variables include interactions of the players, choices for valorization technologies and different cost models. In search of Nash
equilibria, an interesting conclusion has been that the players often converge at errant and deviant equilibria unless waste valorization is involved. In other words, circularity brings stability. In the case where valorization is involved, bilevel optimization has been applied to evaluate the dependence of profit share on market elasticity, options to subcontract waste upgrade to third parties, the cost of processing technologies, and the choices of products. Results indicate a strong dependence of the profit share on market conditions and player interactions. Solutions include cases where leaders choose to subcontract followers, cases that indicate the impact of controls to divert profit share, and the impact of cost and process efficiency in the network development.)
Keywords: circular economy, game theory, bilevel optimization, waste management

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Agile Process Systems Engineering (PSE) education – 1. What should be taught to achieve desired outcomes mastery by graduates?

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Abstract

Process Systems Engineering (PSE) is the branch of the chemical engineering discipline that harnesses computational methods and tools for the analysis, design, control, optimization, and effective operation of processing systems, and the design of products, across different scales and dimensions. PSE binds basic science and engineering and helps integrate in an effective way different subjects that student engineers pass through, thus giving context and meaning to their studies. One of the curriculum challenges in many institutions is that PSE-focused instructors do not convincingly cover the integrative nature of systems thinking and application of computational tools within the curriculum. This two-part paper proposes a "game plan" for teaching of PSE topics that addresses what should be taught and how these topics should be taught effectively in a classroom setting. We base our recommendations on: (a) A comprehensive survey of the teaching methods used in leading universities to teach PSE, and our collective experience of the most effective ways that should be used to cover such topics (the "how"); and (b) Surveys of the actual topics and application areas covered in the courses taught in academia, both from an academic point of view and also from the perspective of the processing and manufacturing/hi-tech industries (the "what").

This first part concerns the "what" – i.e., which specific key PSE topics should constitute the core requirement of the first degree in chemical engineering – either a BSc, but in many cases, an MSc, and the coverage of which application areas should be included. The teaching of PSE courseware has traditionally used example applications from rather well-established process industries, usually involving only steady state considerations. More recent applications of PSE, both in industry and in academic research, have increasingly involved other industries, including for example biotech, pharmaceuticals, electronics, energy, environmental applications, food engineering, and water treatment.

The gap between modern applications of PSE and the way that it is taught, particularly to undergraduates, undersells the role and importance of PSE as a central driver for innovation and development of the chemical and biochemical engineering profession, accounting for other major innovations such as the Industry 4.0 paradigm that facilitates the implementation of all the PSE contributions.

The two-part paper suggests a working plan for academic activity in preparing the next generation of engineers and researchers to be better aligned with the needs of academic research, industry and society, without requiring additional time-on-task beyond that allocated currently for the coverage of PSE topics. The process systems community needs to openly share best practices and resources; otherwise, we will be back talking on this subject in 5- or 10-years' time (Cameron and Lewin, 2009, Cameron et al., 2019, Kiss and Grievink, 2020).

Keywords: PSE Education, curriculum, active learning.

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You have nothing to lose: Worry-free flipping for PSE

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Abstract

All topics taught under the PSE umbrella benefit from more time-on-task made available for students to learn by class discussion, experimentation, and cooperative solution of open-ended problems – basically by "getting their hands dirty" as a key component of their own learning process. Courses taught using the conventional teacher-centered, lecture-based approach have less time available for these crucial activities, and thus may achieve lower levels of learning outcomes.

The flipped format moves the lecture material online, to be completed by students as homework. Thus, the main justification to move to flipped format is the desire to increase the proportion of the student-staff contact time in which students are actively learning, rather than just listening to lectures (Felder and Brent, 2015). This makes better use of the shared time between teacher and students, which has a huge impact on students' engagement, as does aiming to maximize the degree to which students are participating actively with the teacher and with each other, rather than passively listening to lectures. There are many existing studies that provide quantitative evidence that active learning improves course outcomes (e.g., Freeman et al, 2014, Velegol et al, 2015; Lewin and Barzilai, 2021).

Since the COVID-19 pandemic forced all teaching to move completely online, one would have thought that this would have motivated the transition to active methods in teaching. In fact, teaching pedagogy has largely not been affected by the potential of technology, with most online teaching still teacher-centered, relying on synchronous lectures delivered over Zoom. The main obstacles to change are the following:

(a) Resistance to change from lecturers: Teachers are discouraged both by the significant investment of time and effort required to prepared quality online materials (prerecorded lectures and online exercises), and by the initial resistance of some students to active learning; (b) Reduced outcomes performances from the non-participants/non-engagers: Quantifiable lower outcomes are attained by students who engage less with the online materials and with class activity (Lewin, 2021).

With the advantages of adopting the flipping approach clear, one is left with the above two issues to resolve, both of which are the focus of the contributions of this paper: (a) Guidelines for the effective and efficient production of the necessary supporting materials (recorded lectures, online quizzes, and class activities); and (b) Guidelines for continuously fostering higher engagement rates from the students. These contributions will be supported by examples from the authors' extensive experience of successful applications of active learning approaches in courses on process design and process control.

Keywords: PSE education, active learning, flipped class.

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Agile Process Systems Engineering (PSE) education – 2. How to teach to achieve desired outcomes mastery by graduates?

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Abstract

This is the second part of a contribution (Kondili et al., 2022) concerning the "how" – what should be the correct teaching sequence of the key PSE modules constituting the core requirement of the first degree in chemical engineering – either a BSc, but in many cases, an MSc. Of equal importance are the methods that should be used to achieve learning objectives that produce graduates that can master and apply those principles in practice. In particular:

- Students should be taught fundamental concepts in detail, ideally self-paced, achieved more efficiently using prerecorded materials.
- Students need to be exposed to computer programming packages ranging from those solving chemical process flowsheets to those specialized in data analysis, optimization, and spreadsheets.
- Students should become familiar with optimization tools earlier in their academic career, so that they can use them to solve practical problems in their senior years.
- Students should apply multivariate statistical and artificial intelligence tools for solving real problems.
- Students need to understand why some software or computer packages may not provide accurate answers in some instances. The fact that they converge to a solution does not necessarily mean that the solution is correct.
- Students should be required to develop critical thinking skills, i.e., to question their solutions/methods and ask themselves if alternative approaches could be used to tackle a particular problem.
- Students should develop professional and personal skills such as teamwork, communication, and project management.

For students to attain mastery in the critical understanding and application of the PSE core materials, time needs to be allocated for them to experiment, get things wrong (and understand why), repeating this process as necessary. Several methods have been advocated that free class time for students to engage in active learning, such as project-based learning, blended teaching, and flipped class approaches. The flipped class paradigm shifts the transmission of basic information to online preparatory tasks, which students complete in advance of class activities.

This study consists of a survey of teaching practices aimed to assess the degree to which active methods are used in practice, to understand the reasons or limitations why they are not, and to identify circumstances where those methods may be more effective. Together, the two-part contribution provides a working plan for academic activity in preparing the next generation of engineers and researchers to be better equipped and aligned with the needs of academic research, industry, and society, without requiring additional time-on-task beyond that allocated currently for the coverage of PSE topics. The process systems community needs to openly share best practices and resources, otherwise we'll be back talking on this subject in 5- or 10-years' time (Cameron and Lewin, 2009, Cameron et al., 2019, Kiss and Grievink, 2020).

Keywords: PSE Education; curriculum; active learning

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Modelling and optimisation decision-making for improved educational resilience under pandemic events

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Abstract

The recent pandemic events have significantly affected people and institutions worldwide. Multiple issues and difficulties arise from this scenario, with an increasing number of challenges. In this work we address the impact of the crisis on the education sector, and we provide guidelines for handling it using a structured framework assisted by data-driven modelling and optimisation decision-making.

The methodology employed for building the educational resilience framework is comprised of five steps: data collection, data analysis, gap formulation, solution development, and implementation structuring. First, a data-driven strategy is proposed using data collected from the internet, literature, previous knowledge on the topic, and presential or online surveys with students, researchers, faculty, and staff. Second, analyses are carried out aiming to find meaningful patterns and insights that can serve as indicatives of issues or gaps that represent potential candidates for improvement (i.e., educational aspects that should be considered and addressed in order to improve the education resilience). Third, the most important or impactful gaps are classified according to a cost-effectiveness criterion. Fourth, guidance is provided on when, where, and how these gaps should or could be handled, whereby proper solutions are developed considering the availability of resources (time, effort, economic) and outcomes (benefits, accomplishments, profit). This includes applying proper modelling and optimisation decision-making approaches for real-life educational problems. Finally, a deployment plan is built using structured solutions that provide benefits in the short-, middle-, and long-term for multiple recipients and institutions.

From the guidelines proposed herein, educational resilience improvements can be achieved for people, academia, industry, and society, in a wide variety of problems and applications, and with multiple significant benefits. The results and conclusions derived from this work illustrate how mathematical modelling and optimisation decision-making can be effectively and interestingly employed towards easier and more efficient educational strategies, methodologies, and policies.

Keywords: Educational resilience, Education in PSE, Learning capabilities, Collective intelligence.

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Teaching courses heavily dependent on computational resources to STEM students during Pandemics

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Abstract

The current pandemic has blatantly affected teaching at all levels. Specifically, in Portugal, for STEM (Science, Technology, Engineering and Mathematics) students attending Universities and taking high learning degrees, it was particularly harsh. Most mandatory courses implied attendance to science laboratory or computational lab lessons that had to be postponed to after lockdown times, rescheduled to late night hours, or simply converted into videoconference sessions. Teachers and researchers had to be very creative and resourceful to keep their students interested and invested in their courses in spite of the disturbing and abnormal situations caused by the pandemic. Operational Research, Simulation, and Actuarial and Financial Mathematics courses were mostly converted to online versions with videoconference lectures supported by elearning platforms. The courses' heavy usage of computational resources and the physical characteristics of the majority of existing computer labs prevented the possibility of faceto- face classes due to social distancing even after the end of the several lockdowns. Unfortunately, online versions of these very hands-on courses revealed to be really bland and having a low appealing to students, leading to pupils' increasingly dropping out of courses and even quitting their attendance for that particular semester. In this work the authors will present the adaptations that they decided to implement on their courses during three long semesters to make the teaching and learning experiences engaging, interesting and effective and the assessment activities reliable and efficient. Lectures being recorded (previously or live), small group assignments during classes, the use of a professional video-conferencing software, each course having its MOODLE page are some of the experimented adaptations, among others. The main goal was to meliorate and even to cease students' drop-outs. This work will explore the experiments and good practices that worked and the ones that did not correspond to the expected outcomes. Additionally, some framing will be made concerning how Portuguese Government and the authors' teaching institution have supported these experiments and good practices. Some comparisons between the students' performances from the affected semesters and from previous years will also be presented.

Keywords: Virtual Education, Teaching Practices, Pandemics, Active Learning, Peer Instruction

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Reflexivity for evaluating complex acting/thinking skills necessary for socio-ecological transitions

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Abstract

Inheriting from a 18th century tradition of engineers aiming at bringing material and social progress to people, French engineers are still mostly assigned the task of assembling knowledge and know-how for producing industrial artefacts (Roby, 2017). Nowadays, multiple crises about climat, biodiversity, energy, inequity, social unrest, etc. set a new frame for addressing engineering problems. Technological recipes of the past are nowadays of limited use. Usages, impacts, etc., are rarely discussed or tackled too late, even though they are crucial aspects of the issues in debate in our society.

Since 2014, Institut National Polytechnique Toulouse University (INPT) offers a 1-year MSEI cursus at graduate level (MSEI, 2014). It focusses on empowering students with engineering capability to tackle complex problems related to the global socio-ecologic transition. It is built around two competencies that concern both the epistemological register in which students address problems and the students themselves.

The first competency '"acting/thinking in complexity" (ATC). It is builds upon Morin' "la pensée complexe" paradigm (Morin, 1977, LeMoigne, 1999, Rossignol, 2018). It aims at practicing engineering *in* complexity rather than practicing engineering *of the* complexity. The former sets a global and systemic perspective of engineering activity and lies in the scope of the pragmatic constructivism epistemological thinking (LeMoigne, 1999, Avenier, 2011), whereas the latter is rooted in cartesianism and bears a reductionist view of a system made de facto complex by the multitude of its elements (Boiera et al. 2019). At MSEI, students experiment the ATC competency in various projects and case studies often backed by an experiential learning approach (Kolb, 1984) and POGIL strategy and using various modelling techniques. As a brief overview of the precepts students implement, one can list: 'link is at least equally and often more important than elements in a system // there exists no universal solution or recipe, no miraculous model // models are not the ultimate purpose but solely a media of intermediation for co-building an understanding of all issue, share by all stakeholders // project objectives or questions must always be questioned at first in the light of social, ecological, technical, economics, climate, landscape and other issues // satisfying rather than optimal solutions should be sought // solutions are integrative and necessarily co-built with all stakeholders // discuss while acting // reassess goals during projects // design relevant indicators from the start // periodically evaluate means of evaluation".

From our experience, it happens that shifting from cartesianism routine to an engineering approach *in* complexity also necessitates that students practice "reflexivity thinking", the second core competency at MSEI. Reflexivity is not new and it is a practice encouraged for addressing many issues, in particular those about sustainable engineering (Kearins

and Springett, 2003, Miller et al., 2011), that has inspired the current socio-ecological transitions concern in engineering. At MSEI, practicing reflexivity has two goals. It helps evaluating the 'acting/thinking in complexity' competency and it questions the students about their professional horizon in relation to their past and present experiences and learning. It takes the form of a free-format portfolio (Michaud, 2010; Gerbaud, 2018) which asks each student an uncommon and sometimes uneasy effort, to write down its own living and thinking. For accompanying the students, several exercises are proposed, such as 'coat of arm' with four quadrants: what they are, what they can rely on, what they fear, what they hope, + their motto; a 'writing of amazement' of what surprised the students since they started the MSEI cursus. Private writing. No evaluation, a 'Kolb experiential learning practice' exercise on a personal experience and two 1-hour interviews using a semi-structured frame. In addition, students and teachers practice self and co-evaluation both during the interviews and in the final portefolio production, for evaluating how students implement the 'acting/thinking in complexity' competency in their past and current experience and how they project it into their future work.
Allowing to product a free format portefolio is a must since it does not constrain the student into fulfilling any teacher's request and it leaves him open to perform reflexivity.

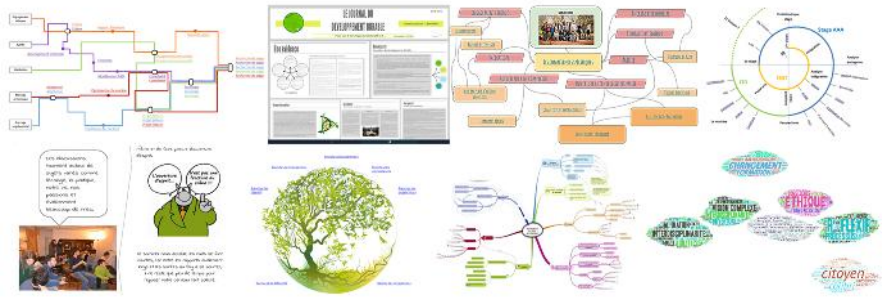

Figure 1. Portfolio production overview

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Keywords: Socio-ecological transition, Engineering, Reflexivity, Experiential learning, Complexity

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