Proceedings of
23rd Nordic Process Control Workshop

16 – 18 March 2022

Control Engineering Group
Department of Computer Science, Electrical and Space Engineering
Luleå University of Technology

Contents

About

The Nordic Process Control Workshop takes place every 18 months. The workshop aims to bring together leading academics, researchers, and industrialists from the Nordic countries to discuss recent advances in process control and its various domain applications. We also very much welcome contributions and participation beyond Nordic countries as well.

Nordic Process Control Working Group

he Nordic Process Control Working Group was founded in Stockholm on October 24, 1994. The group initiates activities 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". The Nordic Process Control Working Group also awards the Nordic Process Control Award to persons who have made a lasting and significant contribution to the field of process control.

Organizing committee

Wolfgang Birk, Luleå University of technology (Chair)
Johannes Jäschke, NTNU, Norway (Co-chair)
Gurkan Sin, DTU, Denmark
Elling W. Jacobsen, KTH, Sweden
Sigurd Skogestad, NTNU, Norway
Jeno Kovacs, Foster Wheeler Co., Finland
John Bagterp Jørgensen, DTU, Denmark
Jan Peter Axelsson, Vascaia, Sweden
Annika Leonard, Vattenfall, Sweden
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Bernt Lie, Telemark Univ. College, Norway
Tore Hägglund, Sweden
Torsten Wik, CTH, Sweden
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Morten Hovd, NTNU, Norway
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The Venue

The 23rd Nordic Process Control Workshop will take place at Luleå University of Technology (LTU). The Porsön Campus area is located 5 km from the center of Luleå. It can be conveniently reached from the airport in Luleå (Bus line 4) or from the city center (Bus lines 4, 5 or 6). You can find more information on how to find us and also some tips for your stay in Luleå in Chapter **Useful Information**.

Tutorial

A Building
A1547 (First Floor)
Campus Porsön
Luleå University of Technology
97187, Luleå

Conference

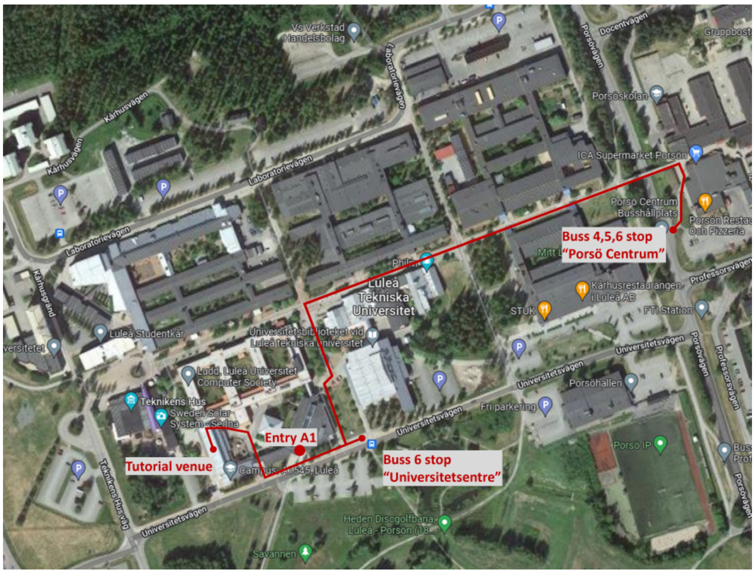
A Building
A117, LKAB salen (First Floor)
Campus Porsön
Luleå University of Technology
97187, Luleå

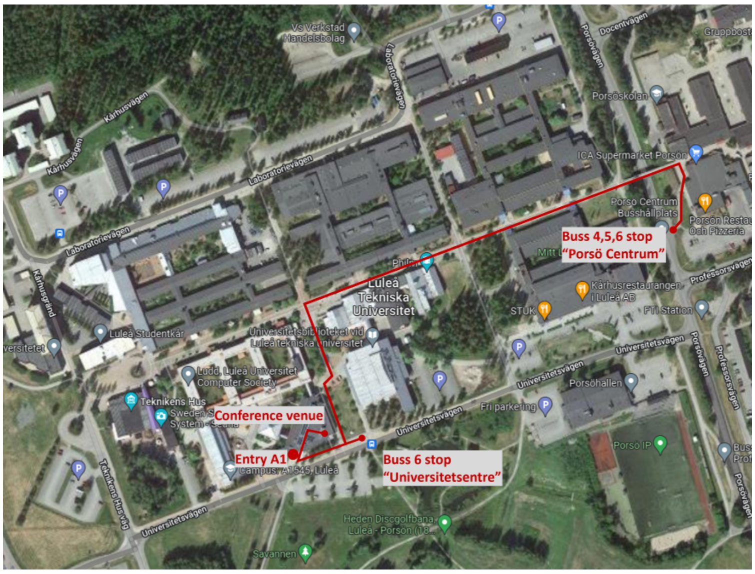
How to get to the 23rd NPCW?

The 23rd Nordic Process Control Workshop will take place at Luleå University of Technology (LTU). The Porsön Campus area is located 5 km from the center of Luleå. It can be conveniently reached from the airport in Luleå (Kallax) or the city center by public transport (Bus line 4, 5 and 6).

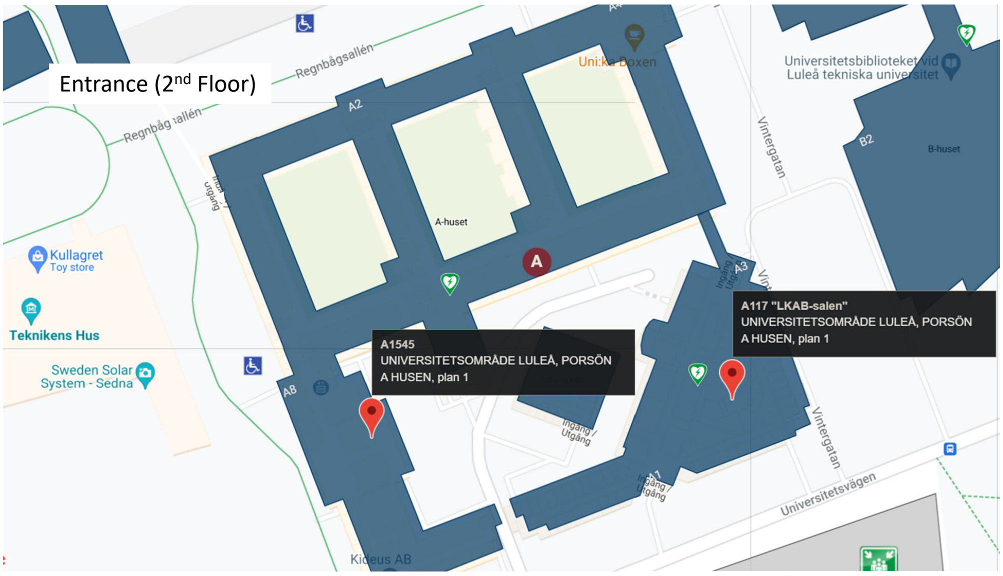
Bus line 4 goes directly to and from the airport.

- Bus: Take line 4, 5, or 6 from downtown "Smedjegatan". Go to either "Universitetsentré" or "Porsö centrum".
- Taxi: Go to "University" and ask for "entry A1" or "Bus stop Universitetsentré"
- Google maps link: https://goo.gl/maps/fbw4VYrqdvRXDUnf8
- Please have a look at the maps below.





Once you managed to enter the A building, you will find yourself in the second floor. The rooms reserved for the Tutorial (A1547) and Conference (A117, LKAB salen) are located in the first floor, and indicated in the building map below. So take a set of stairs down when you find one and try to follow the map!



Program

CT: Contributed Talk, IT: Invited Talk.

Wednesday, 16 March - Tutorial Day

Model generation for complex processes - in the context of simulation, control and monitoring

10:00–10:30	**Coffee/Tea**		
10:30–10:40	**Welcome and introduction**		
10:40–12:30	IT	**Roland Hostettler** UU	Introduction to Gaussian Processes
12:30–13:30	**Lunch**		
13:30–14:30	CT	**Khalid Atta** LTU	Optimization example using Gaussian Processes
14:30–15:30	CT	**Johan Simonsson** LTU	Automated Equation-Based Modeling and Simplification
15:30–16:00	**Coffee break**		
16:00–17:00	IT	**Peter Lingman** Optimation	Model development for control system design - a practical exampel from pulp and paper industry
17:00–17:30	**Discussion and reflections**		
17:30	**End of the Tutorial**		

Thursday, 17 March - Conference Day 1

08:00–08:30	**Coffee/Tea & Registration**		
08:30–08:35	**Opening ceremony, Wolfgang Birk**		
08:35–08:45	**Welcome address, Pär Weihed (Pro Vice-Chancellor, LTU)**		
08:45–08:55	**Nordic Process Control Award, Wolfgang Birk**		
08:55–09:40	IT	**Thomas F Edgar**	Awarde Seminar: Power Systems, Carbon Emissions, Smart Grids, and Process Control
09:40–10:00	**Short break**		
10:00–12:00	**Session 1: Control Theory**	**Chair: Andreas Johansson**	
10:00–10:20	Generalized Primal-dual Feedback-optimizing Control with Direct Constraint Control **Risvan Dirza, Sigurd Skogestad**		
10:20–10:40	Supervisory control for optimal operation under changing active constraints **Lucas Ferreira Bernardino, Dinesh Krishnamoorthy, Sigurd Skogestad**		
10:40–11:00	Adaptive Horizon Multistage NMPC: Stability and Recursive Feasibility **Zawadi Mdoe, Dinesh Krishnamoorthy, Johannes Jäschke**		
11:00–11:20	On Consensus of Positive Multi-Agent Systems **Amirreza Zaman, Wolfgang Birk, Khalid Tourkey Atta**		
11:20–11:40	Nonlinear input transformations for linearization, decoupling and feedforward control with application to compact steam generators **Sigurd Skogestad, Cristina Zotică, Rubén M. Montañés, Nicholas Alsop**		
11:40–12:00	Global sensitivity analysis using deep learning on industrially relevant large datasets – A case study of N2O emissions from WWTPs **Adem Rosenkvist Nielsen Aouichaouia, Gürkan Sin**		
12:00–13:00	**Lunch, Main restaurant, B-Building**		
13:00–15:00	**Session 2: Optimization**	**Chair: Andre Yamashita**	
13:00–13:20	A Study of Scenario Decomposition of Robust Model Predictive Control using Parametric Nonlinear Programming Sensitivities **Simen Bjorvand, Johannes Jäschke**		
13:20–13:40	Speed Optimization for Cruise Ships considering the Hotel Load **Axel Waris, Jari Böling, Mikael Manngård, Jerker Björkqvist, Janne Huotari, Teemu Manderbacka, Mathias Pirttikangas, Wilhelm Gustafsson**		
13:40–14:00	Optimizing thermal power production in district heating and cooling systems considering flexibility **Maryam Razi, Khalid Tourkey Atta, Wolfgang Birk**		
14:00–14:20	What GEA learned from 10 years with Advanced Process Control (APC) **Lars Norbert Petersen, Signe Munch, Christer Utzen**		
14:20–14:40	Neural network control policies for uncertain systems **Evren M. Turan, Johannes Jäschke**		
14:40–15:00	Control and Optimization of Nitric Acid plants **Knut Wiig Mathisen, Bjørn Glemmestad**		
15:00–15:30	**Coffee/Tea**		

15:30–17:30	**Session 3: Posters**	**Chair: N/A**
	Which surrogate models to use? – Benchmarking of Superstructure Optimization Approaches for Process Design **Nikolaus I. Vollmer, Gürkan Sin**	
	Digitalization of Pilot Plant Facilities to Develop Methods and Tools that Improve Data Utilization in Chemical- and Biochemical Processes **Mads Stevnsborg, Peter Jul-Rasmussen, Yuanmeng Duan, Jakob Kjøbsted Huusom**	
	Model Predictive Control for Zero-emission Industrial Processes **Zhanhao Zhang, Steen Hørsholt, John B. Jørgensen**	
	Process Simulation and Optimization of NH3/CO2 separation with ionic liquids **Yuanmeng Duan, Jens Abildskov, Jakob Kjøbsted Huusom, Xiangping Zhang**	
	Nonlinear State Estimation for the Modified Four-Tank System **Marcus Krogh Nielsen, John Bagterp Jørgensen**	
	Bayesian analysis of the physics-based process models: A case study on multiphase pipe flow **Md Rizwan, Christian Holden, Johannes Jäschke**	
	A Dual-hormone Artificial Pancreas based on Nonlinear Model Predictive Control and Maximum Likelihood Estimation **Asbjørn Thode Reenberg, Tobias K. S. Ritschel, Emilie B. Lindkvist, Christian Laugesen, Ajenthen G. Ranjan, Jannet Svensson, Kirsten Nørgaard, John Bagterp Jørgensen**	
	Hybrid modelling of industrial scale fermentation process **Atli Freyr Magnússon, Stuart M Stocks,Gürkan Sin, Jari Pajander**	
	Interpretation of responses to bolus-feeding during CHO-fedbatch cultivation using an extended bottleneck model and simulations with Bioprocess Library for Modelica **Jan Peter Axelsson**	
	Fast Charging Control of Li-Ion Batteries: Effects of Input, Model, and Parameter Uncertainties **Yao Cai, Changfu Zou, Yang Li, Torsten Wik**	
	A tuning strategy for advanced control of grinding circuits based on multiobjective optimization **Andre S. Yamashita, Wellington T. Martins, Thomás V. B. Pinto, Thiago A.M. Euzébio**	
	Electrochemical Model-Based Fast Charging for Lithium-Ion Batteries: Physical Constraint-Triggered PI Control **Yang Li, Evelina Wikner, Torbjörn Thiringer, Torsten Wik, Changfu Zou**	
	Approximations to the solution of the Kushner-Stratonovich equation for the stochastic chemostat **Augusto Magalhães, Muhammad Fuady Emzir, Francesco Corona**	
	Forward sensitivity analysis of a supercritical extraction process **Oliwer Sliczniuk, Pekka Oinas, Francesco Corona**	
17:30–18:00	**Bus to Gammelstad Churchtown**	
18:00–19:00	**Guided tour to Churchtown**	
19:00–22:30	**Banquet, Kaptensgården, Churchtown Gammelstad**	
22:30	**Bus back to central Luleå**	

Friday, 18 March - Conference Day 2

08:15–08:20	**Opening Day 2, Wolfgang Birk**	
08:20–10:00	**Session 4: Bioprocesses**	**Chair: Gürkan Sin**
08:20–08:40	Optimal Control of Water Quality in a Recirculating Aquaculture System **Allyne M. dos Santos, Sigurd Skogestad, Kari J.K. Attramadal**	
08:40–09:00	Microalgae production systems: modelling and control issues **José Luis Guzmán, Manuel Berenguel, Francisco Gabriel Acién**	
09:00–09:20	Designing control models of fed-batch bioreactors based on dFBA using interior-point solvers **Caroline S. M. Nakama, Johannes Jäschke**	
09:20–09:40	Closing the loop: Online model predictive control strategy with real-time monitoring of experimental bioreactors **Pedro A. Lira-Parada, Andrea Tuveri, Che Fai Alex Wong, Christopher Sørmo, Nadav Bar**	
09:40–10:00	Bioprocess Monitoring: A Moving Horizon Estimation Experimental Application **Andrea Tuveri, Haakon Eng Holck, Caroline S.M. Nakama, Jose' Matias, Johannes Jaschke, Lars Imsland, Nadav Bar**	
10:00–10:20	**Coffee/Tea**	
10:20–12:00	**Session 5: General processes**	**Chair: Amirreza Zaman**
10:20–10:40	Optimal Control of a Smart House using MPC-based Reinforcement Learning* **David Pérez-Piñeiro, Sebastien Gros, Sigurd Skogestad**	
10:40–11:00	Closed-Loop Treatment as a Diagnostic Tool in Type 2 Diabetes **Sarah Ellinor Engell, Tinna Björk Aradóttir, Henrik Bengtsson, John Bagterp Jørgensen**	
11:00–11:20	A receding-horizon framework for optimal control and estimation of a common class of activated sludge plants **Otacilio B.L. Neto, Michela Mulas, Francesco Corona**	
11:20–11:40	Modelling and Optimization of large-scale alkaline CO_2 electrolysis systems **Lucas Cammann, Isabell Bagemihl, Mar Pérez-Fortes, J. Ruud van Ommen, Volkert van Steijn**	
11:40–12:00	Automated modeling and simulation of district energy systems **Johan Simonsson, Wolfgang Birk, Khalid Atta**	
12:00–13:00	**Lunch, Main restaurant, B-Building**	
13:00–14:20	**Session 6: Estimation and Control**	**Chair: Fransesco Corona**
13:00–13:20	Why tuning rules for feedforward control are required **José Luis Guzmán, Tore Hägglund**	
13:20–13:40	A simple and efficient PID control loop decoupler **Tore Hägglund**	
13:40–14:00	Adaptive Tuning of Nonlinear Kalman Filters **Halvor Aarnes Krog, Johannes Jäschke**	
14:00–14:20	Robust Active Set Identification for Mathematical Programs with Complementarity Constraints **Peter Maxwell, Johannes Jäschke**	
14:20–14:30	**Next NPCW, Johannes Jäschke**	
14:30–14:40	**Closing ceremony, Wolfgang Birk**	

Nordic Process Control Award

Thomas F. Edgar

The Nordic Process Control Award is given to outstanding process control professionals who have made a lasting and significant contribution to the field of process control.

Thomas F. Edgar is the George T. and Gladys H. Abell Chair Emeritus in Chemical Engineering at the University of Texas at Austin and former Director of the UT Energy Institute. For nearly 50 years, Edgar has concentrated his academic work in process modeling, control, and optimization, and has published over 500 articles and book chapters in the above fields applied to separations, chemical reactors, energy systems, and semiconductor manufacturing. His research has focused on control theory and computation for nonlinear and large-scale systems where he has supervised more than 80 Ph.D. students.

Edgar has co-authored two leading textbooks: Optimization of Chemical Processes (McGraw-Hill, 1988 and 2001) and Process Dynamics and Control, 4th ed. (Wiley, 2016) with Dale Seborg, Duncan Mellichamp, and Frank Doyle. Tom Edgar was co-founder of the Smart Manufacturing Leadership Coalition (SMLC; https://smart-process-manufacturing.ucla.edu/), which develops software tools for saving energy in industrial plants.

Abstract, Awardee seminar

Power Systems, Carbon Emissions, Smart Grids, and Process Control

Thomas F. Edgar

The University of Texas at Austin

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Trends in power production are discussed and economic driving forces in the decarbonization of the grid are highlighted both for the U.S. and Europe. Automation, process control, and real-time optimization are critical technologies to operate power plants in the most efficient way. The increased use of intermittent renewable energy sources such as solar or wind power reduces carbon usage but adds a dynamic element to power production. Time of day pricing of power and use of demand response techniques to flatten demand curves will be important ingredients of smart grids. Increased usage of thermal and other energy storage systems along with automatic control can give large energy users degrees of freedom to deal with dynamic power conditions and improve energy efficiency and sustainability.

List of Awardees

1. Howard H. Rosenbrock (UK) (Aaland, Finland, August 1995)
2. Karl Johan Åstrøm (Sweden) (Wadahl, Norway, January 1997)
3. F. Greg Shinskey (USA) (Skeviks Gård, Stockholm, 24 August 1998)
4. Jens G. Balchen (Norway) (Lyngby, Denmark, 14 Jan. 2000)
5. Charles R. Cutler (USA) (Åbo, Finland, 23 Aug. 2001)
6. Roger W. Sargent (UK) (Trondheim, Norway, 09 Jan. 2003)
7. Ernst Dieter Gilles (Germany) (Gothenburg, Sweden, 19 Aug. 2004)
8. Manfred Morari (ETH, Switzerland) (Lyngby, Denmark, 26 Jan. 2006)
9. Jacques Richalet (France) (Espoo, Finland, 23. Aug. 2007)
10. John MacGregor (Canada) (Porsgrunn, Norway, 29 Jan. 2009)
11. Graham Goodwin (Australia) (Lund, Sweden, 26 Aug. 2010)
12. Lawrence ("Larry") T. Biegler (USA) (Lyngby, Denmark, 26 Jan. 2012)
13. James B. Rawlings (USA) (Oulu, Finland, 22 Aug. 2013)
14. Rudolf Kalman (ETH, Switzerland) (Trondheim, 15 Jan. 2015)
15. Wolfgang Marquardt (Germany) (Sigtuna, Stockholm, 25 Aug. 2016)
16. Dale Seborg (USA) (Turku (Åbo), Finland, 18 Jan. 2018)
17. Nina Thornhill (UK) (DTU, Lyngby, Denmark, 22 Aug. 2019)
18. Thomas F. Edgar (USA) (LTU, Luleå, Sweden, 13 Jan. 2022)

Session 1: Control Theory

Generalized Primal-dual Feedback-optimizing Control with Direct Constraint Control

***Risvan Dirza**, Sigurd Skogestad*

Dept. of Chemical Engineering, Norwegian Univ. of Science Technology (NTNU), NO-7491, Trondheim, Norway

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This work proposes a strategy to track steady-state changes in active constraints and minimize dynamic constraint violations in order to achieve system-wide optimal operation of coordinated oil and gas production systems using simple feedback control structures and logic blocks. One possible approach is the reduced gradient approach or region-based control. This method is easy to implement for a simple case with a few regions. Moreover, this method enables tight active constraint control. However, this method can be problematic for a complex and large case as the number of the region increases. Alternatively, we can use the recently proposed primal-dual feedback-optimizing control scheme. This scheme consists of local gradient and central constraint controllers. The local gradient controller is responsible for controlling the the gradient of Lagrange function w.r.t the physical input (primal variables) to 0 in order to satisfy KKT stationary condition by manipulating the physical input. The gradient is a function of Lagrange multipliers that are the manipulated variables (dual variables) for the central constraint controller. Thus, the central constraint controller is responsible for controlling the constraint in a slow time scale by manipulating the Lagrange multipliers. When the constraint is not active, we introduce a selector to assign 0 for the Lagrange multipliers. This strategy ensures KKT dual feasibility and KKT complementary slackness conditions, and thus, this scheme can optimally handle steady-state changes in active constraints. However, controlling the constraint in a slow time scale may lead to dynamic constraint violations during the transient. To minimize these constraint violations, we need to provide direct access to control the active constraint tightly. Thus, we propose an improved primal-dual scheme with explicit control of hard constraints. We show that this improved scheme can reduce profit loss in the long run by allowing for smaller back-off from hard constraints. To assist the designer in determining the pairing between the primal variables and the constraint, we can use systematic pairing selection for economic-oriented constraint control. To overcome input saturation issues, we generalize the improved scheme by introducing multiple input direct constraint control. To conclude, our proposed method or scheme is both flexible in handling steady-state changes in active constraints and able to control the active constraint tightly.

Supervisory control for optimal operation under changing active constraints

Lucas Ferreira Bernardino[1], ***Dinesh Krishnamoorthy***[1], ***Sigurd Skogestad***[1]

[1]Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway

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In the context of optimal operation, it is well-known that active constraint control has a fundamental role. Active constraints are usually tied to quality specifications or other key process variables, and therefore infeasible operation leads to huge economic losses. In addition, avoiding constraint violation through the use of a big back-off also leads to considerable economic losses, as the loss has a linear relationship with the implementation error in the constraint value. The implementation error in the unconstrained degrees of freedom, on the other hand, has a quadratic influence on the economic loss, and is therefore less relevant so long the operation is kept in the proximity of the optimum. This has motivated approaches of supervisory control layer design that take the unconstrained degrees of freedom into account, as the implementation error from approximating the cost gradient by measurements becomes almost negligible in terms of loss. These approaches fall under the umbrella of self-optimizing control.

The field of self-optimizing control has been very successful in designing procedures for optimal operation, given that the set of active constraints is known beforehand. In principle, when the active constraints change, the whole control structure should change to accommodate the new controlled variables. However, in simple systems, active constraint changes can be dealt with through the use of logic control elements, such as selectors and split-range blocks, given that an analysis of all possible regions is performed during design. In addition, one may think of adaptive control structures based on the direct tracking of optimality conditions. Here, motivated by a case study with constraints that need to be dealt with during operation, we discuss the implementation of such types of control structures for optimal operation.

The considered case study is a heat exchanger network, consisting of three exchangers in parallel with different hot fluid supplies, and the goal is maximizing the outlet temperature of the cold fluid, by manipulating the split valves that dictate the fraction of cold fluid that goes in each exchanger. We further consider that each exchanger is subject to a constraint of maximum allowed temperature of the cold fluid. In this system, with two manipulated variables and three constraints, it was impossible to devise a control structure solely based on simple selectors, as the constraints may become active independently, and thus an adaptive pairing strategy was required. We propose then a primal-dual feedback optimizing control structure, that consists of two layers. The first layer deals with the constraints, generating estimated Lagrange multipliers. The second one takes the estimated Lagrange multipliers and plant gradients to generate control variables that are equivalent to directly tracking the optimality conditions. The proposed control structure allows for optimal operation in all possible active constraint regions. There are, however, limitations to it mainly regarding the timescale separation between layers, making the convergence fundamentally slower than a traditional region-based approach.

Adaptive Horizon Multistage NMPC: Stability and Recursive Feasibility

Zawadi Mdoe [1], ***Dinesh Krishnamoorthy*** [1], ***Johannes Jäschke*** [1]

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This work presents a computationally efficient and robust model predictive controller (MPC). Our goal is to reduce the computational cost of the multistage MPC by performing an online adaptation of the prediction horizon. The multistage MPC problem is a stochastic program that optimizes over several likely scenarios in the prediction horizon determined by a scenario tree. The resulting optimization problem has large size with high complexity causing computational delay which is undesirable for online implementation. Most systems are nonlinear, and the use of a nonlinear model forms a nonlinear MPC (NMPC) problem that has further increased complexity and the computational delay. However, the multistage NMPC problem is a nonlinear program (NLP) parametric in the initial state, so we can estimate a sufficient prediction horizon for the subsequent MPC iteration using NLP sensitivities. Usually, a system is controlled to a setpoint that is eventually approached with time. Therefore, as the system progresses the adaptive horizon algorithm reduces the prediction horizon resulting into a smaller NLP problem size. The online prediction horizon update is expected to reduce the computational delay especially when the system is closer to the setpoint.

First, we combine the adaptive horizon algorithm with multistage MPC by determining a terminal region around an optimal equilibrium point for each uncertainty realization, and a terminal cost for the quasi-infinite horizon multistage NMPC. Then using parametric NLP sensitivities, we estimate the multistage NMPC solution at the next iteration, and from that determine the sufficient prediction horizon at which all trajectories for all scenarios enter their respective terminal regions.

Secondly, under some specific conditions we show that the controller is recursively feasible and robustly stable using the input-to-state practical stability (ISpS) framework. Therefore, our controller retains the stability and recursive feasibility properties of the multistage NMPC as desired.

Lastly, we demonstrate the performance of this controller by comparing it with the original multistage NMPC using two numerical examples. One is the control of a jacket-cooled continuously stirred tank reactor (CSTR) and the other is level control of a four-tank system. In both cases, it is evident that the controller is more computationally efficient (fast solve times per iteration) and as robust as the original multistage NMPC.

On Consensus of Positive Multi-Agent Systems

Amirreza Zaman[1]**, *Wolfgang Birk***[1]**, *Khalid Tourkey Atta***[1]

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The distributed cooperative control approach of multi-agent systems (MASs) has been investigated previously in many cases. These systems are applicable in control, sensing, communication network technologies, and district heating and cooling networks. Other substantial perspectives of analyzing distributed MASs are using consensus or synchronization control problems in recent years since most of the coordination control problems can be stated into consensus problems. Besides, by considering the physical features of technical systems such as nonlinearity, actuation, and model uncertainties, the latest consensus studies have been developed based on these physical factors to improve the networks' performance.

Positive MASs are introduced when the state variables in MASs remain non-negative. Recently, positive MASs have been remarkably gained attention to the study, including

- Solving the containment control problem of MASs by applying positive systems' fundamentals under heterogeneous and unbounded communication delays.
- Developing the positive edge-consensus approach for nodal networks by employing output feedback schemes.
- Studying the discrete-time positive edge-consensus for both directed and undirected nodal networks for simple and complex networks.

Another interesting application of positive MASs is in providing smart control strategies for distributed energy management networks or investigating smart homes' flexible energy systems. Besides, since in complex networks, using pinning control only requires applying controllers on a small fraction of the nodes, the pinning control strategy has an advantage over other techniques.

This presentation introduces the distributed pinning consensus solution for directed nonlinear positive MASs with nonlinear control input, including observer-based control protocols. The network topology is considered as a directed and fully connected structure. By considering sector input nonlinearities and various forms of topologies, two kinds of state observers involving standard observer and distributed pinning observer are presented for each regarded nonlinear agent by applying a novel analysis directly dealing with the nonlinear input and nonlinear system dynamics. The measured local output detail outlines the first observer, and the other observer is achieved via the corresponding output detail of its adjacent agents.

Acknowledgements

Funding received from the Horizon 2020 Research Programme of the European Commission under the grant number 956059 (ECO-Qube) is hereby gratefully acknowledged.

Nonlinear input transformations for linearization, decoupling and feedforward control with application to compact steam generators

[1] ***Sigurd Skogestad***, [1,2] ***Cristina Zotică***, [2]***Rubén M. Montañés***, [3]***Nicholas Alsop***

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3 Senior Process Control Engineer, Borealis AB, Stenungsund, Sweden
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This work introduces very powerful nonlinear input transformations which transform a nonlinear process with relative order at most 1 (the input u directly affects the output y or $\frac{dy}{dt}$) into a system that is linear, decoupled and independent of disturbances both at steady state and dynamically. For systems with relative order higher than 1, we introduce cascade control which gives similar performance, although perfect disturbance rejection cannot be achieved because of fundamental control limitations. We also introduce static transformations, which makes the transformed system linear, decoupled and independent of disturbances at steady state, and for systems that are linear in the output (y) also give perfect disturbance rejection dynamically. The transformations have some relationship to the nonlinear control method of "feedback linearization", but we emphasize their nonlinear feedforward properties related to disturbance rejection and decoupling. All disturbances and states that directly affect y or $\frac{dy}{dt}$ are assumed to be measured. This may seem restrictive, but it actually holds for many process systems. In hindsight, most of the results in this work seem trivial, especially since it can result in ratio, cascade or nonlinear feedforward control which are frequently used in the industry. Nevertheless, a systematic theory for deriving these nonlinear control strategies is lacking in the open literature. As an example, we apply the proposed method to control the temperature of steam generated in a compact heat-exchanger which recovers waste-heat from a source with high variability.

Global sensitivity analysis using deep learning on industrially relevant large datasets – A case study of N2O emissions from WWTPs

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Global sensitivity analysis (GSA) is now playing an increasingly prominent role in the development and assessment of complex simulation models. Among its other uses, GSA is widely employed to generate insights into the contributions of individual model inputs, or sub-groups of inputs, to the variations in the output of a mechanistic model (Saltelli et al., 2019). However, when such models fall short of explaining a particular process phenomenon, sensitivity indices derived from these models become unreliable. One good example is nitrous-oxide emissions (N2O) from wastewater treatment plants (WWTP), for which the mechanistic understanding is still in its infancy(Daelman et al., 2015;Sin and Al., 2021). The recent breakthroughs achieved in deep learning (DL), on the other hand, offer an exciting possibility to bring new light to such poorly understood process phenomena. To this end, here we present a new software tool, named deepGSA, incorporating well-established variance-decomposition-based global sensitivity analysis methods, such as Sobol sensitivity indices, with the plant data-driven deep learning modeling techniques.

The deepGSA aims at enabling non-specialist practitioners to leverage DL-based models for GSA application purposes. To this end, the tool builds on an earlier GSA framework of the authors, easyGSA (Al et al., 2019), and is based on a recently proposed framework for DL-based and big data-driven process modeling (Hwangbo et al., 2020). By using these two frameworks, the deepGSA streamlines a number of tasks into a deep learning pipeline, such as data cleaning and preparation, model building and discrimination, model validation, Monte Carlo simulations, Sobol sensitivity analysis, Derivate-based global sensitivity analysis and effective visualizations of GSA results. The capabilities of the tool are highlighted with a case study from WWTPs concerning study of nitrogendioxide (N2O) emissions which is a potent greenhouse gas. In this project we have performed a monitoring campaign for measuring, quantifying and analysing N2O emissions at Ornum plant (Kalundborg, Denmark) for 6 months long from March until September 2021. The monitoring campaign showed that the N2O emission factor –defined as the ratio of N2O emitted from the plant over the total influent nitrogen load to the plant, is 0.06% on average. This emission factor is quite low compared with the threshold considered in IPCC 2019 report (1.6%) or Danish environmental agency recom-mendation of 0.32%. This finding is robust against a huge uncertainty (two sigma deviation in estimated value) in the estimation of mass transfer coefficient for N2O (that gives a 95% confidence level assuming the estimators are normally distributed).

A deep learning model is then trained successfully using the deepGSA tool, which provided a training R2 of 0.81, which is comparable to N2O models reported in literature. The model is deemed qual-itative and sufficiently well to perform sensitivity analysis. A global sensitivity analysis using Sobol sensitivity method is conducted with this model. The model indicated that the most important factor is dissolved oxygen, which explains by itself 40% of the variation in the liquid N2O concentration. The results also showed that all other inputs namely temperature, NH4, nitrate and influent flowrate were also important but mainly through their interaction effects. All these inputs are relevant and important to monitor to study N2O dynamics in the plant. Regarding understanding this low N2O emissions, some empirical observations of the plant design and operation e.g. high COD/N ratio, a good aeration regime (not limited by aeration with DO setpoint around 1 mg/L) which may explain low N2O emission. However a better understanding of the underlying biological processes and their interactions with process operating conditions and environment will require a focused multidisciplinary work across microbial community analysis and process engineering/first principles modeling among others.

References

[1] Al, R., Behera, C.R., Zubov, A., Gernaey, K. V., Sin, G., 2019. Meta-modeling based efficient global sensitivity analysis for wastewater treatment plants – An application to the BSM2 model. Comput. Chem. Eng. 127, 233–246. https://doi.org/10.1016/j.compchemeng.2019.05.015

[2] Chen, X., Mielczarek, A.T., Habicht, K., Andersen, M.H., Thornberg, D., Sin, G., 2019. Assessment of Full-Scale N 2 O Emission Characteristics and Testing of Control Concepts in an Activated Sludge Wastewater Treatment Plant with Alternating Aerobic and Anoxic Phases. Environ. Sci. Technol. 53, 12485–12494. https://doi.org/10.1021/acs.est.9b04889

[3] Daelman, M.R.J., van Voorthuizen, E.M., van Dongen, U.G.J.M., Volcke, E.I.P., van Loosdrecht, M.C.M., 2015. Seasonal and diurnal variability of N 2 O emissions from a full-scale municipal wastewater treatment plant. Sci. Total Environ. 536, 1–11. https://doi.org/10.1016/j.scitotenv.2015.06.122

[4] Hwangbo, S., Al, R., Sin, G., 2020. An integrated framework for plant data-driven process modeling using deep-learning with Monte-Carlo simulations. Comput. Chem. Eng. 143, 107071. https://doi.org/10.1016/j.compchemeng.2020.107071

[5] Saltelli, A., Aleksankina, K., Becker, W., Fennell, P., Ferretti, F., Holst, N., Li, S., Wu, Q., 2019. Why so many published sensitivity analyses are false: A systematic review of sensitivity analysis practices. Environ. Model. Softw. 114, 29–39. https://doi.org/10.1016/j.envsoft.2019.01.012

[6] Sin, G., Al, R. (2021). Activated sludge models at the crossroad of artificial intelligence—A perspective on advancing process modeling. npj Clean Water, 4(1), 1-7.

Session 2: Optimization and control

A Study of Scenario Decomposition of Robust Model Predictive Control using Parametric Nonlinear Programming Sensitivities

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In this work we address efficient computational schemes for robust scenario-based nonlinear model predictive control. In scenario-based nonlinear model predictive control the realizations of uncertainty is represented by a scenario tree, where the size of the tree grows exponentially with the amount of uncertainties considered, so efficient methods of to compute it is necessary. Primal decomposition is considered, where the full problem is split into several sub-problems coupled by the non-anticipativity constraints with a master algorithm coordinating the different sub-problems. The computational trade-off between solving the different sub-problems and solving the master algorithm is compared for different schemes of decomposing the full problem. The schemes being considered are decomposing the problem into individual scenarios or bundles of several scenarios. In addition to considering primal decomposition, the possibility of using fast nlp sensitivity updates to further speed up computations is studied. The decomposed problems are parametric NLPs, so parametric programming techniques can be used. These techniques are only computationally efficient for problems with certain conditions. We study if these conditions are meet for a quad-tank case study.

Speed Optimization for Cruise Ships considering the Hotel Load

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The maritime industry strives to greatly reduce emissions, and efficient energy management as well as improved route planning is essential in this objective. On cruise ships, the hotel load is a significant part of the total power consumption. We present a model for estimation of the hotel load on a cruise ship with a diesel-electric propulsion system. The model is based on real-world historical data from a cruise ship sailing in the Caribbean and the Mediterranean. The electric energy consumption on different systems was analyzed and grouped into propulsion, hotel, and auxiliary systems. The aim is to achieve fuel savings through more efficient voyage optimization. With the different power consumers accurately predicted, an optimal route and speed profile can be planned, in which the engines can run at optimal load levels. A dynamic programming approach was taken for speed profile optimization in varying environmental conditions, but with a fixed route and a fixed arrival time. Instead of running the ship at constant speed, the route is divided into smaller parts with different (but constant) cruise speeds. This allows for optimization of the speed profile using a dynamic programming approach, by taking into account both the changing environmental conditions, and the predicted energy consumption profile on board the ship. This serves as a first investigation of whether a full route optimization might gain from considering the energy consumption profile on board cruise ships. Furthermore, it is also taken into account that the ship uses multiple engines, with efficiency varying with the load, so the starting and stopping of engines also introduces a degree of freedom that is utilized in the optimization.

Optimizing thermal power production in district heating and cooling systems considering flexibility

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This work presents thermal power optimization in a district heating and cooling system (DHCS) considering flexibility in the grid. We formulate an optimization problem to minimize power production cost while taking account of the electricity market's income and flexibility. Time delay of temperature change in pipelines and thermal energy storages (TESs) are considered as flexibility in the system. The problem is stated in a model predictive control (MPC) framework as a mixed-integer linear program (MILP). It is subject to constraints on models of the pipelines, heat exchangers, buildings, and TESs, and provision of demanded thermal power on heating and cooling sides of DHCS. There are limitations on thermal power produced by generation units, including combined heat and power (CHP) plants and boilers on the heating side and chillers on the cooling side, electricity production by CHPs, and their heat to power ratio too. Furthermore, ramp-up and ramp-down limits on thermal power and electrical power and the minimum duration of time for which every unit must be kept on and off are considered in the problem.

To verify the optimization, the district heating system (DHS) in Luleå is used as a test case. A simulator replicates all three main parts as a combination of physics-based models, machine learning models (black box), namely the generation, the distribution, and the consumer side (end users). Since the city is geographically quite large, several generation units are distributed over the city and connected to the same thermal grid. The scenario for the test case is the simulation of the optimization problem and usage of the storage tank on some cold winter days when the outdoor temperature falls rapidly. Because the flow rate of the medium in the pipes is not constant, the transport time delay on the DHCS is variable. Measuring the flow in a large number of pipelines at every instant is impossible, and for DHS in Luleå, it is only measured in some pipes near the generation units. Moreover, estimating flow in all pipes using a model is not realistic. Then, at every time instance, an average time delay is calculated. The future delay is estimated as the mean value of the samples of flows in the last instant. Some controllers control the pressure of the medium supplied by pumps in DHS in Luleå. Therefore, the optimization problem is not subject to the models of the pipelines and heat exchangers. Moreover, the model of the buildings is not considered in the simulation.

The optimization problem is solved at every time instant using Matlab, and the optimal on/off state of the generation units and optimal power produced by them are obtained. Simulation results are compared to a case without optimization and the TES. The results show that the production cost decreases considerably using optimization and considering flexibility.

What GEA learned from 10 years with Advanced Process Control (APC)

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It is now 10 years ago that GEA started its endeavors into APC with a master's student project in collaboration with DTU. So, what have we learned and how did we respond to that? The benefits of APC are clear in almost all cases in the process industry. The software can increase throughput, and quality as well as reduce energy consumption. It may even reduce the efforts for the operators of the processes. The business case is therefore easy to build with short payback time. Yet, we found that the long-term business case did not hold because shortly after commissioning customers stopped using our APC solution. The APC solution did not stay up to date as the plant did mechanically, IT security changed, staff changed, and the technology also evolved all the time. To be successful over time we had to aim for a solution that was performing as well year-on-year as at the time of installation. To deliver that, we had to revise both the technology and the business model.

In the engine room of the APC we changed our models to so-called grey-box models that have built-in physics behind the process that we control. Therefore we can do model training and retraining in a much more efficient way using less data while obtaining a higher model quality. To incorporate that in our software we also developed the APC solution in-house with DTU doing PhD projects. Also, the usability of the user-interface for the operator was improved considerably compared to our old solution. We wanted to make a UI that was intuitive and focused on what the operator needed and want to know about the process – instead of aiming at a commissioning engineer. Last but not least we had to connect the APC to the cloud in order to have APC experts review the data from the site and make suggestions and actions related to modelling, upgrades etc. in a pro-active manner.

Neural network control policies for uncertain systems

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Nonlinear model predictive control (NMPC) problems that explicitly consider uncertainty, e.g. multi-stage NMPC, are difficult to solve in real-time due to their large computational cost. An alternative to solving these problems online is to use a surrogate which approximates the solution of the NMPC problem. Use of a surrogate shifts the computational load offline, allowing one to simply evaluate a function online. As neural networks are universal approximators they are commonly used as surrogates. Training the network in an imitation learning approach would require computing a dataset of solutions of the NMPC problem at many points in the state space. This dataset can be very costly to generate, as it should fully describe the system behaviour and cover the state space.

In this work, we consider NMPC problems with uncertainty in the parameters and/or initial state. We parametrize the control policy by a neural network, and optimise this network in a single shooting approach, using the NMPC objective and constraints. This means we do not have to form a dataset of MPC solutions. We use a Koopman operator approach to evaluate the expectations, arising due to uncertainty, at a desired tolerance. Three problems are used to demonstrate the proposed method. The optimised neural network controllers can be evaluated within 4 microsecond (on average), and shows good performance.

Control and Optimization of Nitric Acid plants

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Yara International ASA produces fertilizers for agriculture and industrial products for e.g., emission reduction. With total product deliveries of 38 million tons, Yara is one of the largest fertilizer companies in the world. Yara has developed various fertilizer processes and holds several patents related to nitric acid production, which is a key intermediate in fertilizer production. Nitric acid plants emit the climate gas N2O and agricultural N2O represent about 4% of global human-caused climate-warming emissions. This paper presents two nitric acid plant APC projects, one in Glomfjord, Norway and one in Köping, Sweden. Degrees of freedom for operation analysis and the main control and optimization objectives are outlined. It is explained how the overall project success depends on regulatory control, local organizational anchoring and a skilled project organization in addition to the APC controller itself. Modelling and understanding the key issues and trade-offs related to main reactors, columns and compressors are important. Benefits are linked to better ratio control of main inputs and optimization of pressure and temperature profiles, and are achieved through variability reduction, identification of active constraints and constraint pushing. Positive effect on throughput, energy efficiency and emissions have been achieved. Monetary value depends on plant operating mode, maximum throughput operation typically has higher value than maximum efficiency operation. However, with quickly increasing climate gas emissions tax, maximum efficiency operation becomes more attractive. How to integrate a standard APC solution with non-linear, plant wide optimization is discussed, and the potential additional benefits are estimated.

Finally the impact of Industry 4.0 and cloud solutions are discussed. Yara's digital production platform, currently in development with partner Amazon Web Services, will be the home for advanced analytics and other applications residing in the cloud. The possible success of these future tools depends on closed-loop identification and that historical plant data have the required excitation for identification.

Session 3: Posters

Which surrogate models to use? – Benchmarking of Superstructure Optimization Approaches for Process Design

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Surrogate modelling is highly popular in process systems engineering. One of the application are in the conceptual process design of biorefineries. Here Superstructure Optimization (SSO) approaches are typically employed to identify optimal process topology. These approaches are inherently limited by the initial search space and the fidelity of the models (Mencarelli et al., 2020). To increase the computational tractability of the SSO, surrogate models can be used instead in the superstructure formulation. The key question resulting from this is which surrogate model to use and how to validate it? We propose to evaluate this question considering potential consequences of a particular model choice within the context of end application. We motivate this problem for the case of SSO. Here we propose a benchmarking framework to determine the most suitable surrogate alternative for a process design task. The first four alternatives comprise 1) a Gaussian Process Regressor and 2) an Artificial Neural Network as a surrogate model, which are respectively fitted to flowsheet simulation data over the input space. The third alternative is a piecewise linear regression model, called Delaunay Triangulation Regression (DTR). Each model is validated, and root mean square error as well as the coefficient of determination are assessed and compared. With the respective surrogate models for each flowsheet option in the superstructure, the underlying optimization problem of the SSO, which is classically a mixed-integer nonlinear program, can be reformulated either as a series of nonlinear programs for the first two models or as a mixed-integer linear program for the last surrogate. The solution of the optimization problem with each surrogate and validation with the original flowsheet model serves as the benchmarking purpose in this study (Vollmer et al., 2020). As a result, despite the excellent predictive qualities of most machine learning surrogates, this is not reflected in the results of the SSO. The DTR model performs best in the benchmark, which indicates a promising potential as surrogate modelling technique for optimization applications as process design or even scheduling. Overall, the crucial role of cross-validation and case-dependent analyses of different surrogate models becomes evident, as sampling size and strategy clearly play a role in the resulting model quality and the optimization results, thus application strategies can hardly be generalized.

References

L. Mencarelli et al., 2020, ‘A review on superstructure optimization approaches in process systems engineering’, Computers Chemical Engineering, Vol 136, 106808.

N. Vollmer et al., 2020, ‘Benchmark of Superstructure Optimization Approaches for a Hybrid Process Design Framework for Biorefineries’, Computer-Aided Chemical Engineering, Vol 50, 475-480.

Digitalization of Pilot Plant Facilities to Develop Methods and Tools that Improve Data Utilization in Chemical- and Biochemical Processes

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The transition of the chemical- and biochemical industry towards industry 4.0 is accelerating as in-line sensor technologies and data storage solutions become more advanced, accessible and affordable. While an increasing number of companies are investing heavily into developing expanded data collection- and storage solutions, there is a scarce focus on how this added volume of data can improve operational efficiency when the production line is running. To address this deficiency, the Department of Chemical- and Biochemical engineering at DTU has initiated a substantial modernization effort of the in-house pilot-scale process equipment, to match the digitalization trend observed in industry. This is achieved by implementing a new centralized data framework that initially, will encompass approximately twenty of the installations in the chemical engineering pilot hall. The scope of the integration will be to centralize the process data and store it in a PostgreSQL database, accessible via the internal network in real-time. Furthermore, the previous hard-wired human-machine-interfaces (HMI), are replaced with Siemens WinCC, which will allow for remote control of the pilot facilities through a wireless connection to the internal network. To manage the communication between the physical equipment, HMI and database, a versatile software known as vNode will serve as an intermediate layer. This software is compatible with most communication protocols, most notably REST and OPC-UA. The implementation will encompass a diverse selection of equipment, including fermentors, filters, distillation columns, evaporators and many additional unit operations commonly found at commercial manufacturing sites in the chemical and biochemical industries.

With a centralized and software agnostic data infrastructure, the pilot plant is expected to serve as a centre for both education and research. Several research projects have therefore already been initiated with a primary focus on developing methods and tools that can improve the utilization of the increasing amount of accessible data. The easy access to both the real-time and historical process data will provide improved facilities for coupling first-principle models with data-driven methods to produce hybrid models that can be validated on pilot-scale. Combining the aspect of hybrid model development with the bidirectional communication via the new SCADA system will provide a solid base for researching and testing digital twin deployment. Another area of research is integrating the real-time experimental process data with dynamic process models from commercial software like Aspen Plus, enabling the direct use of pilot experimentation in process scaling- and design. Great effort has also been put into generalizing the SQL database infrastructure to easily include new sensor readings, equipment or pilot setups. The database has also been harmonized with software packages like Riffyn that allows for easy analysis of inter-equipment process data for production line emulation, and AnIML that can integrate raw data from most third-party sensors into the database. It is the vision that this investment will align the academic research facilities at DTU to address the demands from the chemical and biochemical industry and provide a general basis for research that encourages external collaboration.

Model Predictive Control for Zero-emission Industrial Processes

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As the underground hydrocarbon reservoir fields in the Danish North Sea mature, the increasing amount of produced water (PW) becomes an important challenge in offshore oil and gas production. The produced water contains oil and other pollutants and must be cleaned before it is discharged to the surrounding sea.

Offshore oil and gas extraction processes consists of the flow line riser unit, the three-phase separator unit and the de-oiling hydrocyclone unit. We combine the engineering knowledge and sysmatic model building methods to model these units. The slug flow phenomenon that might arise in the riser as a consequence of a Hopf bifurcation. Large production variations are caused by the slug phenomenon, which must be avoided. We develop an economic model predictive control (MPC) based advanced process control (APC) system for offshore oil and gas production processes that can significantly reduce oil concentration in discharged water and maintain high oil and gas production without violating legislative requirements of the discharged water.

We investigate and test the models and controllers using industry standard digital twins as well as in a pilot plant at Aalborg University in Esbjerg to demonstrate how the developed technologies can be combined with novel sensors in an APC system to maximize production while having zero emissions in upstream oil and gas facilities.

Process Simulation and Optimization of NH3/CO2 separation with ionic liquids

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With the development of industry, the emission of tail gas such as CO2, NH3, SO2, etc. from industrial tail gas is becoming more serious, which is harmful to human body and environment. Melamine production produces tail gas will a significant amount of both NH3 and CO2. At present, the main treatment methods are water scrubbing and urea co-production technology but these methods face the difficulties of high energy consumption, equipment corrosion and secondary pollution. As a new type of solvent, the ionic liquid is designable structure, extremely low vapour pressure, and high gas solubility, it has received wide attention in the field of tail gas cleaning and gas separation.

Therefore, two new process technologies based on ionic liquids treatment of melamine tail gas are employed and evaluated for energy and cost efficiency. In this work, a protic ionic liquid with high NH3 absorption performance named [Bim][NTf2] is selected for the simulation and evaluation on the melamine tail gas cleaning process. Based on experimental data, a thermodynamic model suitable for process simulations is regressed with the NRTL equation. The two steady-state model of the process (ionic liquid-based process and enhanced ionic liquid process)are built and investigated through sensitivity analysis in Aspen Plus, energy/economic evaluation are also carried out by making a comparison with the more traditional water scrubbing technology. The two ionic liquid based process can both lower the separation cost compared with the water scrubbing process. In addition, the enhanced ionic liquid process with stripping can achieve a lower purification cost which is reduced as 61% of that of water scrubbing process. Moreover, the flowsheet based on the two ionic liquid are simpler than water scrubbing method and avoid the wastewater discharge.

Moreover, in order to decrease the energy consumption in the ionic liquid-based separation process, a multi-objective optimization (MOO) research was carried out using Aspen Plus and Matlab for the ionic liquid-based process. This process was optimized by the nondominated sorting genetic algorithm II (NSGA-II) algorithm after the simulation. The minimum total separation cost (TSC) and total process CO2 emission (TPCOE) were set as two objective functions. With the constraints and several operational parameters optimized, the Pareto front displays a set of nondominated optimal design parameters that satisfy the specification of the NH3 concentration standard in purified gas. The results show that the effect of desorption pressure and the ratio of lean solvent to total solvent are critical for both TSC and TPCOE. After the MOO, the TSC of the ionic liquid-based process can be decreased by 5%, and TPCOE is reduced by 7% compared with the base case. The optimization results support the optimal design and operation of the NH3 and CO2 separation process with ionic liquids considering environmental and economic objectives. For the the phenomenon that fluctuation of tail gas concentration and gas volume will have effect on the ionic liquid-based process, corresponding process dynamic control scheme will be established in the next step work and finally provides detail support for the industrial application of the process.

Nonlinear State Estimation for the Modified Four-Tank System

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In this work, we present methods for state estimation in nonlinear system described by continuous-discrete stochastic differential equations. For nonlinear state estimation, we present the extended Kalman filter, the unscented Kalman filter, the ensemble Kalman filter, and the particle filter. Furthermore, we present a simulation model for the modified four-tank system. In the modified four-tank system, a grid of coupled tanks are filled with liquid which drains from the bottom of each tank into either another tank or a reservoir below. The tanks are filled in known proportions by a set of manipulated input flows and a set of unmeasured disturbance flows flowing into the tanks from the liquid reservoir below. The height of the liquid column inside the tanks are measured for the full set of tanks in the system or for a subset hereof. To ensure non-negativity in the states and disturbances in the model of the modified four-tank system, the states and disturbances are transformed using an exponential transform and a Lamperti transform respectively. Finally, we implement the four different methods for state estimation in nonlinear systems, the transformed model for the modified four-tank system in Matlab, and test and compare the state estimation methods in simulation.

Bayesian analysis of the physics-based process models: A case study on multiphase pipe flow

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In this work we present application of Bayesian inference and parameter estimation for tuning a first principles model of a three phase (oil, gas and water) pipe flow. This three-phase steady state model is based on the drift-flux approach and represents a multiphase pipe flow process. Such process models are commonly used for modeling of pipe and well flow behavior in oil and gas production fields. The main motivation for this work is that the physics-based models of a process system are almost never sufficiently accurate and require tuning of involved model parameters. Traditionally, this is done by considering the unknown model parameters as fixed values and the data from an actual plant as a random variable. This framework is often referred to as frequentist approach and aims to find point estimates of the unknown model parameters. If the conditions change, which is common in practice, the model becomes inaccurate and needs to be re-tuned. In this work we present an alternate framework which allows to tune the first principles models to the process conditions using Bayesian inference and parameter estimation. Our approach estimates the expected values of the first principles model parameters and quantify the uncertainty associated with these estimated values. This is quite useful in practice as this modeling approach help us to know how certain the model is about its prediction which enables to make accurate decisions to operate a plant in safe and reliable manner.

A Dual-hormone Artificial Pancreas based on Nonlinear Model Predictive Control and Maximum Likelihood Estimation

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In this work, we present a switching nonlinear model predictive control (NMPC) algorithm for a dual-hormone artificial pancreas (AP) and we apply maximum likelihood estimation (MLE) to identify the system. A dual-hormone AP consists of a continuous glucose monitor (CGM), a control algorithm, an insulin pump, and a glucagon pump. We have designed an app for an android smartphone, that 1) is a graphical user interface, 2) communicates with the sensor and pumps, and 3) solves the optimal control problem as well as estimates the states with a continuous-discrete extended Kalman filter (CD-EKF). The AP is designed with a heuristic to switch between insulin and glucagon as well as state-dependent constraints. We use a glucoregulatory model with glucagon and exercise for simulation and we use a simpler model for control. In this work we test the MLE and the performance of the AP using in silico numerical simulations on virtual patients. The AP is being tested in clinical trials, but the results are not available yet.

Hybrid modelling of industrial scale fermentation process

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The production of pharmaceuticals has always had a strong focus on quality. A common method for producing Active Pharmaceutical Ingredients (API) is via biological processes or fermentation of high producing bacteria or fungal strains. These processes have been subject to mechanistic modeling for use in batch optimization, monitoring and control Gernaey (2010). However, the metabolic pathways responsible for the main product can lead to accumulation of related substances in the batch that hamper the final product quality and may be impossible to remove in the downstream process. Mechanistic models rarely take batch quality into account and most model development is focused on main product only. Additionally, biological systems are notoriously complex so sufficient knowledge is often lacking for production strains. The biotechnological industry increasingly applies mechanistic models because it has realized their significance. Due to the complexity of the biological systems a hybrid model approach is used as an alternative. The concept of hybrid modelling in this context is the combination of a first principles mechanistic model and machine learning models into single model. Machine learning and Artificial Intelligence algorithms such as Artificial Neural Networks (ANN) have seen an increase in popularity in various research fields and the use of Hybrid modelling has seen success in chemical engineering such as in particle processes Nielsen (2020). This study focuses on the application of a hybrid modelling framework on the fermentation of a filamentous fungi that produces Fusidic Acid. A first principles biochemical model is built influenced by existing literature based on penicillin fermentation models Birol (2002). Sophisticated ANN models are subsequently trained to predict the kinetic expressions for the evolution of by-products. The fully integrated hybrid model is subsequently for predicting productivity and quality of industrial scale batches currently in production and further process optimization to maximize the yield of a single batch without compromising the quality of the final product.

Interpretation of responses to bolus-feeding during CHO-fedbatch cultivation using an extended bottleneck model and simulations with Bioprocess Library for Modelica

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A workhorse in biopharmaceutical industry is cultivation of recombinant CHO-cultures to produce proteins and antibodies. There are also some covid-19 vaccines produced this way. The specific oxygen uptake rate of CHO-cultures is a measure of respiratory metabolism in general. Respiration has a limited capacity. A common industrial practice is to give the culture feed once a day and called bolus-feeding and the cultivation goes on for typically two weeks. The daily bolus-feed challenge the respiratory capacity of the culture. Continu-ous feeding is an alternative, but bolus-feeding is still used and has practical advantages without affecting culture quality much. The amount of feed given for each bolus follows a profile that is slightly adjusted for the measured substrate level in the reactor just before the new bolus. Feeding affect mainly product yield. Bolus-feeding is used in lab-, pilot- and production scale. Data from industrial pilot scale is used in this paper. The bioreactor is equipped with automatic control of variables like temperature, dissolved oxygen, and pH. The dynamic response of the control system to the bolus-feeding varies during the cultivation. In this paper we try to interpret the changes in the response of the control system in terms of status of the culture and whether the culture is over- or under-fed. In this way we may get information to complement, or even eliminate, the need for off-line measurement of substrate levels before bolus. We make use of a simplified bottleneck model, see Amribt et al (2013) and Axelsson (2019). The model is in this paper extended to capture O2 an CO2 as well as by-product lactate consumption. The extended model used here is also used to describe a CHO-culture run in pilot scale equipped with exhaust gas analysis using mass spectrometer and run with daily bolus-feeding, see Goh et al (2020). The model is manually fitted to their data and bring quali-tative check of the extended model. The connection to earlier work with microbial cultures and super-imposed pulses on the continues feeding is also discussed, see Åkesson et al (2001). This is a technique to monitor the status of the culture in relation to its respiratory capacity and can be seen as an “internal standard” and base for feedback control.

References

Amribt Z., Niu H., Tan W., Bogaerts P. (2013): “Macroscopic modelling of overflow metabolism and model-based optimization of hybridoma cell fed-batch cultures”, Biochem. Eng. Jour.

Niu H., Amribt Z., Fickers W., Tan W., Bogaerts P. (2013): ”Metabolic pathway analysis and reduction for mammalican cell cultures – towards macroscopic modeling”, Chem. Eng. Science.

Axelsson J. P. (2019): “Simplified Model of CHO-cultivation in Bioprocess Library for Modelica – some experience”, Proceedings of the 22th NPCW, Lyngby, Denmark, August 22-23, 2019.

Goh H.-Y., Sulu M., Alosert H., Lewis G. L., Josland G. D., Merriman D. (2020): “Applications of off-gas mass spectrometry in fed-batch mammalian cell culture”, Bioprocess and Biosystems Engineering 43:483-493.

Åkesson M., Hagander P., Axelsson J. P. (2001): ”Avoiding acetate accumulation in Escherichia coli cultures using feedback control of glucose feeding.”, Biotech. Bioeng. 73: 223-230.

Fast Charging Control of Li-Ion Batteries: Effects of Input, Model, and Parameter Uncertainties

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The foundation of onboard advanced battery management is control-oriented models that capture the key battery characteristics and are computationally efficient. In addition to their orders, the selection of appropriate battery models will also depend on input and parameter uncertainties, which is often overlooked. This work aims to pinpoint the minimum model complexity for health-conscious fast charging control in the presence of sensor biases and parameter errors. Starting from a high-fidelity physics-based battery model that describes both the normal Li-ion intercalation reaction and the dominant side reactions, Pad ́e approximation and finite volume method are employed for model simplification, with the number of control volumes as tuning parameters. For given requirements of modelling accuracy, extensive model-based simulations are conducted to find the simplest models, on which the effects of current sensor biases and parameter errors are systematically studied. The results show that relatively low-order models can be well qualified in voltage, state of charge (SOC), and temperature control, whereas high-order models are necessary for health control, particularly during fast charging. Furthermore, when the applied current drifted largely, the choices of safety margin need to take these biases into consideration, when the parameters have a certain extent of uncertainties, increasing the model order will not help but complicate the system.

Electrochemical Model-Based Fast Charging for Lithium-Ion Batteries: Physical Constraint-Triggered PI Control

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A new fast charging control strategy for lithium-ion (Li-ion) batteries is proposed. The approach relies on an experimentally validated high-fidelity model describing battery electrochemical and thermal dynamics that determine the fast charging capability. Such a high-dimensional nonlinear dynamic model can be intractable to compute in real-time if it is fused with the extended Kalman filter or the unscented Kalman filter that is commonly used in the community of battery management. To significantly save computational efforts and achieve rapid convergence, the ensemble transform Kalman filter (ETKF) is selected and tailored to estimate the nonuniform Li-ion battery states. Then, a health- and safety-aware charging protocol is proposed based on successively applied proportional-integral (PI) control actions. The controller regulates charging rates using online battery state information and the imposed constraints, in which each PI control action automatically comes into play when its corresponding constraint is triggered. The proposed physical constraint-triggered PI charging control strategy with the ETKF is evaluated and compared with several prevalent alternatives. It shows that the derived controller can achieve close to the optimal solution in terms of charging time and trajectory, as determined by a nonlinear model predictive controller, but at a drastically reduced computational cost.

A tuning strategy for advanced control of grinding circuits based on multiobjective optimization

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In this work we investigate the application of a tuning technique based on multiobjective optimization originally developed for petrochemical processes [1] in the mineral processing industry. Consider a $ny \times nu$ MIMO systems with ny outputs and nu inputs. In order to design a Model Predictive Controller (MPC) for the system, one must specify its tuning parameters, usually a control horizon (m), a prediction horizon (p), and weighting matrices on the outputs and input moves, $Q_y \in R^{ny \times ny}$ and $R \in R^{nu \times nu}$, respectively. The tuning task is not straightforward, as the weights in Q_y and R do not correlate directly to the control performance of the output variables, i.e. setting a large $q_{y,1}$ does not necessarily mean that y_1 will have good closed-loop performance. Several strategies have been developed to tune MPCs, considering heuristic methods, multiobjective optimization and practical guidelines [2]. In many industrial applications, it is not uncommon to rely on trial and error.

In the proposed strategy, the tuning problem is cast as a multiobjective optimization problem and solved using compromise optimization. The optimal solution is calculated minimizing the Euclidean distance between a viable solution and the Utopia solution. We calculate optimal values for Q_y and R and select m and p considering the open-loop dynamics of the system. One of the advantages of our method is the intuitive definition of the tuning goals as a function of the desired behavior of the closed-loop output tracking performance. First, the output variables are sorted by descending relevance order and then paired with appropriate input variables. This step takes into account both process knowledge and mathematical pairing strategies e.g. Relative Gain Array. Second, the open-loop response of the pairs are approximated by First Order Plus Dead Time (FOPDT) transfer functions. Finally, the gains of the FOPDT transfer functions are multiplied by response factors f_i, $i = 1, \ldots, ny$ that determine whether the closed-loop response of an output should be faster or slower than its open-loop behavior.

The partial results demonstrate that it is possible to apply the tuning method in grinding circuits and that the strategy to select the tuning goals based on the desired closed-loop performance is suitable for applications in grinding circuits in the mineral processing industry. We compare the obtained results with a tuning strategy from the literature [3] in a linear system and tune the DMC of a nonlinear system.

References

[1] Yamashita, A. S., Zanin, A. C., & Odloak, D. (2016). Tuning the Model Predictive Control of a Crude Distillation Unit. *ISA Transactions*, 60, 178–190. https://doi.org/10.1016/j.isatra.2015.10.017.

[2] Alhajeri, M., & Soroush, M. (2020). Tuning Guidelines for Model-Predictive Control. *Industrial & Engineering Chemistry Research*, 59(10), 4177–4191.

[3] Wojsznis, W., Gudaz, J., Blevins, T., & Mehta, A. (2003). Practical approach to tuning MPC. *ISA Transactions*, 42(1), 149–162.

Approximations to the solution of the Kushner-Stratonovich equation for the stochastic chemostat

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In order to characterise the dynamics of a biochemical system such as the chemostat, we consider a differential description of the evolution of its state under environmental fluctuations [1, 2]. We consider the chemostat with Monod-Haldane reaction kinetics, subjected to geometric Brownian motion. Under this modelling assumption, our best knowledge about the state of the system is given by its conditional distribution in time, given the distribution of the initial state. Such a function solves a deterministic partial differential equation, the Kolmogorov forward equation [3].

Our focus, however, is to refine our knowledge about the state of the chemostat when additional information about the system is available in the form of measurements. To describe how measurements and states are related, we augment the dynamics with an observation model in which the measurements are also subjected to Brownian motion. When measurements are collected, our estimate of the state is given by its conditional distribution, now given the distribution of the initial state and the collected measurements. A currently successful and versatile method to numerically estimate this function is to approximate it with an empirical distribution based on a set of particles. In such approximation, the particles firstly evolve according to the dynamics, and then, they interact selectively in accordance with their likelihood with respect to the measurements [4].

More formally, we are interested in obtaining the distribution of the state as the solution to a nonlinear stochastic partial integral differential equation, the Kushner-Stratonovich equation. For the chemostat, this solution is not available in closed form and it must be approximated. One common approximation consists of replacing the nonlinear dynamics with a linearised counterpart for which a closed-form solution exists. A less common approach consists of solving an associated stochastic partial differential equation, the Zakai equation. This solution is an unnormalised density function, given the distribution of the initial state and the collected measurements. Also in this case, however, the solution is not available in closed form for our system and it must be approximated numerically.

In this work, we present solutions to the Kushner-Stratonovich and Zakai equations based on partial differential equation methods. We compare the solution with a classical sequential Monte Carlo method known as the Bootstrap particle filter.

References

[1] Imhof, L., Walcher, S. Exclusion and persistence in deterministic and stochastic chemostat models. Journal of Differential Equations, 217, 26 (2005).

[2] Wang, L., Jiang, D., Wolkowicz, G., O'Regan, D. Dynamics of the stochastic chemostat with Monod-Haldane response function. Scientific reports, 7(1), 13641 (2017).

[3] Bain, A., Crisan, D. Fundamentals of Stochastic Filtering. Springer (2009).

[4] Del Moral, P., Miclo, L. Branching and interacting particle systems. Approximations of Feynman-Kac formulae with applications to non-linear filtering. Séminaire de probabilités de Strasbourg, Tome 34, pp. 1-145 (2000).

Forward sensitivity analysis of a supercritical extraction process

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We consider the extraction process of valuable components from biomass using supercritical CO2 as a solvent. We are interested in the extraction of essential oils from carqueja seeds in cylindrical extractorS operated in semi-batch mode. We focus on the sensitivity of the extraction process and yield to process parameters and operating conditions.

For the task, the process is represented using a distributed-parameter model consisting of a three partial differential equations: two mass balances relative to the mobile fluid phase and the fixed solid phase, and the heat balance of a single pseudo-homogeneous phase. In state-space sense, the systems's state consists of the local concentrations of solute in the fluid and solid phases, and the local temperatures of the pseudo-homogeneous phase. A plug-flow model for the velocity and no pressure drop along the extractor are assumed. We also consider only axial diffusion for both mass and heat. As for the mass transfer from the solid to the fluid phase, a kinetic term based on two-film theory for a single solute component is used. Such a model augments what commonly found in the literature [1] in relation to material balances, by adding a heat balance to describe changes in concentration of solute due to a potentially varying temperature of influent CO2 and pressure in the extractor. This is achieved by assuming that certain parameters characterising the properties of the fluid and pseudo-homogeneous phase are dependent locally on temperature and pressure. The Peng-Robinson equation of state is used to describe the thermodynamics of the fluid phase. The thermal properties of the pseudo-homogeneous phase are assumed to vary along the extractor, though always remaining equal to the corresponding mean values between the fluid and solid phase. The system is controllable by manipulating the flowrate and temperature of CO2 in the feed, and the pressure in the extractor. We also assume that extraction yield at the effluent is measurable.

To study the influence of parameters and operating conditions on the time evolution of the system's state, a sensitivity analysis is performed on a spatial discretisation of the model. This is achieved by jointly solving a set of ordinary differential equations whose solutions consist of the evolution of discretised state variables and sensitivity functions. The sensitivity functions are partial derivatives of the state variables with respect to parameters, and operating conditions: They solve the sensitivity ordinary differental equations and quantify how the state trajectory is affected by individual changes in parameters, and operating conditions, over time. As for the measurements' sensitivities, they are determined algebraically by using the sensitivity functions in the total derivative of the output equations. We restrict our analysis to first-order sensitivities [2,3].

References

[1] E. Reverchon (1996). Mathematical modeling of supercritical extraction of sage oil. AIChE Journal, 42(6):1765–1771.

[2] R.P. Dickinson, R.J. Gelinas (1976). Sensitivity analysis of ordinary differential equation systems - A direct method. Journal of Computational Physics, 21(2):123–143.

[3] T. Maly, L.R. Petzold (1996). Numerical methods and software for sensitivity analysis of differential-algebraic systems. Applied Numerical Mathematics, 20(1-2):57–79.

Session 4: Bioprocesses

Optimal Control of Water Quality in a Recirculating Aquaculture System

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This study compares nonlinear model predictive controls, using setpoint tracking objective function (NMPC), and economic objective function (E-NMPC), with a hierarchical control structure of PI controllers applied to the water treatment of a Recirculating Aquaculture System (RAS), which consists of a tank, a biofilter, a stripper and an oxygen cone. Two of the three control structures used in this work consist of an optimization layer on top of proportional integral (PI) control loops or NMPC. The optimization layer reduces the degrees of freedom with an economic objective function by deactivating some of the manipulated variables when choosing between buffer and base addition and location of addition to the system. The third structure consists of a single layer with E-NMPC. The PI control structure is easy to design once we know the relationship between the variables. The PI controllers' performance were satisfactory, but a small back-off would be needed, if the constraints would not be soft constraints, or use of buffer with base would be necessary to improve speed and avoid constraint violation, as some components took more than 6 days to reach the optimal concentration. The NMPC and the E-NMPC performed better: the E-NMPC provided a mixture of smooth trajectory, as the PI controllers did but with optimal economic cost, although some responses had offset; and the NMPC was much faster on conducting the controlled variables to optimal conditions, despite not providing optimal economic cost during the trajectory.

Why tuning rules for feedforward control are required

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Feedforward control to deal with load disturbances is a very old topic with more than 100 years of history. Most industrial processes are affected by disturbances and feedback can be inefficient to reject them because of the reactive behavior of the control loop. Feedforward control approaches have become like a standard and simple solution to improve the disturbance rejection effect when disturbances are measurable, since the feedforward control contribution is injected before affecting the process output. In fact, under perfect situations, the disturbance effect can be completely removed.

Nevertheless, those perfect situations are seldom possible and the feedforward is not realizable in most occasions. In those cases, static feedforward compensators are typically used in industry, but with this solution non-desirable overshoots are obtained and the performance is not the expected one. So, could the feedforward compensator be tuned in those cases in order to improve the disturbance rejection response? The answer is, yes.

This work motivates why feedforward compensators should be tuned and how different tuning rules can be proposed. First, it is shown that when inversion problems arise, the feedforward compensator should not be designed in open loop anymore. Now, a connection between the feedback controller and the feedforward compensator is required. This analysis will lead to two different groups of tuning rules based on closed-loop or open-loop designs. So, this paper summarizes these two groups of tuning rules as a result of the research on this topic during the last 10 years. Numerical simulation results and experimental tests on the greenhouse temperature control problem will be shown to illustrate the main contributions.

Designing control models of fed-batch bioreactors based on dFBA using interior-point solvers

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Model-based control is an important strategy that can improve production efficiency of bioprocesses. Implementation of this type of control is usually based on unstructured models, which employ specific growth rates and fixed yield parameters, being only valid for narrow ranges of process conditions and cellular behavior. Dynamic flux balance analysis (dFBA) is a modeling technique that can overcome this limitation, since it uses the metabolic network of the microorganism and can describe physiological changes in the cell. dFBA models consist of a set of ordinary differential equations for the mass balance of substances external to the microorganism and a linear programming (LP) model for representing the internal fluxes in the metabolic network. When using dFBA as the control model, a bi-level optimization problem is obtained. A possible approach for solving this class of optimization models is to replace the LP model with its first-order optimality conditions (KKT conditions), relax the inequality-multiplier complementarities and employ a nonlinear solver. In this work, we analyze this solution strategy for when a line-search interior-point solver, such as IPOPT, is used. This analysis is based on a case study that seeks to the maximize growth of *Escherichia coli* on glucose considering both open-loop and closed-loop formulations for the control problem. We discuss limitations of the selected type of nonlinear solver and show that it is important that the stoichiometry matrix used for representing the metabolic network has full row rank and that carefully initializing the model can avoid convergence issues. In addition, we analyze two reformulation methods for relaxing the complementarity constraints derived from the KKT conditions: the penalty method, that removes complementarities of the form $a^T b = 0$ and adds a penalty term $a^T b$ to the objective function, and the relaxation method, which replaces the complementarities with inequalities such as $a_i b_i \leq \varepsilon$ with ε being a small positive value. The results show that both reformulation approaches are suitable for the fed-batch bioreactor control problem; however, they present some relevant differences, while the relaxation method is able to set a desired complementarity satisfaction, the penalty-term approach can converge faster when a good initialization of the model is not available.

Closing the loop: Online model predictive control strategy with real-time monitoring of experimental bioreactors

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The technology involved in bioprocesses has significantly evolved in the recent decades. Simple batch fermentation techniques initially dominated the bioprocess industry, in which medium and initial feeding were added to an initial microbial culture, based on user's experience, and with no measurements or control on the process. In fact, although this technique still dominates industrial fermentation processes, newer technology and digitalization have appeared in cultures that require highly scrutinized growth and production conditions, such as in the pharma industry.

Tight control of microbial cultures requires models of the biological process, online measuring techniques, control algorithm, supplemented by hardware controlling the manipulated variables and software interface that can communicate with the bioprocess in real-time. However, online monitoring of highly dynamic cell cultures is still in its infancy, and real-time control interface with bioreactor is still very limited. Therefore, it is a challenge to apply advance control, including nonlinear and optimal control of microbial cultures.

In this presentation we explore beyond the state-of-the-art technology for monitoring and control of bioproceses. Models of microbial culture are usually simply but highly non-linear such as the Monod growth model. We present here the challenges and successes of a complete feedback nonlinear control strategy in bioprocesses, developed and implemented as part of a large H2020 project iFermenter. This includes technologies that keep online, *in-situ*, invasive and non-invasive monitoring and algorithms that can provide feedback for such highly nonlinear systems. Automatic sampling devices, liquid chromotography, accurate dilution and filtering devices are coupled with online near infrared probes that estimate biomass, and with measurements of carbon dioxide and oxygen that indicate cellular respiration, all were integrated with an advanced software system. Furthermore, unscented Kalman filter, extended Kalman filter and moving horizon estimators were explored in this complete feedback system, aiming to serve as digital twins, supplementing, and to some extent replacing, complex online measurements techniques, and improving the quality of the feedback information.

We also discuss different control implementations of this process. The control strategy aims to close the loop and keep stable growth, high production and healthy respiration, by applying control on substrate feeding, inducers and essential media nutrients, all keep the cell factories at desired conditions. A set of dedicated control experiments of *C. glutamicum* is presented, and possible improvements needed to move the technology forward.

Bioprocess Monitoring: A Moving Horizon Estimation Experimental Application

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Microbial fermentation processes are most often described by nonlinear time-varying dynamics, which require the implementation of nonlinear state estimators to infer unmeasured metabolites in the cultivation broth. Among the various nonlinear available estimator strategies, the Moving Horizon Estimator (MHE) is an *on-line* optimization approach that easily allows to enforce hard constraints, an important feature that helps to avoid unfeasible concentrations. In this work we implemented an MHE by using experimental data from a fed-batch cultivation process of *Corynebacterium glutamicum*. Available real-time measurements of biomass and CO_2 formation were used to infer sugar concentrations by combining the available measurements with a simple Monod model. We found that the MHE was able to estimate all the three variables of interest, including the unmeasured sugar concentrations, during the entire fed-batch cultivation process. Moreover, we show that the estimates are accurate in comparison to the reference *off-line* samples. This work demonstrates the benefits of MHE as a soft sensor that can monitor bioprocesses in real-time.

Session 5: General processes

Optimal Control of a Smart House using MPC-based Reinforcement Learning

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With the modernization of the energy infrastructure, buildings are increasingly becoming not only consumers of electricity but also producers and participants in the electricity market (Powell, 2014; Anderson et al., 2011). Energy management in smart buildings requires making decisions (buying, selling, and/or storing electricity now to be used later) in the presence of variability and uncertainty associated with forecasts, weather conditions, electricity demand, and electricity prices. This makes these problems challenging from an optimal control perspective. We propose to combine model predictive control with reinforcement learning techniques to learn the optimal energy management policy in the presence of variability and uncertainty.

In this work, we consider the energy management in a smart house that can produce electricity using photovoltaic panels, store electricity using a battery, consume electricity, and buy and sell electricity to and from the market. The electricity prices are assumed to be known in the next 12h, but we consider uncertainty associated with the solar irradiance and the demand forecasts as well as with the battery efficiency.

To solve this problem, we deploy an actor-critic architecture where the critic uses the LSTDQ method (Lagoudakis and Parr, 2003) to evaluate the current policy and the actor uses the deterministic policy gradient method (Silver et al., 2014) to make a policy improvement over the current policy. The optimal policy is approximated using a parametric MPC (Gros and Zanon, 2019) and the optimal action-value function is approximated using an affine compatible function approximator (Silver et al., 2014). Our simulations show that the proposed MPC-based reinforcement learning method is effective in decreasing the long-term economic cost of this smart house problem despite its variability, uncertainty and plant-model mismatch.

References

Anderson, R. N., Boulanger, A., Powell, W. B., and Scott, W. (2011). Adaptive stochastic control for the smart grid. Proceedings of the IEEE, 99(6):1098–1115.

Gros, S. and Zanon, M. (2019). Data-driven economic NMPC using reinforcement learning. IEEE Transactions on Automatic Control, 65(2):636–648.

Lagoudakis, M. G., Parr, R. (2003). Least-squares policy iteration. The Journal of Machine Learning Research, 4, 1107-1149.

Powell, W. (2014). Energy and uncertainty: Models and algorithms for complex energy systems. AI Magazine, 35(3):8–21.

Silver, D., Lever, G., Heess, N., Degris, T., Wierstra, D., Riedmiller, M. (2014, January). Deterministic policy gradient algorithms. In International conference on machine learning (pp. 387-395). PMLR.

Closed-Loop Treatment as a Diagnostic Tool in Type 2 Diabetes

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In late-stage type 2 diabetes (T2D), treatment with long-acting insulin can become necessary to avoid long-term complications. However, initiating treatment, an iterative process known as titration, is a taxing and time-demanding procedure for the individual. As a result, not all adhere to treatment and less than 60% successfully reach treatment targets. We propose that automating the titration process can improve adherence. In our work, we present a method to select a safe and effective insulin dose with long-acting insulin through short-term use of fast-acting insulin in a closed-loop (CL) system. To illustrate this concept, we simulate the glucose response to fast- and long-acting insulin in people with T2D. We apply a model-free control algorithm to adjust the insulin infusion rate during fasting periods. We simulate insulin-naïve T2D patients on CL treatment for one week, gradually adjusting the insulin infusion rate. After one week, we convert the insulin infusion rate to a daily injection of long-acting insulin. We compare our method to titration with standard of care algorithms. Our simulations indicate that CL treatment can safely shorten the titration period, whilst easing the burden on the patients through automation.

A receding-horizon framework for optimal control and estimation of a common class of activated sludge plants

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Increasing population and erosion of diversity exposes our planet to unsustainable stresses on renewable water resources. Because central in a broad cycle in which water should be replenished at the same rate at which it is extracted from the resources, we are interested in municipal wastewater treatment plants and their use as water resource recovery facilities. Water resource recovery refers to the capture of energy and nutrients from otherwise unused wastewater streams [1,2]. Being an infrastructure common to most urban areas, biological treatment through activated sludge processes is an important platform for recovering resources from municipal wastewater. The optimal operation of wastewater treatment plants (WWTPs) has been extensively studied thanks to support tools that provide a simulation protocol for real-world facilities: The Benchmark Simulation Model no. 1 (BSM1, [3]), specifically, singled out as the reference platform for controlling activated sludge plants subjected to typical municipal influents. While the availability of the BSM1 has stimulated numerous control strategies for satisfying regulatory constraints, its performance for resource recovery is still under active research. We research control solutions to operate WWTPs as efficient water resource recovery facilities [4,5,6]. Towards this goal, we present an output model predictive controller that operates activated sludge plants to produce effluent water of specified quality on demand. 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) over noisy measurements [7]. The tracking of the desired effluent profiles is enforced by stabilizing the system around optimal steady-state points that satisfy the output reference trajectories. We specialise the control problem by considering quadratic cost functions and linearisations of the process dynamics around each set-point. Similarly, we consider estimation problems with linearised dynamic constraints in which the initial state, disturbances, and measurement noise, are Gaussian. We illustrate the controller behaviour when operating a large-scale plant to produce water and sludge of varying quality. Given the generality of the approach, this controller can also be configured to achieve alternative goals.

References

[1] G. Sarpong et al., Near future energy self-sufficient wastewater treatment schemes. International Journal of Environmental Research, 14:479-488, 2020.

[2] S. Kundu et al., Source and central level recovery of nutrients from urine and wastewater: A state-of-art on nutrients mapping and potential technological solutions. Journal of Environmental Chemical Engineering, 10(2):107146, 2022.

[3] K.V. Gernaey, et al., Benchmarking of Control Strategies for Wastewater Treatment Plants. IWA Publishing, 2014.

[4] O.B.L. Neto, et al., About the classical and structural controllability and observability of a common class of activated sludge plants. Journal of Process Control, 111:8-26, 2022.

[5] O.B.L. Neto, et al., Predictive control of activated sludge plants to supply nitrogen for optimal crop growth. IFAC-PapersOnLine, 54(3):200-205, 2021.

[6] O.B.L. Neto, et al., A receding-horizon framework for optimal control and estimation of a common class of activated sludge plants. Under preparation.

[7] J.B. Rawlings, et al., Model Predictive Control: Theory, Computation and Design, 2nd

Edition. Nob Hill Publishing, 2020.

Modelling and Optimization of large-scale alkaline CO_2 electrolysis systems

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Electrochemical $\mathrm{CO_2}$ reduction offers the promise of becoming one of the enabling technologies for the dire needed energy transition by producing valuable carbon products from $\mathrm{CO_2}$, water and renewable electricity. However, given the relative infancy of the technology, many uncertainties regarding its large scale implementation still exist. As such, the question of how to optimally design and operate the electrolyzer and the overall process is still mostly unanswered. Providing answers to such questions will not only require to scale up experimental systems, but also to develop multiscale models which allow to quantitatively describe the complex interactions between all process levels.

This work intends to advance current system design efforts for electrochemical $\mathrm{CO_2}$ reduction through two contributions. The first consists of a multiscale model of the electrolysis process, which is synergized by coupling a previously published financial model to herein developed models of an alkaline flow electrolyzer and the local reaction environment. The second contribution builds on this model and consists of an optimization framework which allows to find economically optimal process and design parameters. This framework is subsequently used to devise an economically optimal electrolyzer design with a target production rate of 100 kg d^{-1} of pure ethylene.

The obtained results show that operational bottlenecks make the large scale implementation of electrochemical $\mathrm{CO_2}$ reduction processes more challenging than anticipated from previous, non-mechanistic techno-economic analysis. One of those bottlenecks comes in the form of a somewhat inverse relationships between the conversion and the selectivity, which manifests itself in low optimal values for the former ($<$ 0.3). A second bottleneck arises in the form of parasitic homogeneous reactions, which are shown to become substantial at higher alkalinities resulting from increased current densities. While neglecting these homogeneous reactions puts the economically optimal current density near values suggested in prior techno-economic analysis ($>$ 2000 A m^{-2}), incorporating them results in considerably lower values of $\approx$ 1000 A m^{-2}. Sensitivity analysis based on these results show that currently envisioned changes in the technological and economic conditions would not suffice to make the considered setup profitable, indicating that more research effort should be put into economically compelling system designs.

While these results are certainly insightful in themselves, the main outcome of this work is considered to be the developed modelling and optimization framework. Not only does it show that preliminary design optimizations can be done with currently available knowledge in the field, but also that they should be done in order to elucidate possible bottlenecks early in the design process. This work therefore lays the foundation for more holistic and model-based approaches towards rationally designed $\mathrm{CO_2}$ reduction systems.

Automated modeling and simulation of district energy systems

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Modeling of district energy systems is considered an essential tool for developing the next generations of district energy networks, and can be used e.g. for urban planning, automatic control and production planning. Modeling of networks is however a tedious process unless many of the required steps are automatized.

The process of automatic modeling of a district energy grid starts with data, that in most cases is not complete. Process knowledge is usually needed to ensure that missing data is replaced using valid assumptions.

From the data, the grid can be automatically modeled in one or several tools and languages of choice. Specialized tools for district energy simulation can be used, but in most cases only consider static scenarios with regards to the thermal dynamics. Languages used for modeling include, but are not limited to, Modelica, MATLAB, Julia and Python.

New technologies and concepts such as 4:th and 5:th generation district heating grids, smart grids, and utilization of waste heat have increased the complexity of the networks, and simulation of the thermal dynamics can provide additional insights in such scenarios. Examples of challenges include many different producers, production that is non-plannable, different supply temperatures and integration with electrical networks.

For most use cases, the complexity of the grid needs to be reduced to meet the demands of computational performance. Many available methods to reduce the complexity are tailored towards restricted use cases, such as only one producer, and might not be applicable.

The complete simulator setup might e.g. include a co-simulated physics-based environment, modeling of human behavior using machine learning methods, interfaces for weather predictions, automatic control simulation, and tools for visualization.

This multi-faceted way of simulation provides many upsides for integrating simulation as a natural tool for the whole life cycle of the process. Tools that are familiar to the user can be employed, that are often more mature than e.g. visualization tools integrated in monolithic simulation environments.

Session 6: Estimation and control

Microalgae production systems: modelling and control issues

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Microalgal-based technology is becoming an emerging and powerful solution for different industrial applications. They can be used to produce high value-added compounds, such as antioxidants, polyunsaturated fatty acids, cosmetics, pharmaceuticals, etc., to produce biomass or bio-diesel, or even to be used in the wastewater treatment process.

Microalgae culture can be cultivated in different type of photobioreactors depending on the final application. For instance, when high-value algal biomass is required, closed photobioreactors, and particularly, tubular photobioreactors, are normally used. On the other hand, when the production volume is most important than the quality, open photobioreactors are employed.

The microalgae production process is a very complex system, where the photosynthesis rate depends on solar irradiance and many other variables, such pH, dissolved oxygen (OD), or medium temperature. In most of the industrial photobioreactors, light requirements and operating temperature cannot be manipulated during normal operation and are determined by the reactor architecture. The rest of the variables should be handled using proper control techniques, especially for the pH and DO. These two variables need to be kept close to their optimal values and depend strongly on the photosynthesis rate.

This work briefly deals with the analysis, study and application of modeling and control strategies for the optimization of the microalgae process production in medium/large scale industrial photobioreactors. The proposed solutions try to achieve optimal work conditions that allow an efficient optimal growth of microalgae to be used for different purposes (cosmetic, human food, fish food and/or the wastewater treatment), pretending to reach an appropriate balance between the energy required for such a process, the injection of CO_2 for the maximization of microalgae production, and the recovery of costs through the resulting products.

Experimental results are presented, with tests performed in facilities available at the University of Almería, Spain.

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A simple and efficient PID control loop decoupler

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This presentation describes a control loop decoupler that decouples PID control loops efficiently, where the original PID controllers, with their tunings, are retained. The method is implemented in an industrial DCS control system. The structure is simple and automatic tuning procedures are provided to tune the decoupler.

A common problem in process control is that control loops interact in an undesired way. An obvious example is when one controller controls the flow in a tube, and another one the pressure. These two controllers will disturb each other. The most common solution to this problem in industry is to decouple the control loops by detuning one of the controllers. This will provide a decoupling, but the control in the detuned loop is deteriorated.

The fact that two control loops interact is normally not discovered until the two loops are tuned and put in operation. At this stage, it is often not desired to replace the two PID controllers by another controller structure such as a TITO PID controller or an MPC controller. In this project, the goal has been to derive a control loop decoupler that makes it possible to retain the two PID controllers with their tunings.

The decoupler is based on the inverted decoupling technique, where the decoupling is obtained by feeding the two control signals forward to the opposite controller. It was found that just static feedforward filters provided a significant decoupling. The two gains were determined in two ways. One way was to calculate the gains from just static relations, and the other one was to find gains that minimize the IAE values for the load disturbance responses obtained in the opposite loops when the loops were subjected to setpoint changes. It was found that these two approaches provided similar feedforward gains in most cases. For this reason, the simple static approach was chosen.

It was possible to retain the PID controller tunings, but the controller gains had to be multiplied by a compensating factor when the decoupler is operating. This is obtained by adding a gain scheduling function to the decoupler.

The control loop decoupler was tested on six TITO processes found in the literature. The IAE values were reduced by between 75% and 93% when the decoupler was introduced.

The project has been a collaboration between Lund University and ABB Process Automation, and the decoupler was implemented in the ABB controller family AC 800N for the DCS system ABB Ability System 800xA. Two automatic tuning procedures to obtain the feedforward gains were also implemented. One is based on open-loop experiments with step changes in the control signals, and the other one on closed-loop experiments with step changes in the setpoints.

Adaptive Tuning of Nonlinear Kalman Filters

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The most complicated part of tuning Kalman filters is to determine the noise statistics, especially the process noise. By assuming that the noise is due to parametric uncertainty in the model, one can approximate the noise statistics by propagating the parametric uncertainty through the state and measurement equations. To minimize the online computational cost, we propose to do this by either i) the Generalized Unscented Transformation (GenUT) or ii) Latin Hypercube Sampling (LHS). These methods require respectively $2n_\theta$ or N_{LHS} online model evaluations at each time step, where n_θ are the number of uncertain parameters and N_{LHS} is the number of samples and it is set by the user. Both approaches work for all kind of distributions, although the basic form of LHS require adjustment for correlated distributions. For the same online computational cost, the GenUT seem to give more consistent results than the LHS.

Robust Active Set Identification for Mathematical Programs with Complementarity Constraints.

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Reliable active set identification is required in several numerical algorithms for Nonlinear Programs (NLPs) such as ‘EQP’ style SQP solvers and as part of path-following algorithms for parametric NLPs. A similar requirement exists for Mathematical Programs with Complementarity Constraints (MPCCs): NLPs that also have one or more complementarity constraints, whereby a disjunctive formulation of inequality constraints are included in the program. We review pertinent results from the literature on active set identification and present new results concerning robust active set identification for NLPs and MPCCs. A feature of our approach is a weakening of the requirement that test points be within a tight neighbourhood of local extrema.