Proceedings of the 25th Nordic Process Control Workshop (NPCW 2025)

January 15–17, 2025
Aalto University, Finland

Aalto University
Department of Chemical and Metallurgical Engineering
Process Control and Automation Group

Contents

Welcome to the 25th Nordic Process Control Workshop

Dear Nordic Process Control community and friends,

Welcome to the 25th Nordic Process Control Workshop (NPCW) at the Aalto University, Finland, January 15–17, 2025. Organized by the Nordic Process Control Working Group, this workshop aims at strengthening the ties between the Nordic process control communities by providing a platform for discussing current research and developments in process control and for meeting old and new friends. This year, Prof. George Stephanopoulos will be awarded the Nordic Process Control Award for his lasting and significant contribution to the field of process control.

NPCW'25 is locally arranged by the Process Control and Automation Group of the School of Chemical Engineering at Aalto University. We wish you a productive and rewarding workshop!

Local organising committee

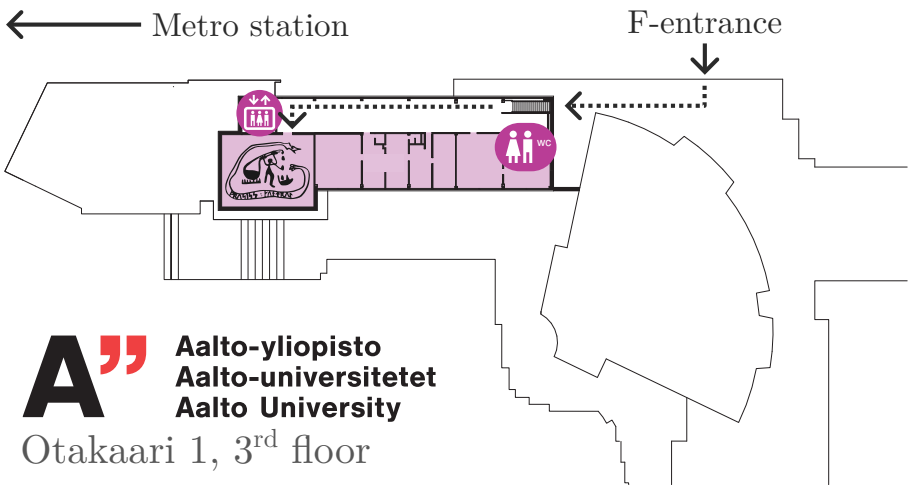
- Francesco Corona (Chair)
- José Augusto Magalhães Fontenele
- Otacilio Bezerra Leite Neto

Venue: Otaniemi campus, Aalto University (Espoo, Finland)

Aalto University is a multidisciplinary university established in 2010 as a merger of the Helsinki University of Technology, the Helsinki School of Economics, and the University of Art and Design Helsinki. The name of the institution is a tribute to the Finnish architect Alvar Aalto, who designed a large part of the Otaniemi campus.

The easiest way to reach Otaniemi is by metro to the Aalto University Station, which is located within the A Bloc shopping mall. The best tool for guiding yourself around Helsinki is the "Helsinki Transportation HSL" website and app. You can buy tickets in the app and at the ticket machines next to metro/bus stations.

The conference will take place in the Room H304 of the Undergraduate Center (Otakaari 1). The room is located on the third floor and can be reached through the stairs next to the F-entrance (see image below). If needed, the information desk in the main lobby can provide you with directions. For more information, including a detailed map of the building, visit the website: `https://aalto.fi/en/locations/undergraduate-centre`. During the conference, lunch will be served at the MOO Restaurant, Otakaari 2 (across the street from the Undergraduate Center). After the main activities on Thursday (16/01), we will provide transport from Aalto University to downtown Helsinki, where we will have the social program.



Nordic Process Control Award

Prof. George Stephanopoulos is the recipient of the NPCW 2025 Award

George Stephanopoulos received his diploma in chemical engineering from National Technical University of Athens (1970), his M.E. from McMaster University (1971), and his Ph.D. from University of Florida (1974). Since 2018, he holds a joint appointment as professor at the School of Molecular Sciences and the School for Engineering Mater, Transport and Energy at Arizona State University (ASU). He is also the Arthur D. Little Post-Tenure Professor of Chemical Engineering at the Massachusetts Institute of Technology (MIT).

His research and teaching interests have covered many aspects of process systems engineering, such as: process synthesis; process modeling and analysis; process optimization; process operations modeling, analysis, diagnosis, and control; process operations scheduling and planning. He is a member of the National Academy of Engineering (1999), Foreign Member of Russian Academy of Technological Sciences (1991), and a fellow of the American Academy of Arts and Sciences (2012). He received an Honorary Doctor of Science degree from McMaster University (2002). In 2009 he received the Ragazzini Award, of the American Automatic Control Council (AACC), 2009. He is a fellow of American Institute of Chemical Engineers (AlChE) and has received the Walker ('03) and Colburn ('82) awards. He was also the 2003 AIChE Institute Lecture and one of the 100 Chemical Engineers of Modern Era. He received the 1993 Computing in Chemical Engineering Award, from AIChE's CAST Division. He has also received the C. McGraw Award for Research from American Society for Engineering Education ('86) and the 1977 Dreyfus Teacher and Scholar Award. The journal Computers and Chemical Engineering selected his papers twice for the Best Paper Award (1987, 1992). He has given honorary lectureships at Princeton University (Wilhelm Lectures, 2009); ETH-Zurich (Stodola Medal Lecture, 2009); Univ. of Delaware (Gerster Lecture, 2004); Imperial College (Sargent Lecture, 2000); Carnegie Mellon (2000); Purdue Univ. (Kelly Lectures, 1999); Univ. of Oklahoma (Fair Lecture, 1999); Rutgers Univ. (Merck Distinguished Lecture, 1992); CCNY (Katz Memoral Lecture, 1989); Univ.of Newcastle (The ICI Distinguished Lecture, 1988); Univ. of Bologna (Distinguished Lecturer for the 900th Anniversary, 1988); Caltech (The Dreyfus Lectures, 1982), and others. Stephanopoulos has authored/co-authored seven books and co-edited eight. He is co-author to more than 210 papers.

List of NPC Awardees

1. Howard H. Rosenbrock (UK), 1995
2. Karl Johan Åstrøm (Sweden), 1997
3. F. Greg Shinskey (USA), 1998
4. Jens G. Balchen (Norway), 2000
5. Charles R. Cutler (USA), 2001
6. Roger W. Sargent (UK), 2003
7. Ernst Dieter Gilles (Germany), 2004
8. Manfred Morari (Switzerland), 2006
9. Jacques Richalet (France), 2007
10. John MacGregor (Canada), 2009
11. Graham Goodwin (Australia), 2010
12. Lawrence T. Biegler (USA), 2012
13. James B. Rawlings (USA), 2013
14. Rudolf Kalman (Switzerland), 2015
15. Wolfgang Marquardt (Germany), 2016
16. Dale Seborg (USA), 2018
17. Nina Thornhill (UK), 2019
18. Thomas F. Edgar (USA), 2022
19. Sebastian Engell (Germany), 2023
20. George Stephanopoulos (USA), 2025

Nordic Process Control Working Group

The Nordic Process Control Working Group was formally founded in Stockholm on 24 October 1994. The group initiates activities in order to strengthen the ties between the Nordic process control communities. One activity of the Working Group is to propose the location, date and organizers of an annual or semi-annual "Nordic Process Control Workshop" (NPCW). The Working Group also awards the "Nordic Process Control Award" to persons who have a made a lasting and significant contribution to the field of process control.

NPC Working Group members

- Francesco Corona, Aalto University, Finland (2019) (Chair)
- John Bagterp Jørgensen, DTU, Denmark (2009; 2015; 2022) (Co-chair)
- Johannes Jäschke, NTNU, Norway (2018; 2023) (Past Chair)
- Wolfgang Birk, Luleå University of technology (2018, 2023)
- Gurkan Sin, DTU, Denmark (2009; 2015; 2022)
- Elling W. Jacobsen, KTH, Sweden (1994; 2000; 2006; 2012; 2018; 2023)
- Sigurd Skogestad, NTNU, Norway (1994; 2000; 2012, 2018; 2023)
- Jeno Kovacs, Sumitomo SHI FW Energia, Finland (2010; 2016; 2022)
- Alf Isaksson, ABB, Sweden (2004; 2010; 2016; 2022)
- Torsten Wik, CTH, Sweden (2013; 2019)
- Christer Utzen, GEA Process Engineering A/S, Denmark (2015; 2022)
- Iiro Harjunkoski, ABB Germany/Aalto Univ., Finland (2016; 2022)
- Morten Hovd, NTNU, Norway (2018; 2023)
- Jakob Kjøbstedt Huusom, DTU, Denmark (2018; 2023)
- Jari Böling, Åbo Akademi University, Finland (2019)
- Nicholas Alsop, Borealis, Sweden (2022)
- Olav Slupphaug, ABB, Norway (2022)

Programme

Wednesday (15/01) – Tutorial "Introduction to Machine Learning"

08:30	**Coffee/tea and registration**	
09:00	**Probabilistic Machine Learning** (w/ coffee break at 10:30)	
	09:00	Part 1.1
	10:50	Part 1.2
12:30	**Lunch**	
13:30	**Statistical Machine Learning** (w/ coffee break at 15:00)	
	13:30	Part 2.1
	15:20	Part 2.2
17:00	**End of Tutorial Sessions**	

Presenter: Francesco Corona
Abstract:

PART 1 - Probabilistic machine learning: The first part of the tutorial aims at providing an introductory account of the probabilistic ideas underlying machine learning and some models that take into account uncertainty and deal with an imperfect description of the problem at hand. Such ideas are fundamental, since our characterisation of the problem will always be limited by our observations and the models we use to describe them. We provide an incremental and easy to follow introduction to the concepts of Bayesian inference for regression (from curve fitting to linear models for regression, via a recap on probabilities and the Gaussian distribution) and classification using neural network learning as an example.

PART 2 - Statistical machine learning: The second part of this tutorial aims at providing a theoretical account of the statistical ideas underlying machine learning and some of the derivations that are used to transform these principles into practical algorithms. We provide an introductory though rigorous presentation of the concepts of learning, from what it is to whether it is always achievable. We introduce the formal model of learning known as Probably Approximately Correct, we discuss learning rules like the Empirical Risk Minimisation and its error (the no-free-lunch theorem), and we quantify the amount of data needed for learning (the VC-dimension).

Thursday (16/01) – 1st Conference Day

08:00	**Coffee/tea and registration**	
09:00	**NPCW 2025 Opening**	
	09:05	NPCW Award Ceremony
	09:15	NPCW Award Lecture
10:00	**Coffee Break**	
10:30	**Session 1: Control and Estimation (I)** Chairs: J. B. Jørgensen, T. Wik	
	10:30	*"Sparse spectral methods for approximating PDE solutions in particle flow"* J. A. F. Magalhães (Aalto University), M. F. Emzir, F Corona
	10:50	*"State estimation for gas purity monitoring and control in alkaline electrolysis systems"* L. Cammann (NTNU), J. Jäschke
	11:10	*"Adaptive reinforcement learning control using tube-based methods for systems with parametric uncertainty"* S. Rastegarpour (ABB Corporate Research), H. Feyzmahdavian, J. Wang, A. J. Isaksson
	11:30	*"Robust economic predictive control of bioreactors using metabolic network models"* R. D. de Oliveira (NTNU), J. Jäschke
	11:50	*"Simple worst case scenario back-off calculation for non-linear model predictive control"* L. L. Carmel (NTNU), N. Bar
	12:10	*"Receding-horizon control of wastewater treatment plants as self-sufficient water resource recovery facilities"* O. B. L. Neto (Aalto University), M. Mulas, F. Corona
12:30	**Lunch** (MOO Restaurant, at Otakaari 2)	
13:30	**Session 2: Process Control Practice (I)** Chairs: I. Harjunkoski, J. Jäschke	
	13:30	*"Techno-economic assessment of sustainable aviation fuel production via H2/CO2-based methanol pathway"* P. Guilloteau (DTU), H. Silva, A. Andreasen, G. Sin, A. D. Jensen
	13:50	*"Operational and control challenges in green hydrogen production: Insights and comparison with conventional energy processes"* K. D. Benam (ABB Oslo), C. Grimholt, M. Omtveit, J. K. Tjoland
	14:10	*"Advances in decision support: Optimization and FMU integration"* K. Vestman (Optimation AB), A. Yamashita, E. Lundgren, J. Simonsson
	14:30	*"Leveraging mill-wide optimization for more informed decision-making at pulp mills"* M. Hultgren (Valmet Automation Oy), G. Fralic
14:50	**Poster session and coffee break**	
17:30	**Transfer to Downtown Helsinki**	
18:00	**Social activity** – Visit to Helsinki City Museum (Aleksanterinkatu 16, Helsinki)	
19:00	**Workshop dinner** – Sofia Helsinki (Aleksanterinkatu 28, Helsinki)	

Friday (17/01) – 2nd Conference Day

08:00	**Coffee/tea and registration**	
09:00	**Session 3: Process Machine Learning** Chairs: J. Böling, I. J. Halvorsen	
	09:00	*"Model-integrated neural networks for battery modelling"* Y. Huang (Chalmers), C. Zou, Y. Li, T. Wik
	09:20	*"Enhancing fault diagnosis for chemical processes via MSCNN with hyperparameters optimization and uncertainty estimation"* J. Liang (DTU), G. Sin
	09:40	*"A probabilistic approach to froth flotation modeling using Gaussian process regression"* J. Lindqvist (Luleå University of Technology), K. Atta, A. Johannsson, D. le Roux
	10:00	*"A two-level approach for plant-wide root cause analysis"* T. Overgaard (DTU; Novo Nordisk), M. Bertran, J. B. Jørgensen, B. F. Nielsen
10:20	**Coffee break**	
10:40	**Session 4: Control and Estimation (II)** Chairs: D. S. Laila, S. Skogestad	
	10:40	*"Generalized feedback Nash equilibrium seeking in partially observed dynamic games"* O. B. L. Neto (Aalto University), M. Mulas, F. Corona
	11:00	*"Uncertainty-based perturb and observe for automated optimization of industrial processes"* L. I. M. Aarnoudse (NTNU), M. A. M. Haring, A. Pavlov
	11:20	*"Minimum energy operation of dividing wall column - application of extremum seeking control"* I. J. Halvorsen (SINTEF Digital; NTNU), L. I. M. Aarnoudse, M. A. M. Haring
	11:40	*"Optimal experiment design for multivariable system identification"* A. J. Isaksson (ABB Corporate Research), M. Lundh, S. Munusamy, G. Sigurdsson, V. S. Pinamaraju, H. Hjalmarsson
	12:00	*"Augmented extended Kalman filter for estimation and model's improvement of a bioreactor fermentation process"* G. Sartori (NTNU), N. Bar
	12:20	*"Estimation of pattern formation in stochastic reaction-diffusion systems with particle flow filters"* J. A. F. Magalhães (Aalto University), O. B. L. Neto, F. Corona
12:40	**Lunch** (MOO Restaurant, at Otakaari 2)	
13:40	**Session 5: Process Control Practice (II)** Chairs: A. Isaksson, G. Sin	
	13:40	*"Dynamic pressure management of CO2 pipelines"* A. Kumaraswamy (NTNU), J. Jäschke
	14:00	*"Constraint-switching control of proton exchange membrane water electrolysis systems"* M. Fredriksen (NTNU), J. Jäschke
	14:20	*"A strategy for accurate estimation of identifiable model parameters and sensor placement in the process industry"* E. Lundgren (Optimation AB), A. Yamashita, J. Simonsson, K. Vestman
	14:40	*"Parallel comparison of control structures: A case study in mining"* F. Norlund (Lund University; Boliden AB), K. Soltesz, M. Bauer
15:00	**Closing ceremony**	
15:30	**End of NPCW 2025**	

List of Posters

P01	*"Dynamic modeling and optimization of microalgae growth in airlift bioreactors"* A. Sehatnia (Luleå University of Technology), A. K. Patel, A. Johansson, D. S. Laila
P02	*"Evaluating hybrid modelling for process safety applications: A novel benchmark model based on renewable ammonia production"* N. Groll (DTU), G. Sin
P03	*"Learning-based health aware operations"* E. Ngowi (NTNU), R. D. de Oliveira, J. Jaschke
P04	*"Machine learning based system modeling in bioprocess control with Corynebacterium glutamicum"* Y. Li (NTNU), V. N. R. Pedreira, N. Bar
P05	*"Model and software in-the-loop testing of engine's speed and load control functionality"* A. Tahir (University of Turku), P. Prinsén, J. Böling
P06	*"Multi-scale virtual flow metering for optimal decision-making"* J. D. Fraihat (NTNU), R. D. de Oliveira, J. Jäschke
P07	*"Nonlinear model predictive control of an industrial BioPower 5 CHP plant boiler in a cloud-based Java Spring environment"* J. Kortela (Aalto University)
P08	*"System simulation of maritime automation systems using co-simulation with FMI and OPC-UA"* K. Klemets (University of Turku)
P09	*"State and parameter estimation of anaerobic digesters based on the modified AMOCO model"* B. Abera (Addis Ababa University), T. Wik, G. Bekele, M. Mamo
P10	*"The Simulation of shipboard microgrids: A practical approach"* M. Asadizadehshiraz (University of Turku)
P11	*"Ultrasound technology based plants quality and health monitoring"* D. S. Laila (Luleå University of Technology), A. Sehatnia, M. A. Sattar

Book of Abstracts

Session 1: Control and Estimation (I)

Sparse Spectral Methods for Approximating PDE Solutions in Particle Flow

José Augusto F. Magalhães* Muhammad F. Emzir† Francesco Corona*

In Sequential Monte Carlo (SMC), one method for performing the Bayesian computation *prior* × *likelihood* is to derive the law of motion of an ensemble of particles—a particle flow [1, 2]. This allows sampling from complex distributions while avoiding common issues in more traditional SMC methods, such as particle degeneracy and the need for resampling. However, some implementations of particle flow require solving a weighted Poisson equation, an elliptic partial differential equation (PDE) whose coefficients depend on the density of particles. In general, the solution to this elliptic PDE must be approximated, as analytical solutions are limited to specific cases, such as Gaussian prior and likelihood. Traditional spectral methods for approximating the solution are usually based on the tensor product formulation, where the solution is represented as a weighted sum of a sufficiently large number of products of univariate basis functions. Using N_B bases in each coordinate of the N_X-dimensional state-space leads to $(N_B)^{N_X}$ unknowns. Thus, even for problems of moderate dimensionality, current computational resources are insufficient to support the full tensor product grid necessary for an accurate approximation. Additionally, tailored choices of bases are often required in order to match the solution's regularity and domain properties, and a systematic basis selection approach is still lacking, with only a few promising studies addressing this issue [3, 4].

In this work, we propose an approximation using a sparse grid/hyperbolic cross technique [5] to solve the weighted Poisson equation in more general settings. The solution is approximated with multivariate polynomials bases, whose span is dense in the space of solutions under mild assumptions on the underlying distribution, such as exponentially decaying tails or finite moments of all orders. We demonstrate the accuracy of this technique when applying SMC to state estimation of a stochastic chemostat. The aim is to reconstruct biomass and substrate concentrations based on noisy observations of biogas production [6]—a state estimation problem with non-linear process and observation models.

References

[1] Fred Daum and Jim Huang. Particle flow for nonlinear filters with log-homotopy. In Oliver E. Drummond, editor, *Signal and Data Processing of Small Targets 2008*, volume 6969 of *Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series*, April 2008. doi: 10.1117/12.764909.

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†Control and Instrumentation Engineering Dept., King Fahd University of Petroleum and Minerals, Dhahran, SA

State estimation for gas purity monitoring and control in alkaline electrolysis systems

Lucas Cammann* Johannes Jäschke*

The need to accelerate the energy transition has become increasingly evident through extreme weather events in recent years. This transition requires the use of renewably generated energy vectors that can be readily produced, stored, transported, and used. One of these potential energy vectors is green hydrogen.

Green hydrogen is hydrogen that is produced through electrolytic splitting of water by means of renewable electricity. This electrolytic splitting takes place in process units called electrolyzers, with alkaline electrolysis (AEL) and polymer electrolyte membrane (PEM) electrolysis being the two most readily available technologies for large scale implementation. While PEM electrolysis systems are generally deemed more flexible than AEL systems, both are limited in their flexibility by a lower load limit, i.e., a minimum power that has to be supplied to the system. This limit is determined by gas purity requirements, where the hydrogen to oxygen (HTO) ratio may not exceed 50% of the lower explosion limit in any part of the process [3]. Incidents in the past have proven that exceeding such limits can lead to fatal explosions [1, 2], and current large-scale green hydrogen facilities face associated flexibility challenges and are frequently turned off to avoid operating below the minimum load limit [4].

Gas composition measurements are readily available in the pure gas phase in process steps that follow the separation of water from the product gases. The gas holdup in these separation units means that it can take up to several minutes before a potentially dangerous upstream disturbance of the gas composition is measured. In this work, we propose the use of an Extended Kalman Filter (EKF) to estimate and control the gas purity in parts of the system where measurements are not available. For this purpose, we develop a simplified non-linear model which estimates upstream composition changes as augmented states, driven by process noise. The proposed estimator is tested in-silico against the full process model and a sequence of relevant disturbances. We show that this approach allows to

a) accurately estimate unmeasured composition changes for different disturbance types,

b) effectively control the composition in parts of the process where measurements are not available.

Subject to the same disturbance sequence, control of the estimated gas purity reduces the time spent in a potentially dangerous operating region considerably when compared to controlling only the measured composition. We find that in the former case, the time spent in out of norm conditions is at most a few seconds, whereas it can be as long as twenty minutes in the latter case.

References

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Adaptive Reinforcement Learning Control Using Tube-Based Methods for Systems with Parametric Uncertainty

Soroush Rastegarpour* Hamid Feyzmahdavian Jiayue Wang Alf J.Isaksson

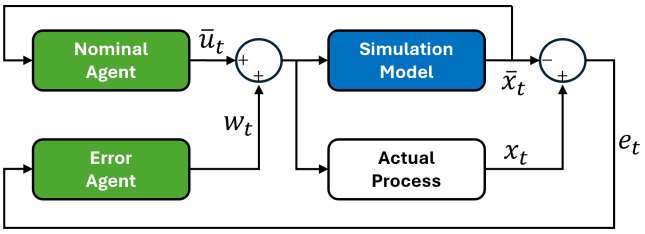

Figure 1: Adaptive Reinforcement Learning Control Framework in implementation.

Uncertainty learning methods use operational data to refine model estimates and update control policies, improving robustness and safety in industrial systems. Techniques such as Gaussian Process (GP) regression improve controller accuracy by providing more precise models of system dynamics [1]. This approach is further extended by integrating GP regression with MPC to manage state and action constraints [2]. Probabilistic safety models incorporate uncertainty and probabilistic constraints, offering a robust framework for ensuring safety in dynamic and uncertain environments [3].

This work presents an adaptive RL control framework for systems with parametric uncertainty. Expanding on the principles of Tube MPC, this framework applies a Tube-Based RL strategy to improve robustness in control systems under uncertain conditions. This approach uses a dual-agent structure to balance optimal control performance with adaptability to real-world conditions. The first agent operates in a simulated environment, optimizing control actions based on a simplified system model to achieve optimal performance under ideal conditions. The second agent complements this by continuously learning to minimize discrepancies between the idealized model's predictions and actual process dynamics, thereby increasing adaptability to real-world scenarios. This cooperative agent structure maintains system stability and performance even in the presence of model inaccuracies or external disturbances. Since direct training on the actual system is impractical, the simulation environment incorporates parametric uncertainties and Gaussian disturbances to closely emulate real-world operational uncertainties. The structure of the proposed Tube-Based RL is shown in Figure 1. The framework's effectiveness is validated through several case studies, highlighting its adaptive response to changing process conditions. Results demonstrate that the Tube-Based RL framework achieves robust performance under uncertain conditions.

References

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Robust economic predictive control of bioreactors using metabolic network models

Rafael D. de Oliveira* Johannes Jäschke*

Bioprocess model-based control technology has not yet achieved maturity [1]. One of the reasons for that is the lack of knowledge regarding cell metabolism, which impacts the development of accurate dynamic models [1]. Structured models based on metabolic networks can improve control performance compared to non-structural classical models (e.g., Monod kinetics type models) [2]. Dynamic Flux Balance Analysis (dFBA) is a metabolic network model mathematically described as an ordinary differential equation system with an embedded optimisation problem [3]. dFBA has an embedded Linear Programming (LP) optimisation problem that optimises some cell's objective function (e.g. biomass yield) through the metabolic network. One issue with the solution of the LP is the degenerate solutions that give rise to multiple possible trajectories of the dFBA states [4]. When the dFBA is used inside a model-based control strategy such as Nonlinear Model Predictive Control (NMPC), the uncertainty on the trajectories can cause constraint violations. This work proposes a robust control strategy based on the Multi-stage NMPC (MS-NMPC) scheme. A new framework was developed to make MS-NMPC suitable for dFBA models. A regularised version of the LP problem was used to obtain the multiple solutions inside the metabolic flux space. After that, the KKT conditions of that new problem were imposed as equality constraints into the optimal control problem. The MS-NMPC was formulated as an NLP problem with complementarity constraints using the direct collocation approach [3]. A case study using a core metabolic network of *Escherichia coli* was used to validate the methodology. MS-NMPC was applied to maximise biomass production in a fed-batch bioreactor, where a constraint on the acetate concentration was imposed. The results show that the MS-NMPC scheme can improve the robust constraint satisfaction on a scenario of multiple state trajectories using dFBA models.

References

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25th Nordic Process Control Workshop (NPCW25): Simple worst case scenario back-off calculation for non-linear model predictive control

Lipe L. Carmel* Nadav Bar*

The implementation of Non-Linear Model Predictive Control (NMPC) in bioprocesses faces challenges due to measurement uncertainty, scarce measurements, and model mismatch. Under certain conditions, these disturbances may lead to constraint violations and operation outside of the measurable range of the instrumentation for several hours, rendering model predictive control unreliable.

Several robust NMPC strategies can address such problems, but typical multi-model and multi-stage formulations introduce a high computational costs to optimize a scenario tree. This costly computations are usually not a feasible solution for real time operations. Automatic back-off calculation NMPC addresses this computational cost by focusing only on constraint violations and further constraining the system by an additional amount, the back-off value, until the original constraint is satisfied even when subjected to random disturbances simulated via Monte-Carlo over a short uncertainty horizon, which is shown to be more efficient than to optimize the entire scenario tree, though it still requires up to thousands of short simulations [1]. We therefore designed an automatic back-off NMPC by substituting the Monte-Carlo procedure with at most 2^n (where n is the number of disturbances) possible worst case scenario disturbance realizations for each time step in the uncertainty horizon. This formulation is guaranteed to yield sufficient back-off for the next time step for discrete models with monotonic output predictions in relation to the disturbances, under the assumption of a structurally correct model, and disturbances bound by box constraints.

An extensive simulation analysis demonstrated that our automatic back-off NMPC successfully prevented constraint violations, even with infrequent substrate measurements and in the presence of plant-model mismatch. While Monte Carlo simulations allow a broader search space and greater flexibility to address non-linearity, our formulation achieved constraint satisfaction with significantly lower computational effort. Additionally, this approach is well-suited for economic NMPC applications in bioprocesses that aim to maximize product formation. In typical continuous fermentation monod-models, the economic optimum may favor high dilution rates, which are impractical for real bioprocesses, as they drive the NMPC towards the lower limit for biomass concentration—a counterproductive control action. It is important to highlight that the back-off can be calculated after the control actions, allowing it to be integrated into most NMPC frameworks just by adding its value to the constraints, making the controllers more tolerant to plant-model mismatch, input implementation errors, and measurement errors, with minimal changes to their formulations, as these disturbances can be directly represented in the back-off computation. Consequently, this formulation offers a straightforward, low-computation-cost solution compared to alternative robust NMPC formulations.

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Receding-horizon control of wastewater treatment plants as self-sufficient water resource recovery facilities

Otacílio B. L. Neto*, Michela Mulas†, Francesco Corona*

The arising paradigm of perceiving wastewater as a sustainable source of water, nutrients, and energy, pressures for the design and operation of treatment plants as water resource recovery facilities (WRRF) [1]. A recovery facility regulates the quality of its effluent to support demands arising from urban, industrial, and agricultural activities (e.g., a request of nitrogen-rich water for crop fertigation). Simultaneously, to ensure a balanced water-energy nexus, the process must recover its energetic costs by processing disposed sludge into biogas, a renewable source of energy; thus enabling a self-sufficient treatment process. While the research on new process designs has been fruitful, the investment required for replacing the existing treatment infrastructure is the main challenge in this transition. In turn, still little has been investigated on how the existing treatment plants can be repurposed to these emerging objectives. Under this context, we are interested in automation solutions that optimally control typical wastewater treatment plants (WWTPs) as energetically self-sufficient WRRFs.

Biological treatment through activated sludge processes, a technology common to most urban areas, is an important platform for recovering resources from wastewater: Their dynamical properties and optimal operation have been extensively studied thanks to the availability of well-established simulation platforms [2, 3]. Based on this class of treatment processes, we propose a receding-horizon controller that operates WWTPs to produce effluents of specified quality on demand while recovering energy through biogas production. Our controller solves state-feedback model predictive control (MPC) problems in which the current process state and disturbances are determined by moving horizon estimation (MHE) [4]. The tracking of the desired effluent profiles is enforced by stabilizing the system around steady-state points that satisfy the output reference trajectories and the energetic constraints. We illustrate the controller's behaviour when operating a full-scale plant to produce water of varying quality while ensuring energetic self-sufficiency.

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Session 2: Process Control Practice (I)

Techno-economic Assessment of Sustainable Aviation Fuel Production via H_2/CO_2-Based Methanol Pathway

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To achieve long-term greenhouse gas neutrality in aviation, replacing fossil aviation fuels with Sustainable Aviation Fuels (SAF) from renewable sources is essential. This study provides a Techno-Economic Assessment of a SAF production process utilizing renewable hydrogen (H_2) and carbon dioxide (CO_2) through the Methanol To Olefins (MTO) and Mobil Olefins to Gasoline Distillate (MOGD) pathway.

We investigated methanol formation kinetics, comparing various models and reactor types. Models incorporating both CO_2-to-methanol conversion and the Reverse Water-Gas Shift reaction demonstrated high accuracy, with a boiling-water reactor achieving optimal conversion (22.4%) at 450 K and 75 bara. This study provides new insight into how methanol reactor design impacts conversion rates and costs. While MTO and MOGD reactors were designed based on conversion model [1], we determined a two-column distillation system was necessary to reach 97% purity of C8-C16 hydrocarbons for 38 kT/year of kerosene in addition to LPG, diesel and gasoline as side products.

Economic evaluation established a Minimum Selling Price of \$2.46/kg using a Monte-Carlo simulation, higher than the current fossil jet fuel of \$0.68/kg [2] but consistent with prior SAF studies [1]. Uncertainty analysis showed high sensitivity to reactant prices, particularly H_2.

Additionally, we studied the dynamics of the process by examining different storage possibilities for hydrogen, carbon dioxide, and methanol and the catalyst deactivation within the different reactors.

This study underscores the economic potential of the SAF production process, demonstrating the importance of developing advanced reactor models and assessing realistic industrial design specifications.

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Operational and Control Challenges in Green Hydrogen Production: Insights and Comparison with Conventional Energy Processes

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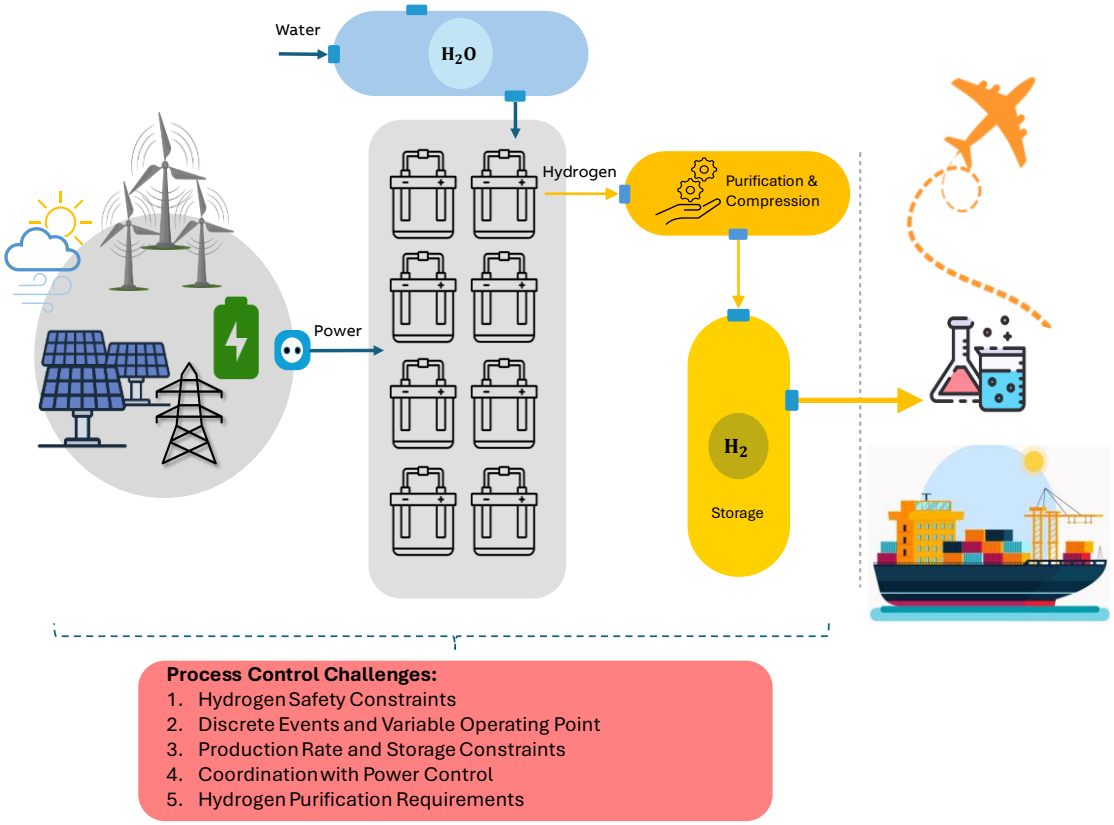

Figure 1 Green Hydrogen Production and Process Control Challanges

Green hydrogen is central to the global effort to reduce carbon emissions and achieve energy sustainability. By leveraging advanced process control techniques and simulating the complete hydrogen production cycle, the study highlights key operational and control challenges, particularly when compared to conventional energy processes. These include the integration of fluctuating renewable energy sources, coordinating multiple electrolyzers in parallel, managing water resources, maintaining process stability under variable conditions, and ensuring safety while meeting production rate requirements. The findings provide crucial insights for engineers and researchers working to scale hydrogen production technologies and process control.

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Advances in Decision Support: Optimization and FMU Integration

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Decision support platforms based on simulation models may serve as a tool during the whole life cycle of a plant and help operators, engineers and managers in their daily work. Based on our previous experiences, decision support platforms should be flexible and interoperable, being able to support models developed by different actors in different programming languages, for example by supporting models imported as functional mock-up units (FMUs). Additionally, a combination of first-order principle and heuristic models is usually needed to enable simulations over long time horizons in a reasonable time. There are many uses for decision support platforms in the industry, for example to evaluate operational goals, assess new CAPEX investments, find bottlenecks and target where and when preventive maintenance is most needed. In short, to reduce waste and energy consumption and to increase a company's profit.

In a recent project, optimization of an iron ore mine has been provided as a decision support service to find optimal production rates. Simplified process models, production constraints and operational goals are implemented as a mixed-integer optimization problem, solved using the Python package GEKKO [1]. The decision support platform delivers a solution calculated by a Model Predictive Control (MPC) algorithm. The same approach has been tested for a co-generation plant, where bypass and turbine steam flow rates produced by a boiler are calculated to maximize the income from selling electricity in the market whilst fulfilling district heating demand.

The next step in decision support is to integrate more complete simulation models into optimization, rather than simplifying dynamics and re-writing system equations. One software that enables import of FMUs to be used for optimization is CasADi [2]. Although some challenges and limitations must be considered before commercialization, promising results following this methodology have been given for a co-generation plant modeled in Dymola using in-house libraries.

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Leveraging mill-wide optimization for more informed decision-making at pulp mills

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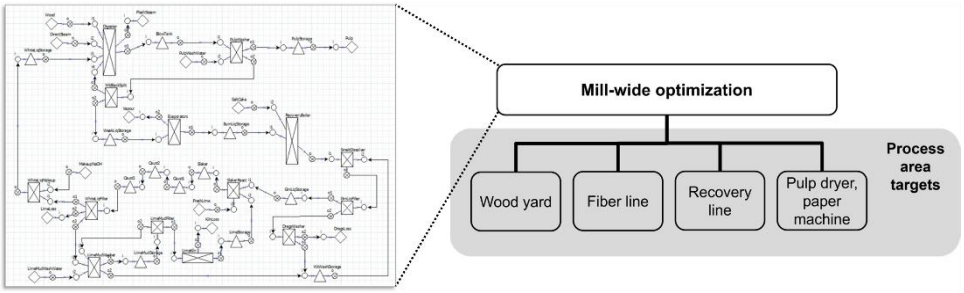

Flowsheet optimization is used for coordinating mill-level process targets.

The present work describes how mill-wide optimization is used for empowering production and quality decision-making in pulp mills. As a result of cost efficiency requirements, changing market conditions, safety and environmental factors, and the challenge of an ageing workforce, pulp and paper mills are aiming at an increased autonomy of their operations to help the personnel understand and control their processes better. An increased level of autonomy should be pursued on all levels of process management and control by implementing modern distributed control systems, optimizing process areas locally through advanced process control, and coordinating the process areas towards high-level targets through mill-level and value chain optimization. Mill-wide optimization (MWO) is discussed here as a real-time advisory solution for the overall optimization of pulp mills.

The MWO approach is based on mathematical flowsheet optimization, where a data-driven flowsheet model is optimized periodically for a given optimization horizon into the future or into the past. The problem is solved on a weighted single-objective equation-oriented basis, subject to both internal and user-defined constraints and objectives. The MWO technology enables the construction of various optimization and simulation concepts, focusing on different model layers, key performance indicators, and production decisions. The MWO platform enables the online implementation and utilization of these concepts directly in the automation system of the mill.

The work presents how mill-wide production planning is enabling more informed production decisions at two reference pulp mills, concerning both the overall impact of the mill-wide operation outlook and more specific use case examples. So far, the results have been promising and have highlighted the benefits of mill-wide optimization. Next, the work expands on how optimized production plans will be used as a foundation for quality optimization in future projects. In particular, fiber line quality tracking is highlighted here as a tool for back-calculating how past disturbances and operations have impacted current pulp quality.

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Session 3: Process Machine Learning

Model-integrated neural networks for battery modelling

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Abstract

The result of detailed modelling of many physical systems is a set of partial differential equations. When reducing such models to a limited set of ordinary differential equations, it is common that this yields a system coupled to algebraic equations due to boundary conditions and state equations set to be in a steady state to avoid high order and stiffness. Although reduced, computational complexity easily still becomes a burden or a hinder for both simulation and control design, because of the need for iterative solutions to the algebraic equations in each time step. In this work, we circumvent this issue by using Neural Networks to approximate the algebraic equations and making them explicit in the state variables.

Integrating physics-based and data-driven approaches has emerged as a promising strategy for modelling dynamic systems. Yet, existing works primarily focus on using data-driven surrogates as replacements for physics-based models, often sacrificing accuracy for computational speed and losing critical elements like generalisability, adaptability, and interpretability, which are often essential for control applications. This work introduces a novel framework for physics-based machine learning, termed Model-Integrated Neural Networks (MINN), designed to learn reduced-order models of the complex physics of systems governed by partial or ordinary differential-algebraic equations (PDAEs and ODAEs). MINN provides a systematic approach to develop optimally simplified models that balance physical insight, numerical accuracy, and computational efficiency. We demonstrate the efficacy of this approach by modelling the electrochemical dynamics of lithium-ion batteries, showcasing the advantages of the MINN battery model. Unlike physics-informed neural networks (PINN), which only approximate solutions to autonomous systems, MINN combines neural networks and physics-based models directly within the network architecture and is therefore neither restricted to autonomous systems nor to conditions of any specific solutions. This integration enables rapid simulations and reduced model orders, and can be extended to a range of control-oriented modelling scenarios.

Keyword: Physics-based learning; Energy storage systems; Reduced order modelling

Reference: Huang, Y., Zou, C., Li, Y., & Wik, T. (2024). MINN: Learning the Dynamics of Differential-algebraic Equations and Application to Battery Modeling. In IEEE Transactions on Pattern Analysis and Machine Intelligence (pp. 1–14). doi:10.1109/tpami.2024.3456475

Enhancing Fault diagnosis for Chemical Processes via MSCNN with Hyperparameters Optimization and Uncertainty Estimation

Jingkang Liang [*] Gürkan Sin [*]

Fault diagnosis is critical for maintaining the safety and efficiency of chemical processes, as undetected faults can lead to catastrophic consequences including equipment damage, environmental contamination, and potential loss of life. Data-driven fault diagnosis methods, especially deep-learning-based methods have been widely used in the field of fault diagnosis of chemical processes [1]. However, these methods often require time-consuming manual hyperparameter tuning [2]. Additionally, existing fault diagnosis methods typically lack uncertainty quantification, which is crucial for assessing prediction confidence in safety-critical applications. This underscores the need for reliable methods that combine improved accuracy with uncertainty estimation in chemical process fault diagnosis. This sets the premise for the research focus in this contribution.

To this end, we present a novel approach combining a Multiscale Convolutional Neural Network (MSCNN) with hyperparameter optimization and Bootstrap for uncertainty estimation. The MSCNN captures complex nonlinear features from chemical processes, while Tree-Structured Parzen Estimator (TPE) automatically optimizes hyperparameters, reducing manual tuning efforts. Bootstrap technique, previously validated for deep learning property predictions [3], was incorporated to enhance model accuracy and provide uncertainty quantification.

The proposed method was evaluated using the Tennessee Eastman Process (TEP) dataset, comprising 21 fault types with 52 variables per sample. From 26,880 total samples, a 60:20:20 split was used for training, validation, and testing. The proposed method was benchmarked against state-of-the-art models including MLP, CNN, LSTM, and WDCNN, with performance evaluated on precision, recall, parameter count, and prediction quality (i.e. uncertainty estimation). Results demonstrated superior accuracy of the proposed MSCNN-TPE-Bootstrap approach, with ablation studies confirming the effectiveness of TPE and Bootstrap in enhancing fault diagnosis performance.

In conclusion, this work paves the way for more robust and reliable fault diagnosis systems in the chemical industry, offering a powerful tool to enhance process safety and efficiency.

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A probabilistic approach to froth flotation modeling using Gaussian process regression

Johan Lindqvist* Khalid Atta* Andreas Johannsson* Derik le Roux†

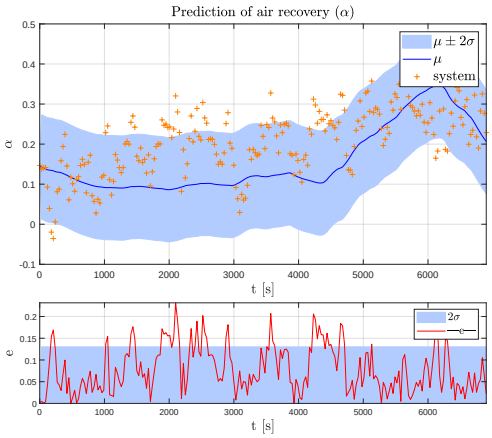

Figure 1: Multi-step ahead simulation of air recovery using a Gaussian process model.

Froth flotation is a method of separation in mineral processing. It is one of the most common methods of separation of minerals. However, a lack of models has historically hampered advanced control of the process. Flotation is a highly complex process with highly nonlinear dynamics, especially related to the physics of the froth. Furthermore, the instrumentation in industry can be sparse and needs to be better maintained. Currently, there are two main models of the process, both of which face challenges because they either assume well-maintained instrumentation or need help balancing accuracy with parameter estimation [1][2]. Due to its ability to handle noisy measurements and model highly nonlinear and unknown dynamics, a Gaussian process framework is ideal for tackling these challenges. Furthermore, the probabilistic nature of such a framework provides a way to evaluate the trustworthiness of the model, information that can be crucial when the plant requires stable and safe operations. To capitalize on the modeling work done so far, this work aims to encode the modeling knowledge into the structure of the Gaussian process covariance function, similar to the methods presented by [3]. Since all the states are measurable, Each state model is trained separately. The models are trained on data generated in simulation and the result is used as a prior for training and validation on industrial data. The resulting validation showed initial promising results.

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A Two-Level Approach for Plant-Wide Root Cause Analysis

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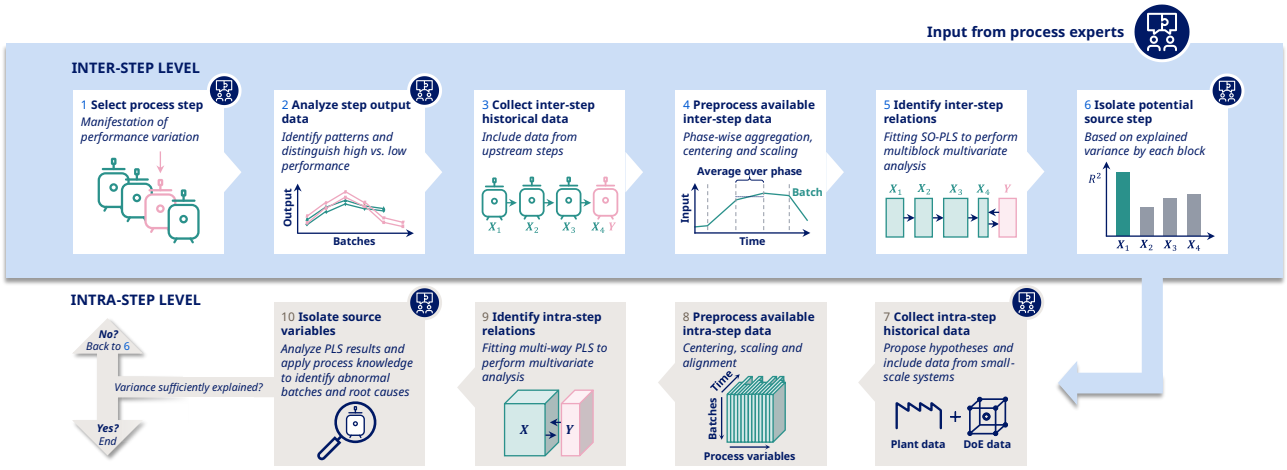

Figure 1: Two-level approach to combine process connectivity information with step dynamics

Detecting and resolving abnormal performance variations in batch bioprocesses involves identifying the responsible process step and analyzing the root cause. While root cause analysis is well-documented, pinpointing the specific step responsible for variations has received limited attention due to complexities like serial-parallel unit arrangements [1]. To address this, we propose a two-level approach using latent-variable techniques that combine process-wide connectivity data (inter-step level) with internal process step dynamics (intra-step level).

At the inter-step level, we identify a process step where performance variations manifest and build a sequential and orthogonalized partial least squares (SO-PLS) model to isolate a process step where the variation likely originates [2]. The SO-PLS model links data blocks across the flowsheet, using orthogonalization to filter correlated information. Once the responsible step is identified, we move to the intra-step level, where another PLS model captures the internal dynamics of the identified step. Here, large-scale production data is paired with small-scale development data. In collaboration with process experts, the PLS model isolates a potential root cause of the abnormal variation.

This approach is applied to a commercial batch bioprocess producing an API. We find that downstream productivity is limited by variability during cell culture production. By pairing bioreactor data from small-scale studies with commercial-scale data, we identify key process variables impacting performance. The validation of process improvement hypotheses is a collaborative effort between process experts and data scientists, thus enhancing transparency and leading to valuable insights.

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Session 4: Control and Estimation (II)

Generalized feedback Nash equilibrium seeking in partially observed dynamic games

Otacílio B. L. Neto*, Michela Mulas†, Francesco Corona*

Modern cyber-physical systems are often comprised of interacting subsystems operated locally by selfish decision-making agents. Ideally, these agents operate according to feedback policies that are (locally) optimal and satisfy global requirements, while being strategically stable to their rivals' interference. The framework of game theory provides the concept of competitive equilibria (e.g., the generalized feedback Nash equilibrium [1, 2]), which allows for describing such control strategies and their properties based on how the agents exchange information. However, computing a feedback generalized Nash equilibrium (GFNE) is a notoriously difficult task. A relevant yet specially challenging class of problems considers stochastic and partially observed dynamic games: When players seek policies that stabilise the system against disturbances while accessing (noisy) partial observations of its internal state. Despite recent progress in solving state-feedback problems [3, 4], a systematic approach to GFNE-seeking in stochastic and partially observed games is still lacking.

In this work, we propose an algorithmic solution to bridge this research gap. Leveraging the framework of system level synthesis (SLS, [5]), our proposal is based on the parametrisation of all jointly-stabilising output-feedback policies for an ensemble of non-cooperative players. Thanks to this parametrisation, each player's policy synthesis problem can be described as a finite-dimensional robust optimisation problem. Under this representation, we define the concept of a variational generalised feedback Nash equilibrium (vGFNE) and reformulate the equilibrium-seeking problem as a monotone inclusion problem. Finally, we design a fixed-point algorithm in which players converge to a vGFNE by optimising local objectives while a central coordinator ensures that the policies are stabilising and do not violate constraints. In addition to enabling GFNE-seeking in stochastic and partially observed games, our approach does not require knowledge of the actual state and actions applied to the system. Thus, this policy learning routine can be performed alongside the game's execution. We demonstrate the behaviour of this algorithm in exemplary problems on the stabilisation of networked systems.

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Uncertainty-Based Perturb and Observe for Automated Optimization of Industrial Processes

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Model-free adaptive optimization methods such as extremum seeking control (ESC) [1] and perturb and observe (P&O) [2] are capable of optimizing industrial processes that many other optimization approaches are not. Common optimization challenges are related to the time-varying nature of the process and the large uncertainties involved, which are caused by an uneven feed composition, environmental changes, a lack of in-depth process understanding, limited sensor measurements, and variations upstream in the production line, among other reasons.

Model-free adaptive optimization methods operate by actively probing the process to find better operating conditions. In typical ESC, a periodic dither signal is added to the values of tunable process parameters to perturb the process and determine a direction of parameter changes that lead to a more favorable state of operation. However, employing a periodic dither signal is inefficient and the resulting optimization is slow. In contrast, P&O steers the process parameters in one direction and only changes direction if the performance degrades. This leads to much faster optimization. However, standard P&O is sensitive to measurement noise and continues switching direction around the optimum, yielding a sustained oscillation in parameter values. Although parameter changes are necessary to track the changing optimal operating setting, both ESC and P&O use many more changes than required, leading to an increased wear of machinery or an unnecessarily large operating cost.

This research aims to develop a model-free adaptive optimization method that diminishes the main drawbacks of traditional ESC and P&O by having a high optimization speed, a low sensitivity to measurement noise, and a vast reduction in unnecessary parameter changes, resulting in a more efficient process operation. Our new method is called uncertainty-based perturb and observe (UP&O) and takes into account the uncertainty due to noisy measurements and the decreasing value of older data due to the time-varying nature of the process. Any proposed parameter changes are the result of maximizing the predicted performance of the process for several time steps into the future. Simulation results in Figure 1 illustrate that UP&O can reduce the number of unnecessary perturbations and the sensitivity to noise compared to P&O, while still tracking the optimal operating point accurately.

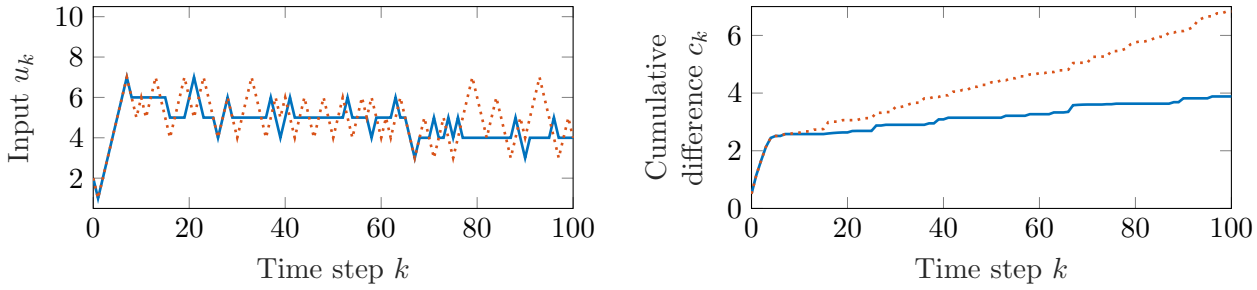

Figure 1: UP&O (—) uses fewer perturbations than standard P&O (····) to track the optimal operating point, thus reducing the cumulative difference $c_k = \sum_{i=1}^{k} f_k(u_k) - \min_u f_k(u)$ with the minimum output $\min_u f_k(u)$.

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Minimum energy operation of dividing wall column - application of extremum seeking control

Ivar J. Halvorsen [*†] Leontine I.M. Aarnoudse[‡] Mark A.M. Haring [*]

The dividing wall column (DWC) is an attractive arrangement since there is a significant energy saving potential compared to conventional column sequences. Distillation column products compositions are usually controlled by applying feedback control from selected temperature measurements since the temperature profile infers information of the actual composition profiles. Controlling conventional binary columns product compositions implicitly leads to minimum energy operations. This is not so for the integrated DWC, and energy consumption is highly dependent on internal flow routing. Thus, the realization of the saving potential requires additional control structures that can track the optimal operation point despite inevitable changes in feed properties, performance characteristics and other uncertainties. The characteristic of the optimum is known, given a good model and key measurements that enable precise information about the internal states [1]. However, there will always be uncertainties, in the model, in the measurements and in the realization of manipulative variables. Moreover, the most informative measurements, related to key composition data inside the arrangement, are usually not directly available. A typical cost function is the energy use per unit of feed constrained at the highest possible production rate. However, temperature profiles may also be direct indicators of optimal operation, are faster to respond to operational changes and may be utilized to formulate a cost function instead. Model-based optimization is a possibility but due to all uncertainties it may be an alternative to use pure data-based methods.

Extremum seeking control (ESC) [2] is a model-free optimization technique that, by active perturbation of selected manipulative variables, infers information about the current location of an extremum of a measured cost function and, by that, enables tracking of a moving optimum. The key point is that for any kind of model-based control and optimization technique there will be remaining uncertainties such that further adjustments by model-free ESC on top will be beneficial. Some structures of ESC for DWC will be analyzed and will be used to plan experiments on a pilot plant. Extremum seeking control can be used also in combination with other approaches, e.g. self-optimizing-control (SOC).

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Optimal experiment design for multivariable system identification

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Having an accurate model of a system is essential for many applications today, especially those related to advanced process control (APC). When executing an industrial delivery project of APC, often significant time is spent performing experiments on the real process to identify a model. By designing higher quality experiments the time needed on site carrying out experiments can be reduced, saving both resources and engineering efforts. In this work, we design a multi-frequency multi-amplitude square wave (multi-square) input based on a nominal model by minimizing the experiment length and placing constraints on the model accuracy (in the frequency domain) and the output amplitudes.

As a first solution a separate design was carried out for each input where the resulting optimization problem has the same structure as a semi-definite program but with the decision variables restricted to integers corresponding to the number of half-periods of each square-wave. For processes with multiple inputs, the corresponding designs are carried out sequentially [1]. In an extension of this initial work focusing on sequential excitation, the effects of using combined simultaneous and sequential excitation have also been investigated [2]. The resulting non-convex optimization problem is relaxed using binary decision variables. An important feature of the approach is that the experiment is carried out in closed-loop using a model predictive controller with zone constraints to further guarantee that the output constraints are not violated. Simulation results indicate that there are many cases where using combined simultaneous and sequential excitation outperforms the previous sequential approach.

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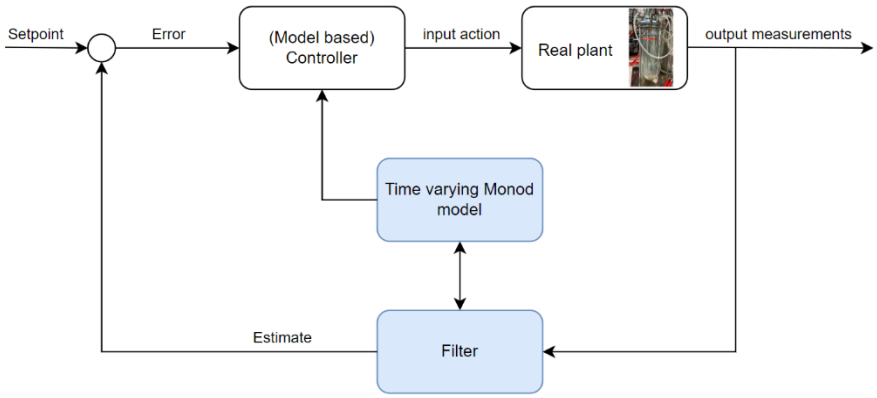
25th Nordic Process Control Workshop (NPCW25): Augmented Extended Kalman Filter for estimation and model's improvement of a Bioreactor fermentation process

Giacomo Sartori[1] Nadav Bar[1]



In automatic bioprocess systems, measuring the substrate concentrations is usually a great challenge because these measurements are infrequent and/or noisy, so -their state estimation is often necessary [1]. Moreover, the typically used Monod-growth based models in bioprocesses are too simple to describe the complex dynamics of microbial processes over time, rendering them infeasible for model-based controllers such as Model predictive control (MPC). The purpose of this work is twofold: to monitor in real time the fermentation process focusing on the substrate and to improve the prediction capability of the Monod model with time. These two objectives were achieved by implementing an Augmented Extended Kalman Filter (AEKF)[2], namely augmenting the state vector system with suitable identifiable parameters, and recursively estimating the entire estimation vector. This, however, also requires imposing state constraints on the estimates: we took care of this by solving an optimization problem that finds the Kalman gain minimizing the a posteriori error covariance matrix [3]. The implementation and tuning of the estimator are described in detail, with focus on the estimation of the model parameters. We compared the results to a Moving Horizon Estimator for Fed-batch microbial bioprocess [4]. Our results show that is possible to solve both problems in real time, guaranteeing good estimation performance (in terms of RMSE indices) while simultaneously adapting the parameters of the simple Monod model during the entire process. This estimator strategy has the potential to significantly improve the performance of real-time model-based controllers such as model predictive control.

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Estimation of Pattern Formation in Stochastic Reaction-Diffusion Systems with Particle Flow Filters

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Adopting reaction-diffusion models in real biochemical applications has been challenging: such models must rely on partial observations of the true system through indirect methods (e.g. light spectrography), and their typical realisations are high-dimensional stochastic systems. Consequently, the task of estimating the state is bound to incur a heavy computational burden, if at all computable. Particle filters (PFs) are popularly used for state estimation of general non-linear stochastic dynamical systems [1]. An ensemble of particles equipped with importance weights undergoes a sampling procedure in two steps: a *prediction* step, which drives the ensemble according to a proposal mapping (the most common being the system dynamics), and the *update* step, in which the ensemble likelihood is assessed every time a new observation is available. Due to the recursive nature of the algorithm, the ensemble presents a degeneracy problem after a few iterations [2]. The issue lies in the update step, where the particles may be situated in regions where they poorly represent the product of the prior and the likelihood. One way to address this is to choose a more informative mapping which includes the observation soon to be assimilated, rather than evolving the ensemble solely under the system dynamics. Additionally, one may leverage the decay-of-correlations property of many high-dimensional systems by performing full-state estimation based on lower-dimensional partitions of the state-space. This class of methods, denoted local particle filters, include the Block particle filter (BPF) of [3].

In this work, we show that the BPF is able to provide accurate estimates of the state under the informative mapping of [4]. However, the resulting ensemble now suffers from another problem—sample impoverishment—which occurs when many particles share the same value after resampling, leading to a low effective number of unique samples. We need to somehow reposition the particles generated during prediction steps, and a particular method is to derive the law of motion—a flow of particles [5]. This avoids particle degeneracy, sample impoverishment, and the need for resampling, albeit it requires solving a particular partial differential equation (PDE) at each update step. This PDE admits a closed-form solution when the informative mapping of [4] has been used in the prediction step. Our results show that the flow of particles provides an alternative to the *vanilla* BPF's update step and can serve as a benchmark for other non-linear filtering techniques in high-dimensional systems. We demonstrate the performance of the resulting PF on a Belousov-Zhabotinskii chemical reaction, with the aim of reconstructing the emerging chemical patterns based on noisy spectral observations.

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Book of Abstracts

Session 5: Process Control Practice (II)

Dynamic Pressure Management of CO_2 Pipelines

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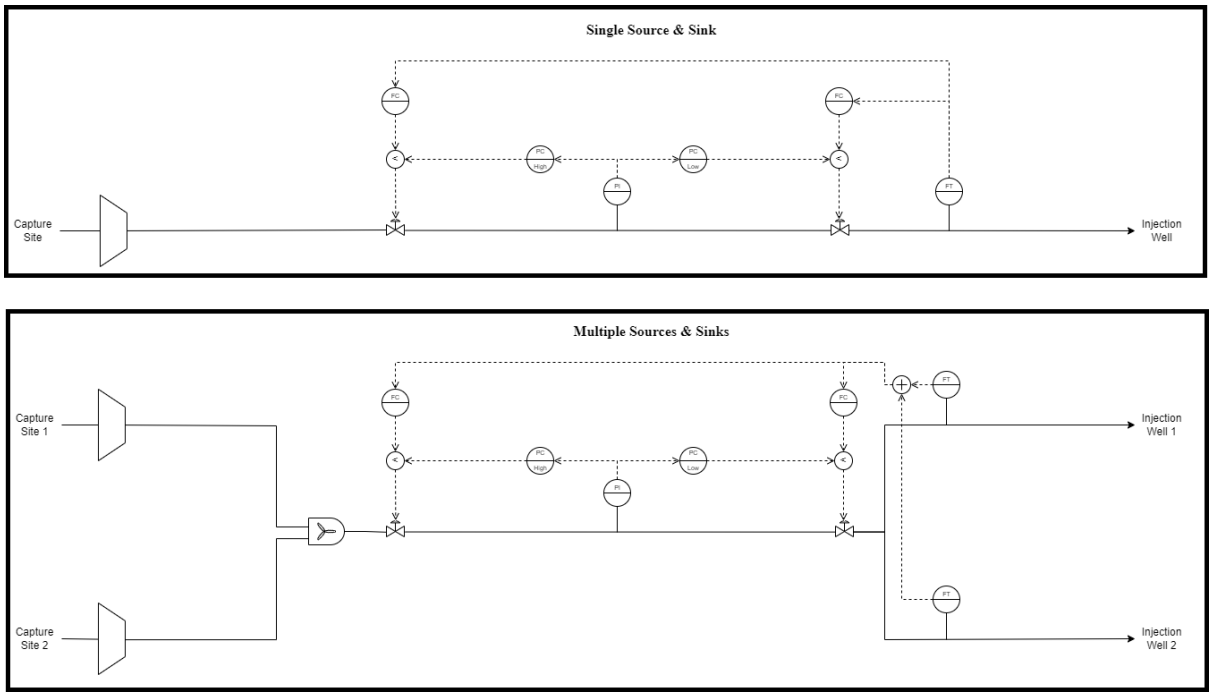

CO_2 transport control structure

Efforts to reduce greenhouse gas emissions are accelerating the deployment of carbon capture and sequestration facilities [1]. Given the spatial distribution of capture and sequestration sites [2], operation of large-scale pipelines for CO_2 transport are critical. Pressure control along these pipelines is important for reliable and cost-minimal operation. Uncertainties in capture and injection flow rates introduce challenges with pressure management. Through the application of simplified mass and momentum balance equations [3, 4], this work seeks to explore the application of a bi-directional control strategy [5] to maximize the throughput of supercritical CO_2 while respecting pipeline operational pressure constraints (see graphical abstract). Specifically, it seeks to determine the available recovery time during critical disruptions such as compressor failures, injection blockages, or changes in capture flow rates. Strategies for pressure management when there are multiple capture or injection streams are also investigated.

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Constraint-Switching Control of Proton Exchange Membrane Water Electrolysis Systems

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Proton Exchange Membrane (PEM) water electrolysis powered by renewable energy sources is a promising technology for green hydrogen production. However, due to the intermittent nature of most renewable energy, developing suitable control structures is crucial for facilitating safe and efficient operation of the PEM system. This work uses the "Top-down" section of Skogestad's plantwide control procedure [4] to suggest a constraint-switching control architecture. From an economic point of view, the active constraints are usually the most important to control due to the penalty related to having a back-off from the optimal constraint value [3]. Constraint-switching control structures may offer several advantages, as they have good disturbance rejection, are relatively easy to scale, are less affected by model accuracy, and are less computationally expensive to implement than control methods such as Model Predictive Control (MPC) [1].

We first developed a steady-state model of a PEM electrolysis system loosely based on the system presented by Crespi et al. [2]. We verified the system's behavior by comparing the polarization curve under different temperatures and pressures with other works in the literature. Following this, we formulated an optimization problem and tested various implementations of the objective function to map the active constraints of the system. We conducted step responses on the different manipulated variables (MVs) to assess their impact on the control variables (CVs) and proposed a control structure for the PEM system. Our simulations show that the PEM system is nearly fully constrained in all operating regions, allowing for implementing the constraint-switching control architecture. The active constraint regions exhibit several similarities with the active constraints identified for alkaline water electrolysis systems, as found by Cammann and Jäschke [1].

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A strategy for accurate estimation of identifiable model parameters and sensor placement in the process industry

Emma Lundgren* André Yamashita* Johan Simonsson* Klara Vestman*

For parameter estimations in dynamic process models for purposes such as model alignment, monitoring machine degradation and tracking simulators, the large number of parameters can create identifiability issues where multiple parameters generate similar changes in the output. This will lead to estimation errors if not dealt with, which lowers the accuracy and usability of the model. To solve this, new physical sensors are in some cases needed in the plant. For this purpose, a method for evaluating what to measure and placement of sensors based on the empirical identifiability Gramian is suggested.

A model of the plant was created in Dymola using the high-end Modelica libraries provided by Optimation AB. Flow rate, pressure and temperature sensors were placed in the model, including both existing and potential positions for new sensors. The model was then exported as a Functional Mock-up Unit (FMU), simulated to steady-state and linearized in Python. From there, the Empirical Gramian (EMGR) Framework [1] was used to compute the empirical identifiability Gramian for identifiability and sensitivity analysis.

A modified version of the Hankel Interaction Index Array (HIIA) through the parameter extended empirical observability and controllability Gramians was used to look at the interactions between the parameters and the output. Using this combination, it was possible to investigate which parameters are fully identifiable and have the greatest impact on a given sensor.

This method has been implemented successfully on a test model where the resulting parameter identifiability could be confirmed analytically, and new sensors could be placed for accurate estimation of more parameters.

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Parallel Comparison of Control Structures: a Case Study in Mining

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When ore is processed to extract a mineral concentrate, a separation process called flotation is commonly used. In series of flotation cells, differences in surface properties is utilized to separate the desired mineral from gauge. The desired minerals attach to air bubbles generated at the bottom of the flotation cells and form a mineral froth on top of the slurry in the cells. This froth is collected as it flows over the rim of the cells, and for this reason, level control of the slurry is foundational for receiving good recovery of the minerals.

In Boliden's concentrator plant at the Aitik mine located near Gällivare in northern Sweden, as in many other industrial plants, the level control of the flotation process has historically been governed by PI-controllers. In Aitik, this control structure consists of one PI-controller for each flotation cell, and a feed-forward therm to the next downstream one. This control structure performs well under normal operating condition, but as bigger inflow variations occur, the deviations of levels in the flotation cells can be quite extensive.

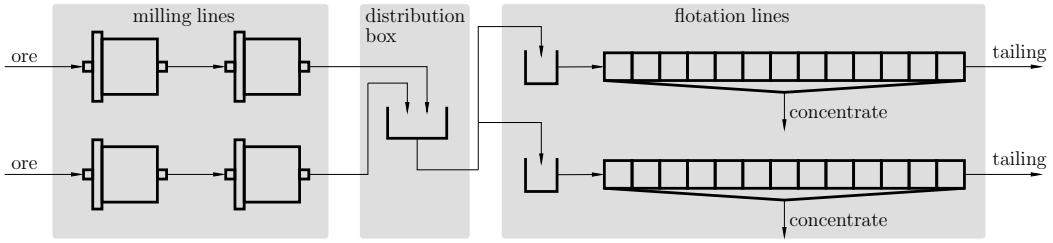

Figure 1: Schematic process overview of the Aitik concentrator plant.

Level deviations are not dangerous per say, but they disturb the recovery of mineral concentrate, and the profit and efficiency of the plant can hence be improved if the level deviations are reduced. The inflow variations that cause the level deviations are typically caused by disturbances in one of the two milling lines that supply flotation with slurry. In the Aitik plant, as illustrated in Figure 1, the slurry from the milling lines is distributed between two identical flotation lines, hence that the inflow variation affect both flotation lines.

To improve the level control performance during the inflow disturbances, a Linear-Quadratic (LQ) controller was introduced. This multi-variable model-based controller was first deployed only on one of two parallel flotation lines. This gave an opportunity to compare the performance of the two control structures side by side.

During a data collection time of 32 days with around-the-clock production, the two different control structures' responses to inflow disturbances could be observed, side by side, hence giving a fair comparison of the control structures.

In this presentation, we take a closer look at what makes this uncommon side-by-side comparison possible, discuss controller tunings, and take a detailed look at the results, both in therms of level deviations, and economic benefit.

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Poster Session

Dynamic Modeling and Optimization of Microalgae Growth in Airlift Bioreactors

Arman Sehatnia* Alok Kumar Patel* Andreas Johansson* Dina Shona Laila*

Schematic diagram for Microalgae cultivation in airlift bioreactors

Microalgae cultivation has emerged as a promising method for sustainable bioresource production, offering potential in biofuel, food, and pharmaceutical industries. In this research, we focus on extracting a dynamic model of an airlift bioreactor by integrating the complex interactions between the reactor's physical dynamics and the biological growth kinetics of microalgae. The study addresses a critical gap in the modeling of microalgae growth, aiming to optimize the cultivation process in airlift bioreactors, which are known for their energy efficiency and scalability.

This research systematically develops a mathematical model that incorporates the dynamic behavior of the airlift bioreactor, including gas-liquid interactions, mass transfer, and nutrient availability, alongside the nonlinear growth kinetics of microalgae species. The primary goal is to predict the biomass yield and optimize operational parameters for increased productivity under varying environmental conditions, such as light intensity, temperature, and nutrient concentrations. Special emphasis is placed on understanding how the reactor's hydrodynamics influence the algae's metabolic activities.

The results will provide valuable insights into the design and control of large-scale microalgae cultivation systems, supporting the development of efficient and sustainable bioprocesses. This research aims to study efficient dynamic models for the microalgae cultivation process in airlift bioreactors. By refining these models and accounting for various operating conditions, the study will extend its scope to design industrial-scale bioreactors with comparable efficiency in microalgae cultivation. The findings will include an exploration of the methods and developments applied to these systems, followed by a discussion of potential avenues for further improvement and optimization.

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Evaluating Hybrid Modelling for Process Safety Applications: A Novel Benchmark Model Based on Renewable Ammonia Production

Niklas Groll* Gürkan Sin*

The emerging hydrogen economy is crucial in the transition towards more sustainability in the process industry. Green hydrogen can serve as both a renewable fuel for process heat and a sustainable feedstock for products like green ammonia. The demand for green ammonia, which can be used as a fertilizer, a fuel, or a chemical energy storage, is expected to grow significantly within the next decades [1]. Accordingly, many efforts are directed toward designing and optimizing hydrogen-based process routes, but implementing innovative process designs also requires rigorous testing to ensure safety.

Safety assessment methodologies are often tested using "benchmark models." Various benchmark processes have been described in the literature to improve process control and monitoring techniques. For instance, the Tennessee-Eastman process replicates a typical chemical process [2], the Fed-Batch Fermentation of Penicillin is used as a benchmark for fed-batch-operated biochemical processes [3], and the COST model allows for the evaluation of wastewater treatment methodologies [4]. However, all established benchmarks lack several relevant aspects of renewable hydrogen pathways, such as integrating intermitting renewable energy supplies and electrochemical reactions. Therefore, the absence of a dedicated benchmark model for the hydrogen industry introduces unnecessary risks when applying process monitoring and control technologies to this emerging sector.

To address this gap, we present a novel simulation benchmark model designed to facilitate safer innovations within the hydrogen industry. Our model integrates green hydrogen production with the Haber-Bosch process for ammonia synthesis, combining electrochemical electrolysis with a conventional chemical process. Hereby, we account for the complete value chain of a typical Power-to-X process from renewable electricity over hydrogen production to a chemical product. The new benchmark model is built with the Aveva Process Simulator, enabling seamless transitions between steady-state and dynamic simulations and easy modifications to process design and control parameters. The model also incorporates controllers, pressure relief valves, and a flare system to simulate the effects of potential failures. By employing failure scenarios, the benchmark is an ideal tool for evaluating risk monitoring and control strategies. Additionally, the new ammonia benchmark model can serve as a foundation for developing new process safety methodologies tailored to hydrogen-based processes.

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Learning-based Health Aware Operations

Ngowi, E.[*] de Oliveira, R. D.[*] Jäschke, J.[*]

Condition monitoring techniques have been evolving through the years. This evolution can be witnessed by the transition of paradigms from the breakdown through preventive to the predictive strategy. The improvement of these strategies has been motivated by the increased understanding of the profit health trade-off [1]. Recently, there has been an increasing trend of embedding the health aspect of equipment into the control layers of chemical processes. Health constraints are imposed on chemical processes while considering the plant's degradation state and the next scheduled maintenance. To implement health-aware control (HAC), degradation models need to be developed for the prognostic of the plant health condition evolution. However, the development of these models is very expensive since they are highly stochastic and process specific. In turn, prognostics become difficult to establish hence failure to estimate the remaining useful life (RUL) of an equipment. Moreover, accommodating the large difference in time scales between the fast regulatory control actions and long-term degradation evaluation requires a long prediction horizon, which further increases the computational burden of Model Predictive Controllers (MPCs) when used in a HAC context [2]. The advent of Artificial Intelligence (AI) and Machine Learning (ML) opens a new avenue for building more accurate process, degradation and prognostic models from already available real plant data. This study proposes a methodology where the HAC is solved one step ahead, and the cost-to-go is approximated by a surrogate model trained offline. Our methodology is evaluated using a case study of a gas-lift well network with choke valve erosion caused by sand particles. The results illustrate how learning-based techniques can be applied to reduce the complexity of HAC optimization problems.

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Machine Learning Based Syetem Modeling in Bioprocess Control with Corynebacterium Glutamicum

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A significant trend in the circular bioeconomy involves leveraging alternative, recalcitrant bioresources for the production of bioactive chemicals. Seaweed, as an abundant marine resource primarily composed of polysaccharides, holds considerable promise as a substrate for sustainable microbial fermentation processes. Understanding bacterial growth and production under varying environmental conditions, such as fluctuations in substrate concentration, respiration rates, and dissolved oxygen, is essential for effective process control. However, real-time measurements of these states are often indirect and can be hindered by practical issues, including time delays, noise, and missing data. Traditional mechanistic models for predicting system states face challenges in accuracy and generalizability when attempting to capture the complex behaviors of bio-fermentation systems.

To address these challenges, we are developing machine learning based models to better capture and generalize the relationship between bacteria behavior and both initial and dynamic conditions in the bioreactor over time. Various modeling approaches will be compared, including hybrid models that integrate mechanistic model and data-driven insights with different weights, input selection and transformation, and model algorithm and architecture optimization. Neural network models, in particular, showed the ability to capture complex patterns, reducing reliance on process-specific parameters and providing complementary insights to mechanistic models. However, the risk of over-fitting and under-generalization due to limited experiment data requires substantial tuning and additional laboratory validations. Therefore our machine learning based models can be a promising alternative to traditional ODEs in order to provide continuous states prediction and support real-time process control. Moreover, an iterative process of model refinement with increasing number of experiments will be a necessary effort for enhancing predictive accuracy and valuable insights to yield high bacteria growth rate and production efficiency.

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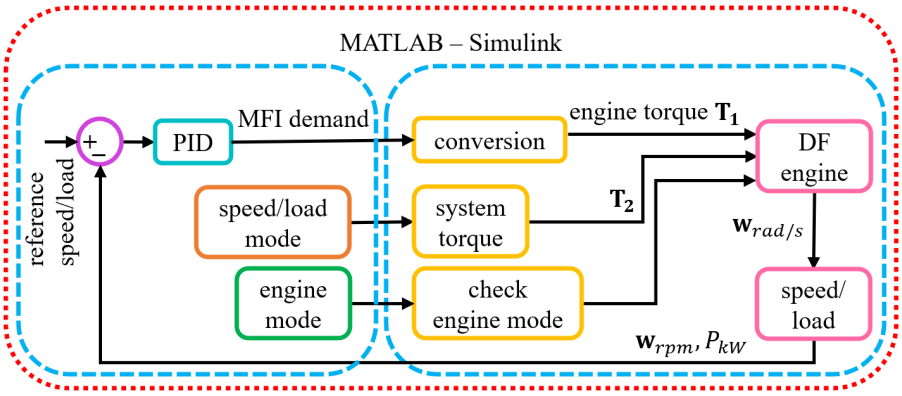
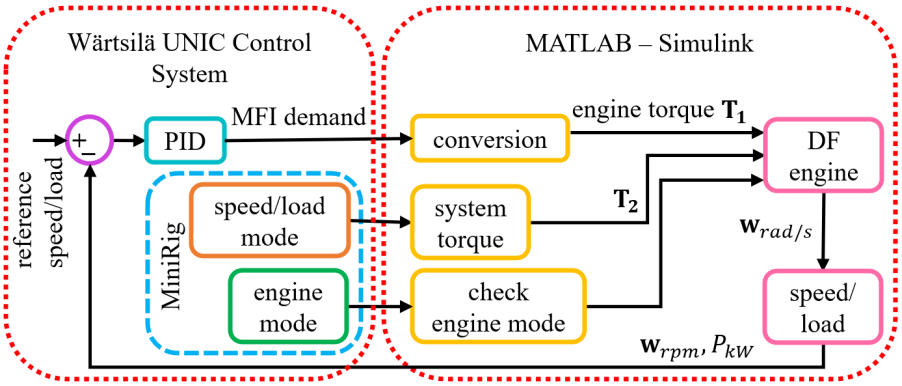
Model and Software In-The-Loop Testing of Engine's Speed and Load Control Functionality

Anam Tahir* Pontus Prinsén† Jari Böling*



(a) MIL testing method



(b) SIL testing method

Figure 1: Proposed engine simulation models.

The goal of this paper is to design the engine simulation models using rated working conditions such as engine speed and electrical load. In this paper, a W31DF first-order engine model is adapted for the proposed X-in-the-loop simulations, operating on torque and the performance output is the engine speed, as shown in Figure 1. The closed-loop system of this model is obtained using two different techniques such as PID manual tuning and PI direct synthesis. This aims to provide the closed-loop control performance by proposing the model-based-testing in MATLAB-Simulink i.e. the MIL simulation. Besides this, another objective utilises the Wärtsilä UNIC control system for the virtual verification of the adapted engine model using co-simulation with MATLAB-Simulink i.e., the SIL simulation. The Wärtsilä's existing real references and PID map-based control parameters from the UNIC control system are taken into consideration. The simulation results show the effectiveness of the proposed testing methods with respect to stability and settling performance. It is found that the system performance with PI direct synthesis control is slightly better than the PID manual tuning control in the MIL simulation. As a concluding remark, both proposed engine simulation models are adaptable to other control functionalities. Furthermore, this work can be extended by using variations of engine models such as higher-order models operating on torque and GT-power engine models.

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Multi-scale Virtual Flow Metering for optimal decision-making

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As the petroleum industry moves from extracting hydrocarbons from a single large field to a multitude of smaller fields, the wells in these smaller fields tie-in to existing infrastructure. [1] This makes the quantification of the hydrocarbon flow from each well interesting, as this information can allow for better economic management of the wells. These flows can be quantified in several ways: well testing, multiphase flow metering (MPFM) and virtual flow metering (VFM). Well testing and MPFM are expensive, with the former requiring to shut down production in the wells and the latter requires installation of expensive equipment. Due to this VFM is an attractive solution, as it only involves the use of mathematical models to estimate these flows and can be implemented based solely on existing measurement. The accuracy of VFM depends on the complexity of the underlying model, as a more complex model can capture more information and represent it with a more detailed understanding of the underlying processes. [2] It is proposed that a combination of differing models can be used to increase the accuracy VFM, as this combination can combats the inaccuracies of each individual model. These models can be first principle, data-driven or hybrid models. This is thought to hold for a combination of models that cross different levels of complexity and time scales.

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Nonlinear Model Predictive Control of an Industrial BioPower 5 CHP Plant Boiler in a Cloud-Based Java Spring Environment

Jukka Kortela*

The European commission has presented a revision of the Renewable Energy Directive as part of the package to implement the European Green Deal. It proposes for a new binding target of a 40 % share of energy from renewable energy sources in total consumption by 2030. The commission is also aiming at a more energy efficient and circular energy system that facilities renewables-based electrification, as well as biomass and waste heat [1].

For biomass combustion, Boriouchkine et al. [2] have developed a simplified model of the BioGrate boiler for the implementation of control and monitoring algorithms, where the fast computational time allows its utilization in online calculations.

Gölles et al. [3] developed a combustion model and a model predictive control (MPC) at small scale boiler. Experimental verification showed that the control strategy was capable to handle step changes of the moisture content of the fuel from 26% to 38% at power load 28 kW without difficulties. Extended Kalman filter was used to estimate the state variables, as only the feed temperature could be measured.

Internal model control with the nonlinear model identifying the essential behaviour of the grate boiler is utilized for control design in [4]. The experimental results prove that the control is able to handle the different loads with high efficiency, and the load changes can be made quickly.

According to the experimental tests, the flue gas oxygen content measurement together with air flow measurements is still the best measure of the fuel power released in the boiler [5]. Therefore, an improved nonlinear oxygen content model was developed for the BioGrate boiler.

In this paper, the novel nonlinear model predictive control (NMPC) is presented for the biomass boiler. The developed NMPC strategy was tested with the simulations in realistic Java Spring environment implemented in the cloud. The test results show that considering the water in the evaporation zone and the dry fuel in the thermal decomposition zone improves the control of the boiler. In addition, by utilizing the more accurate nonlinear model of the flue gas oxygen connect, the optimal air ratio between the primary air and secondary air flows is possible. The test results are presented, analyzed, and discussed.

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System Simulation of Maritime Automation Systems using Co-simulation with FMI and OPC-UA

Kristian Klemets*

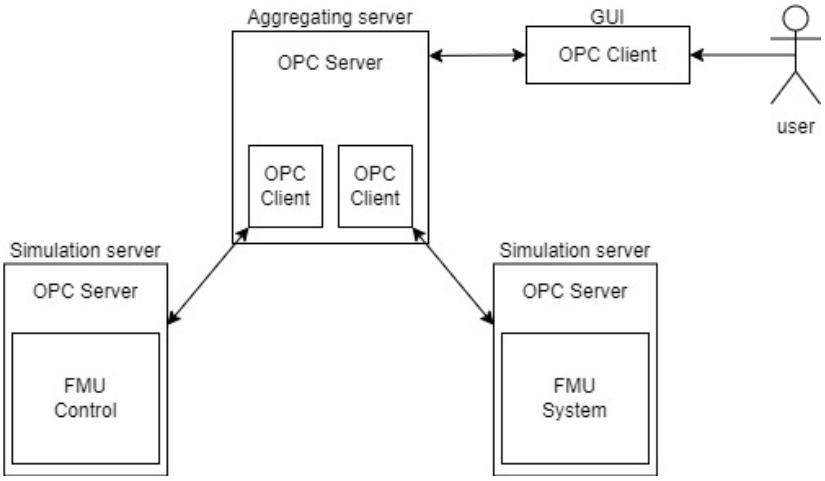

Fig 1. Proposed architecture of the co-simulation using FMI and OPC-UA.

Shipbuilding is a highly complex and multi-disciplinary process involving collaboration across various systems, applications, and organizations. The projects often include hundreds of system vendors and subcontracting companies, making the system simulation of entire ship systems a complex and challenging task. This complexity has contributed to the growing interest in co-simulation for ship prototyping and testing, which is discussed in a literature review conducted during this research on the system simulation of ship automation [1]. Co-simulation expands the possibilities for testing multiple ship systems concurrently and does not limit users to a single simulation platform. Additionally, the use of the Functional Mock-up Interface (FMI) as a model interface standard facilitates model exchange by allowing models to be treated as black boxes, thus preserving proprietary details while enabling integration. Therefore, the proposed architecture aims to promote these benefits by utilizing FMI and Open Platform Communications Unified Architecture (OPC-UA).

Figure 1 illustrates the proposed architectural demonstration, which is comprised of three key components: a User Interface (UI), an Aggregating Server, and two Simulation Servers. The UI serves as the front-end for user interaction, while the Aggregating Server manages and coordinates the data flow between the two Simulation Servers. The simulation servers model both the physical and control components of a lube oil cooling system. The lube oil temperature is controlled using a PI controller adjusting a control valve. Additional system inputs include engine load, mass flow rate, and the temperature of the cold circuit, all of which influence the behavior of the lube oil cooling process.

The communications between the simulation and the aggregating servers are done at one-second intervals, utilizing the OPC-UA protocol for all data exchanges. This communication framework enhances scalability since most of the off-the-shelf controllers and modeling software offer support for OPC-UA. This allows for the seamless addition of software and hardware components to the simulation and enables Hardware-In-the-Loop (HIL) and Software-In-the-Loop (SIL) simulations in the future.

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State and parameter estimation of Anaerobic digesters Based on the modified AMOCO model

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Biogas production through anaerobic digestion (AD) presents a promising renewable energy source with the potential to mitigate global warming. However, the inherently nonlinear nature of AD demands precise monitoring to maximize biogas yield while minimizing costs. The limited availability of affordable, accurate measurement systems for AD process variables, largely based on concentration metrics, necessitates the development of state and parameter estimators [1, 2]. Mathematical models are instrumental in this effort, as they clarify AD's complex biochemical and physicochemical mechanisms.

This study utilizes a modified version of the AMOCO (Advanced Monitoring and Control) model, originally developed for monitoring and control applications [3], which has been modified to align with experimental and simulated data for the design of a state estimator [4, 5]. State and parameter estimation is performed using a discrete Extended Kalman Filter (EKF). Although the modified AMOCO model is relatively simple, containing seven states and twenty parameters, sensitivity analysis within this study identified six key parameters for estimation, enhancing the estimator's robustness and accuracy.

To further enhance performance, particle swarm optimization (PSO) was applied to tune the state and measurement covariance matrices. Results demonstrate that the PSO - tuned EKF estimator accurately estimates all seven states and the selected parameters, offering an effective and economical approach to real - time AD process monitoring.

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The Simulation of Shipboard Microgrids: a practical approach

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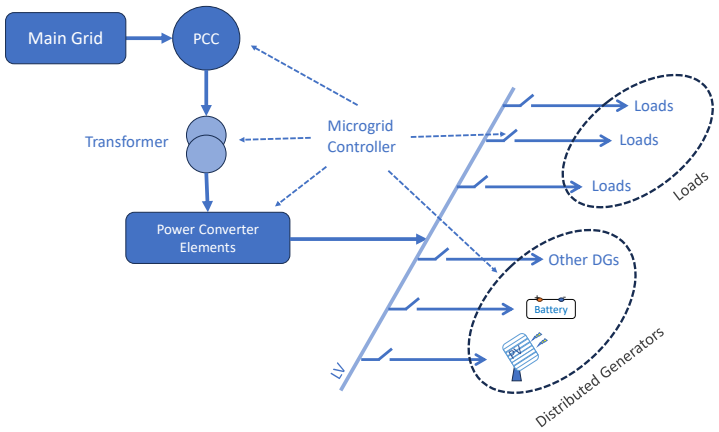

structure of a microgrid

The application of microgrids in electrical power systems has grown significantly in recent years. To increase the efficiency and reliability of ship power systems, the use of microgrid technology has become a fundamental goal in the maritime industry. A microgrid works in two different modes. In one mode, it is islanded and operates independently and in the other, it is connected to the main grid that allows for efficient energy management.

Microgrid control consists of three key components: primary, secondary, and tertiary control. Primary control is responsible for managing the local distributed generator (DG) to ensure that power output remains stable and within specified limits. The tertiary control regulates the power of the whole electrical system when DGs are connected to the main grid. The secondary control is responsible for adjusting and applying reference values for DGs in the absence of tertiary control, effectively returning them to their normal state when in islanded mode [1]. therefore, various methods have been investigated for system stabilization and power regulation, such as feedback linearization and model predictive control (MPC).

In this presentation, we aim to simulate a microgrid system in Open-DSS based on the data received from the Meyer, which is in the form of an Excel file. For this purpose, we will first convert the data in the form of Open-DSS commands, in part of which Matlab software will be used [2]. Then, by completing the Open-DSS program, we will obtain an approximate model using the data. (The model is not yet completed).

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Ultrasound Technology Based Plants Quality and Health Monitoring

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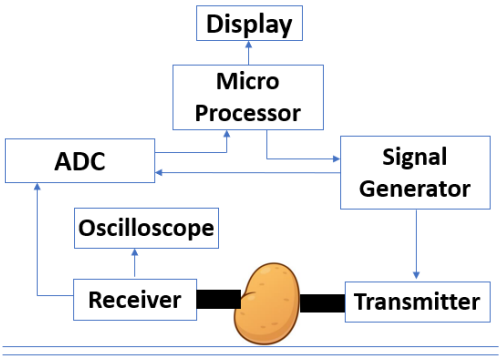

Schematic diagram for an ultrasound based plant part inspection and monitoring.

Ultrasound technology, perhaps best known for its application in biomedical imaging, has gained significant and widespread interest in wider applications in various fields including in agriculture technology particularly in food and plant health and quality monitoring. The increase of its popularity and its emergent as sustainable technology is also because it is also quite safe compared to other methods such as X-ray and other radiography-based technologies.

While some existing studies have shown the potentials of the technology to use for plant health and quality monitoring, no consistent results have been achieved as the existing results mostly rely on ad hoc approaches. Constructive and systematic framework to use these technologies for this application has not existed. Another challenge comes from the characters of plant materials that are different from other materials that are commonly evaluated using ultrasound, such as metal and concrete that are completely solid, or human or animal internal organs that are soft but dense. Plant materials are neither completely solid nor dense. While they have similar appearance to some internal biological organs, they are porous. Hence, they require non-trivial set-up, which is different from the well-known ultrasound non-destructive monitoring and testing applications, in terms of the type of transducers and the range of frequencies.

This research attempts to study methods for effective ultrasound transmission through plant materials and develop methods for ultrasound characterization of the plant materials, particularly the leaves, in which plant metabolism activities occur the most. Selection of transducers, range of frequencies and control of the positioning between the transducer and the specimens being monitored are studied. Some theoretical and experimental results will be presented and discussed, and ideas for further development will be shared.

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