24th Nordic Process Control Workshop 2023

16-18 August 2023
Trondheim

Program and Book of Abstracts

Welcome

Dear Nordic Process Control community and friends,

Welcome to the 24th Nordic Process Control Workshop held 16-18. August in Trondheim. The workshop aims to bring together the Nordic process control community, and to provide a rather informal forum for presenting recent and ongoing work in the process control area. We encourage the presentation of new results, ongoing research, planned research or open problems where further work is needed. We hope the presentations and posters will stimulate good discussions and new collaborations.

The Nordic Process Control Workshop is organized by the Nordic Working Group on Process Control. It takes place every 18 month and aims to bring together academics, researchers, and practitioners from the Nordic countries to discuss recent advances in process control and its various domain applications. We also welcome contributions and participation beyond Nordic countries.

This year, the 19th Nordic Process Control Award will be presented to Prof. Dr.-Ing. Sebastian Engell for lasting and significant contributions to the field of process control. In particular his outstanding contributions to robust and optimizing process control methods are honored. A short biosketch of Professor Engell is given on page 2.

This workshop is arranged by the Department of Chemical Engineering at the Norwegian University of Science and Technology (NTNU) and is partially sponsored by the Center for research-based innovation *Subsea Production and Processing* (SFI SUBPRO).

Venue

The 24th Nordic Process Control Workshop will take place at Norwegian University of Science and Technology (NTNU). The Gløshaugen campus can be conveniently reached from the city center by public transport (bus lines 3 and 22, Bus stop: "Gløshaugen").

The **Tutorial, on Wednesday 16 August** will take place in the Auditorium K5 in the Kjemistry building (link to map: https://link.mazemap.com/YIIOlXhG). After the tutorial we will go to Peppe's restaurant (https://goo.gl/maps/1omCvX3Mq9zxKU1C6) for dinner (all participants at the tutorial and NPCW are welcome)

The **Workshop, 17-18 August** will take place in the Natural Science Building (Realfagbygget) in the Auditorium R5. (link to map: https://link.mazemap.com/7gqKN8e2)

After the main conference activities on **Thursday 17th August**, we will have a social programme. At **1730** we have a tour at Nidaros Cathedral (https://goo.gl/maps/m34xX7r1URJKQgmt8). One can take a bus directly from Gløshaugen campus or walk down to the cathedral. After the tour we have a tour and dinner at **1830** at Gubalari (https://goo.gl/maps/oLxg3P9b4S4G8Yqq9).

Local Organising Commitee

- Johannes Jäschke (Chair)
- Evren Mert Turan
- Lucas Ferreira Bernardino
- Igor Gabriel Ito Iwakiri
- Rafael David de Oliveira

The Nordic Process Control Award 2024

The Working Group awards the "Nordic Process Control Award" to persons who have a made a lasting and significant contribution to the field of process control.

Sebastian Engell

Sebastian Engell received the Dipl.-Ing. degree in Electrical Engineering from Ruhr-Universität Bochum, Germany in 1978 and the Dr.-Ing. degree in Mechanical Engineering from Duisburg University, Germany in 1981 for a thesis on the relationship between information theory and optimal filtering. 1984/85 he spent a year at McGill University, Montréal. In 1987, he received the venia legendi from Duisburg University for a monograph on the limits of the performance of linear control systems.

From 1986 to 1990 he was a group leader at Fraunhofer Institut IITB, Karlsruhe, Germany, responsible for process automation and production scheduling. 1990 he was appointed as Full Professor of Process Dynamics and Control in the Department of Biochemical and Chemical Engineering at TU Dortmund, Germany. 2002-2006 he served as Vice-Rector for Research and International Relations of TU Dortmund. He led several EU-funded projects, including a project which defined a roadmap in Cyber-physical Systems of Systems and the project CoPro – Improved energy and resource efficiency by better coordination of production in the process industries. Up to now, 86 young scientists under his supervision obtained a doctoral degree at TU Dortmund.

Sebastian Engell was appointed Fellow of IFAC in 2006. He received an ERC Advanced Investigator Grant in 2016 for the project MOBOCON (Model-based optimizing control – from a vision to industrial reality) and Best Paper Awards from Journal of Process Control and Computers and Chemical Engineering. In 2021, he received the Arnold Eucken Medal from the German Association of Process Engineering for his impact on the theory and practice of process control. His interests span a broad range in the field of process system engineering, including process control, real-time optimization, distributed optimization, scheduling, and optimization-based process design. A pertinent topic in his work has been how to handle uncertainty in control and optimization.

List of Nordic Process Control Award recipients

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 (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 (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) (Luleå University of Technology, Sweden, 17 March 2022)
19. Sebastian Engell (Germany) (Trondheim 17. Aug. 2023)

Nordic Process Control Working Group

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

NPC Working Group members

- Johannes Jäschke, NTNU, Norway (Chair)
- Francesco Corona, Aalto University, Finland (Co-chair)
- Wolfgang Birk, Luleå University of technology
- Gurkan Sin, DTU, Denmark
- Elling W. Jacobsen, KTH, Sweden
- Sigurd Skogestad, NTNU, Norway
- Jeno Kovacs, Sumitomo SHI FW Energia, Finland
- John Bagterp Jørgensen, DTU, Denmark
- Alf Isaksson, ABB, Sweden
- Bernt Lie, Telemark Univ. College, Norway
- Torsten Wik, CTH, Sweden
- Christer Utzen, GEA Process Engineering A/S, Denmark
- Iiro Harjunkoski, ABB Germany/Aalto Univ., Finland
- Morten Hovd, NTNU, Norway
- Jakob Kjøbstedt Huusom, DTU, Denmark
- Jari Böling, Åbo Akademi University, Finland
- Nicholas Alsop, Borealis, Sweden
- Olav Slupphaug, ABB, Norway

Program

Wednesday 16. August 2023

Tutorial: Optimal operation and advanced control using decomposition and simple elements

Presenters: Sigurd Skogestad and Lucas F. Bernardino

09:40	Coffee/tea and registration
10:00	Introduction (part 0)
10:10	Part 1: Introduction to APC. The three main inventions of process control
11:05	Break (10 min)
11:15	Part 2: Typical hierarchy, Decomposition approaches, CV selection, cascade, time scale separation
12:10	Lunch (40 min)
12:50	Part 3: Constraint switching, standard control elements
13:45	Break (10 min)
13:55	Part 4 : More elements
14:50	Coffee and tea (20 min)
15:10	Part 5: More examples, Inventory control
16:05	Break (10 min)
16:15	Part 6: ESC. RTO. Model-based methods (non-MPC). Input transformations, Dual EMPC?
17:10	Summary
17:20	End of tutorial
18:30	American pizza at Peppe's restaurant (all participants at the tutorial and NPCW are welcome)

Thursday 17. August 2023 – Workshop Day 1

08:00	Coffee / Tea and registration		
08:30	Opening		Johannes Jäschke
08:35	Award Ceremony		Johannes Jäschke
08:45	Award Lecture		Sebastian Engell
09:0	Coffee break		
09:50	Session 1: Industrial Practice		Chair: Sigurd Skogestad
	09:50	How to make control work in practice Krister Forsman (Perstorp AB, Sweden; NTNU), M. Adlouni	
	10:10	Advanced Control and Real Time Optimization in Ammonia Plants Brittany Hall (Yara International ASA), K. W. Mathisen, V. Alstad	
	10:30	Towards Autonomous Process Control - Experiences from Oil and Gas J.B. Jensen, Olav Slupphaug (ABB Energy Industries)	
	10:50	Online production planning for pulp mill through mill-wide optimization Matias K. Hultgren (Valmet Automation Oy), G. Fralic, L. Kouvo, S. Lehtonen	
	11:10	GEA Advanced Process Control (APC) for Continuous Freeze Drying (CONRAD) Marcus K. Nielsen (GEA), L. S. Theisen, C. Utzen	
11:35	Lunch		
12:40	Poster session (All authors present their posters		
13:40	Session 2: Process Control and Optimization		Chair: Lars Imsland
	13:40	A new method to deal with the saturation problem in feedforward control for measurable disturbances A. Hoyo, H. Hägglund, Jose Luis Guzman (University of Almeria), J.C. Moreno	
	14:00	Decentralized control for optimal operation under changing active constraints Lucas F. Bernardino (NTNU), S. Skogestad	
	14:20	Dynamic optimization of aluminium extrusion using a progressor transformation Trym A. L. Gabrielsen (NTNU), L. Imsland	
	14:40	Improving Primal Decomposition for Multistage MPC Using an Extended Newton method Simen Bjorvand (NTNU), J. Jäschke	
	15:00	Comparison of RTO-APC and Deep Reinforcement Learning for a simulated CSTR Soroush Rastegarpour (ABB Corporate Research), A. Isaksson, S. Munusamy, D. Patil, N. Kubal	
	15:20	Systematic selection of controlled disturbances in multi-stage model predictive control by online sensitivity analysis Halvor A. Krog (NTNU), J. Jäschke	
15:40	Coffee break + continuation of poster session		
16:30	End of poster session		
17:30	Social Activity: Guided tour in Nidarosdomen		
18:30	Conference Banquet		Gubalari

Friday 18. August 2023 – Workshop day 2

08:10	Session 3: Bio- and Medical Applications		Chair: Gürkan Sin
	08:10	Biosolutions I: A benchmark dynamic simulation model for bio-manufacturing processes Mohammad R. Boskabadi (DTU), A. Siavram, P. Ramin, J. Kager, G. Sin, S.S. Mansouri	
	08:30	Real-time Moving Horizon Estimation as a Soft Sensor in fed-batch Bioprocess Nadav Bar (NTNU), H. Bø, A. Tuveri	
	08:50	Data-driven modelling and predictive control solutions for pH control in microalgae-based processes Pablo Otálora B. (University of Almería), J.L. Guzmán, J.D. Gil, M. Berenguel	
	09:10	Model-based engineering and AI for bio-based manufacturing Gürkan Sin (DTU)	
	09:30	Safe System Identification through Model-Based Design of Experiment: A Type 2 Diabetes Case Study Sarah E. Engell (DTU), H. Bengtsson, J.B. Jørgensen	
09:50	Coffee break		
10:10	Session 4: Control and Estimation		Chair: Francesco Corona
	10:10	Enhancing Process Monitoring in Dynamic Membrane Systems for Wastewater Reclamation: A Framework for Data-Driven Fault Detection Morteza Zadkarami (DTU), K.V. Gernaey, A.A. Safavi, P. Ramin, O.A. Prado-Rubio	
	10:30	Comparison of Different Identification Algorithms for a Closed-Loop Stirred Tank Heater System Seyedarash Marashian (Åbo Akademi University), A. Marashian, K.H. Sadeghi, A. Razminia, J. Böling	
	10:50	Efficient Online Identification of PID Controllers and Plant Dynamics in Feedback Control Structures using Multi-Recursive Least Squares Estimation from Closed-Loop I/O Data Amirreza Zaman (Luleå University of Technology), K.T. Atta, W. Birk	
	11:10	Input estimation applied to selective catalytic reduction Alex Pesu (Åbo Akademi University), J.M. Böling, D. Rosenström, J. Torrkulla, T. Farjam	
	11:30	Estimation of absolute and distributed time delays in differential equations based on the linear chain trick Tobias K. S. Ritschel (DTU), J. Wyller	
	11:50	A System Level Approach to Closed-Loop Best-Response Dynamics Otacilio B. L. Neto (Aalto University), M. Mulas, F. Corona	
12:10	Lunch		
13:10	Session 5: Applications		Chair: Torsten Wik
	13:10	Analysis of potential lifetime extension through dynamic battery reconfiguration Albert Skegro (Chalmers University of Technology), T. Wik, C. Zou	
	13:30	Oscillating operation points in a pilot scale multiple dividing wall distillation column Lena-Marie Ränger (Ulm University), J. Hildenbrand, T. Grützner	
	13:50	Implementation and evaluation of model-based control of copper flotation Frida Norlund (Lund University), K. Soltesz	
	14:10	Control issues in solar furnaces Manuel Berenguel (University of Almería), J.D. Gil, J.L. Guzmán, L. Roca, I. Cañadas	
	14:30	Applicability of Ammonia Reactor Types for Power-to-Ammonia Joachim Weel Rosbo (DTU), A. Jensen, J. Jørgensen, J. Huusom	
14:50	NPCW 2025		Francesco Corona
14:55	Closing and Farewell		Johannes Jäschke

List of posters

Poster ID	Title and Authors
P01	Control-oriented 2D thermal modeling of battery cells for optimal tab and surface cooling Godwin K. Peprah (Chalmers University of Technology), T. Wik, Y. Huang, F. Altaf, C. Zou
P02	Applying control at molecular level: A reinforcement learning framework for optimally controlled natural flavor design Luana de Pinho Queiroz (University of Porto), C.M. Rebello, E.A. Costa, V.V. Santana, B.C.L. Rodrigues, A.E. Rodrigues, A.M. Ribeiro, I.B.R. Nogueira
P03	A Real-time model predictive control for the microbial bioprocess production of Pediocin Nadav Bar (NTNU), P. A. Lira-Parada
P04	Closed loop optimisation of uncertainty aware economic control policies Evren M. Turan (NTNU), J. Jäschke
P05	Approximate Model Predictive Control of Hybrid Systems using Multitask Deep Neural Networks Faiq Ghawash (NTNU), M. Hovd
P06	A plantwide control structure for improved flexible production of green Hydrogen Lucas Camman (NTNU), J. Jäschke
P07	Digital Twin Framework for Optimal and Autonomous Decision-Making in Cyber-Physical Systems: Enhancing Reliability and Adaptability in the Oil and Gas Industry Carine de Menezes Rebello (NTNU), J. Jäschke, I.B.R. Nogueira
P08	Integration of urban planning and design of energy systems using optimization-based control as an aid for decision-making Johan Simonsson (Luleå University of Technology), C. Ramos Càceres
P09	Novel Framework for Simulated Moving Bed Reactor Optimization Based on Deep Neural Network Models and Metaheuristic Optimizers: An Approach with Optimality Guarantee Vinicius Viena Santana (NTNU), M.A.F. Martins, J.M. Loureiro, A.M. Ribeiro, L.P. Queiroz, A.E. Rodrigues, I.B.R. Nogueira
P10	Model Predictive Control for bioreactors based on Escherichia coli core metabolic network model Marius Fredriksen (NTNU), J. Jäschke, R.D. de Oliveira, C.S. Nakama
P11	Virtual Reality for training hands-on operations of pilot plant - a digital educational tool. Jakob Kjøbsted Huusom (DTU), M. Stevnsborg, O.A. Pardo-Rubio, J. Kager, J. Dreyer
P12	Discrete-to-Continuous Dynamics Reconstruction for Bilinear Systems in Process Control Dina Shona Laila (Luleå Tekniska Universitet), P. Rumchinski, A. Johansson, R. Findeissen
P13	A Robust Learning Methodology for Uncertainty-Aware Scientific Machine Learning Models Erbet Almeida Costa (NTNU), C.M. Rebello, M. Fontana, L. Schnitman, I.B.R. Nogueira
P14	Recirculated gas-lift optimization using Self-optimizing Control Risvan Dirza (NTNU), K. Ødegård, E. Altamirada, S. Skogestad
P15	Simulation of ion-exchange chromatography for teaching purpose using Bioprocess Library for Modelica Jan Peter Axelsson (Vascaia AB), K.J. Brink

Paper ID	Title and Authors
P16	Sensor bias detection, isolation, and estimation in a gas-lifted oil well network Rafael David de Oliveira (NTNU), H.A. Krog, J. Jäschke
P17	Realistic Fault Simulation Platform for Testing Monitoring Strategies in Wastewater Treatment Plants Pedram Ramin (DTU), E. Ramin, U. Jeppsson, K.V. Gernaey, X. Flores-Alsina
P18	Online optimization of froth flotation processes Johan Lindqvist (Lulea Technical University)
P19	DEDS-Systems and Workflows Heinz A. Preisig (NTNU), V. Gautam, T.F. Hagelien, M. Horsch
P20	DEDS-Control and Desired State Orchestration in Cloud Computing Systems Vinay Gautam (NTNU), H.A. Preisig
P21	Receding-horizon control of full-scale wastewater treatment plants as water resource recovery facilities with energetic constraints Otacilio Bezerra Leite Neto (Aalto University), M. Mulas, F. Corona
P22	Mesoscopic thermodynamics of single-particle enzymatic reactions Francesco Corona (Aalto University)

Workshop

Optimal operation and advanced control using decomposition and simple elements.

Presenters: Sigurd Skogestad, and Lucas Ferreira Bernardino
Affiliation: Norwegian University of Science and Technology (NTNU)
Contact email: Sigurd Skogestad, sigurd.skogestad@ntnu.no

Control engineers rely on many tools, and although some people may think that in the future there will be one general universal tool that solves all problems, like economic model predictive control (EMPC), this is not likely to happen. The main reason is that the possible benefits of using more general tools may not be worth the increased implementation costs (including modelling efforts) compared to using simpler "conventional" advanced regulatory control (ARC) solutions. In particular, this applies to process control, where each process is often unique. In addition, for a new process, a model may not be available, so at least for the initial period of operation a conventional scheme must be implemented.

Control is about implementing optimal operation in practice under varying conditions (disturbances, prices, etc.). Most people think that on-line optimization (RTO) is needed to achieve this, but in many cases, it is possible to put the optimization into the control layer using the magic of feedback.

Since its introduction in the 1940's, about 80 years ago, advanced regulatory control (ARC) has largely been overlooked by the academic community, yet it is still thriving in industrial practice, even after 60 years with model-based multivariable control (MPC). So it is safe to predict that conventional ARC (including PID control) will not be replaced by MPC, but will remain in the toolbox along with MPC.

Thus, it is time to give conventional advanced regulatory control (ARC) a "new beginning" in terms of strengthening its theoretical basis and training engineers and students on how to use it in an effective manner. Conventional ARC includes the standard control elements that industry commonly uses to enhance control when simple single-loop PID controllers do not give acceptable control performance. Examples of such control elements are cascade control, ratio control, selectors, split range control, valve position control (VPC), multiple controllers (and MVs) for the same CV, and nonlinear calculation blocks.

This workshop takes a systematic view on how to design a conventional ARC system. The starting point is usually optimal steady-state economic operation. The process may have many manipulated variables (MVs) for control (typically valves), but usually most of these are used to control "active" constraints, which are the constraints which optimally should be kept at their limits at steady state. For the remaining unconstrained degrees of freedom, we should look for self-optimizing variables, which are measured variables for which the optimal values depend weakly on the disturbances.

In terms of control system design, we usually start by designing a good control system for the normal (nominal) operating point, preferably based on single-loop PID controllers where each manipulated variable (MV), which is not optimally at a constraint, is paired with a controlled variable (CV). To handle interactions, disturbances and nonlinearity, one may add cascade control, ratio control, feedforward control, decoupling and more general calculation blocks. However, during operation one may reach new (active) constraints, either on MVs or CVs, which may be easily observed from measurements of the potential constraints. Since the number of control degrees of freedom does not change, we will need to give up the control of another variable, which will either be another constraint (on CV or MV) or an unconstrained CV (self-optimizing variable). The key is then to know which variable give up, and in many cases we may observed by feedback and implemented using standard ARC elements.

A key new observation is that there are only four cases of constraint switching and these may be handled by using standard ARC control elements.

For CV-CV switching we use selectors (overrides), for MV-MV switching we use split range control or two other alternatives, for simple CV-MV switching (where the CV no longer needs to be controlled when the MV saturates) we don't need to do nothing (except for including anti-windup in the controller), and for "complex" CV-MV switching we need to make a "repairing of loops" by combining CV-CV and MV-MV switching.

The main disadvantage with conventional ARC compared to MPC is that it is based on single-loop controllers, so one needs to pair outputs (CVs) with inputs (MVs). For most processes this works well, but for more complex cases with many constraint switches one may get significant benefits and simplifications with MPC. Other cases where MPC may offer significant benefits compared to conventional ARC are for interactive processes and for cases with known future disturbances.

In summary, optimal economic operation may in many cases be achieved by use of simple conventional ARC elements, but there is a lack of understanding, both in industry and academia, on how such control systems should be designed. The workshop offers a new beginning in terms of providing a systematic approach.

Main reference: S. Skogestad, "Advanced control using decomposition and simple elements - An important and challenging research area". Annual Reviews in Control (2023).

About the presenters

Sigurd Skogestad received his Ph.D. degree from the California Institute of Technology, Pasadena, USA in 1987. He has been a full professor at Norwegian University of Science and Technology (NTNU), Trondheim, Norway since 1987. He is the principal author, together with Prof. Ian Postlethwaite, of the book "Multivariable feedback control" published by Wiley in 1996 (first edition) and 2005 (second edition). His research interests include the use of feedback as a tool to make the system well-behaved (including self-optimizing control and stabilization), limitations on performance in linear systems, control structure design and plantwide control, interactions between process design and control, and distillation column design, control and dynamics. His other main interests are mountain skiing (cross country), orienteering (running around with a map) and grouse hunting. He has received several awards and is a Fellow of the American Institute of Chemical Engineers (2012) and IFAC (2014).

Lucas Ferreira Bernardino received his M.Sc. degree from the Federal University of Rio de Janeiro (UFRJ), Brazil in 2019 and is now working on his Ph.D. degree on the topic of this workshop. His other interests are music (singing and playing the keyboard) and downhill skiing.

Presentations

How to make control work in practice

Authors: Forsman, K., Adlouni, M.
Affiliation: Perstorp
Contact email: Krister Forsman, Krister.Forsman@perstorp.com

To make automatic control solutions work in process industry some challenges need to be addressed:

- the final decisions on whether to use automatic controls are taken by operators, who need to believe in the solution implemented
- the specialists designing the control solutions need to work in cross-functional teams with well defined and efficient work processes
- performance indicators need to be defined to evaluate changes, and to find improvement areas

In this talk we describe how each of those challenges were addressed in a recent "Kaizen event" at a Perstorp production site.

For example we have seen from experience that working the "agile way" as is frequently done in software development is also well suited for process control optimization.

Advanced Control and Real Time Optimization in Ammonia Plants

Authors: Hall, B., Mathisen, K. W., Alstad, V.
Affiliation: Yara International ASA
Contact email: Brittany Hall, brittany.hall@yara.com

The majority of Yara's ammonia plants currently utilize Model Predictive Controllers (MPC) for Advanced Process Control (APC). While this type of controller is good at controlling the plant towards its hard constraints (pump capacities, valve openings, design temperatures, etc.), it is not able to fully optimize the operation (optimal production load to minimize energy usage, optimal methane slip from primary reformer, etc.). Instead, operators are left to manually make adjustments based on their experience. This is the motivation behind the development of a Real Time Optimization (RTO) layer for our ammonia plants. While RTO layers have long been used in e.g., refineries, petrochemicals, and NGL/LNG producers, they have not been taken widely into use in the chemical industries and there are no reported applications from the fertilizer industries. This is probably due to a combination of process complexity and limited benefits. However, with the increased focus on emission reduction, improving energy efficiencies, and making our existing plants as profitable as possible, the motivation for implementing a RTO layer has increased. We decided to develop a RTO application in-house to utilize our process knowledge and competencies in process modelling, control and optimization, as well as in data science, and data engineering. The RTO layer will consist of several components: data fetching and validation, data reconciliation (mass, component, and energy balance), performance monitoring, and technical or monetary optimization. We will present the current project status and results from the pilot implementation in one of our modern European ammonia plants.

Towards Autonomous Process Control - Experiences from Oil and Gas

Authors: Jensen, J.B., Slupphaug, O.
Affiliation: ABB Energy Industries
Contact email: Olav Slupphaug, Olav.Slupphaug@no.abb.com

We will share experiences from design, implementation and operationalization of close to fully automatic start-up of complex oil and gas production systems. The perspective taken is from the panel operator point of view.

Online production planning for pulp mill through mill-wide optimization

Authors: Hultgren, M., Fralic, G., Kouvo, L., Lehtonen, S.
Affiliation: Valmet Automation Oy
Contact email: Matias Kristian Hultgren, matias.hultgren@valmet.com

The present work describes the outcomes of a mill-wide optimization project in a pulp mill. Individual process areas are increasingly being optimized through advanced process control in the pulp and paper industries, but process areas also interact with each other and generate bottlenecks that limit the overall production. Mill-wide optimization is introduced as a solution for coordinating process areas through the prediction, optimization, and visualization of future operations across the mill. Therefore, it is an important step in the general development towards autonomous mills.

A systematic mill-wide optimization approach is presented in this work. The solution is based on single-objective equation-oriented flowsheet optimization, with fitted unit operation models based on historical data, and discrete states for shutdowns and grade changes. The optimization simultaneously evaluates the future trajectories of selected production variables for the defined optimization horizon, with respect to time-variant constraints. Mill-wide optimization was solely employed here for production planning, but application concepts like quality planning and grade scheduling have also been developed.

The mill-wide production planning solution was implemented for the first time as an online advisory system in a market pulp mill, where eleven process area production rates were continuously optimized for three-day periods to maximize pulp production and additional secondary objectives. A mill-wide optimization audit was conducted to evaluate the process area bottlenecks based on historical data, and the constructed process model and optimization setup were subsequently used in the online production planning application. Results proved the feasibility of the technology on an industrial scale and clearly demonstrated the production efficiency improvement potential, with use cases for production debottlenecking, fiber line and recovery line coordination, and maintenance planning. The results form a solid foundation for the global optimization of pulp mill performance based on production, quality, and energy in the future.

GEA Advanced Process Control (APC) for Continuous Freeze Drying (CONRAD)

Authors: Nielsen, M. K., Theisen, L. S., Utzen, C.
Affiliation: GEA
Contact email: Marcus Krogh Nielsen, marcuskrogh.nielsen@gea.com

It is now more than 10 years ago that GEA started development of APC solutions for the process industry. Today, GEA delivers APC software-as-a-service (SaaS) to spray drying customers world-wide. The software is based on model predictive control (MPC) and steady-state real-time optimisation (RTO). The product portfolio started with industrial spray dryers, but today the portfolio also includes other processes in the drying line, e.g. evaporators. The software can increase throughput, quality, stability, as well as reduce energy consumption. At GEA, we have experienced that for an APC solution to continue to deliver value to customers, the software must be continuously maintained and improved to meet new product specifications, process changed, operator changed, as well as modelling and controller tuning. Therefore, GEA today delivers a subscription-based APC SaaS solution. 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.

The latest addition to the APC product portfolio is the OptiPartner CONRAD. The CONRAD is a continuous freeze drying process. In the process, frozen granulate enters a vacuum tunnel at approximately -40 degrees Celsius. In the vacuum chamber, the frozen granulate is exposed to radiated heating from heating plates as it travels through several heating zones of varying temperatures. After spending several hours in the chamber, the granulate exits the vacuum chamber with desirably low moisture levels. The process contains significant delays, making it an ideal candidate for predictive model-based control applications. The APC solution for the CONRAD manipulates the temperature of the heating plates in 10 heating zones to maintain a stable and low residual moisture level of the final freeze dried product, while constraining inputs and outputs meet equipment and product specifications as well as costumer and process demands. The large delays of the CONRAD makes it practically inconvenient to perform step response experiments. As a result, the MPC uses a linearised grey-box model that has built-in physics behind the process that we control.

A new method to deal with the saturation problem in feedforward control for measurable disturbances

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This works treats the problem of control signal saturation caused by feedforward control from measurable load disturbances. An efficient feedforward compensator will often give significant peaks in the control signal at fast changes in the load disturbance. These peaks may cause the control signal to reach a saturation limit. Typically, when feedforward compensators are combined with PID controllers, the saturation problem is managed by the anti-windup control scheme. In the work, we show that the anti-windup function may cause unnecessarily sluggish responses in those cases. To face this problem, a modification of the classical feedforward control scheme is suggested, based on the reduction of the feedforward compensator gain during periods when the control signal is in saturation. A method to calculate this gain reduction is given based on the process parameters. The proposed idea is evaluated first through several simulated examples and is also tested on a lab-scale temperature control system to demonstrate the noticeable practical capabilities.

Decentralized control for optimal operation under changing active constraints

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Optimal economic operation of chemical plants requires control of active constraints, which may change because of disturbances. In addition, one should ensure optimality with respect to the unconstrained degrees of freedom by driving the reduced cost gradient to zero. One solution is to use on-line optimizing control, but the preferred approach in industry is to use decentralized control and selectors whenever possible. In this paper, we consider a new framework based on identifying the cost gradient projections that can be left uncontrolled when each specific constraint becomes active, leading to a decentralized logic. The proposed framework is applied to the optimal operation of the Williams-Otto reactor, which has two degrees of freedom and two constraints. The projection matrices, which depend on the gradient of the constraints, are assumed constant, resulting in a simple control structure. The approach works well in simulations and is able to switch between the four active constraint regions. Even though a small economic loss is observed because the constraints are not linear in the inputs, this loss may be eliminated by relinearizing the constraints' model and updating the projection matrices for the reduced cost gradient during operation.

Dynamic optimization of aluminium extrusion using a progressor transformation

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Motivated by dynamic optimization of aluminium extrusion, this paper demonstrates how a progressor transformation of dynamical models can simplify the implementation of simultaneous methods for dynamic optimization. The implementation of direct collocation becomes difficult when the model exhibits known discontinuous changes, but at unknown times. If the model changes happen at known values in another progressor, the model can be transformed and implemented effortlessly. An example from the extrusion process is given, where the extrusion process model is transformed from time to extrusion length. The transformation allowed the implementation of direct collocation. In addition, the predictability of the transformed model allowed nearly a 50 percent reduction in state variables for describing the aluminium billet throughout the extrusion phase

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Improving Primal Decomposition for Multistage MPC Using an Extended Newton method

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Multistage model predictive control is a ro- bust MPC formulation that takes into account parametric uncertainty by constructing a finite set of coupled scenar- ios. As the amount of scenarios increase so does com- putational cost and real-time implementation might not be possible. Scenario decomposition has been proposed to distribute computations and make real-time implementa- tion possible, however, typically the subproblems are co- ordinated using the steepest descent method with slow convergence properties. In this paper a primal decompo- sition algorithm is improved by the use of a nonsmooth Newtons method for continuous nonsmooth equations. The proposed algorithm is applied to a gas-lift optimization sys- tem and compared to the standard primal decomposition method using steepest descent.

Comparison of RTO-APC and Deep Reinforcement Learning for a simulated CSTR

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Deep Reinforcement Learning (RL) techniques have gained popularity in recent years for their ability to learn from a given environment and provide optimal actions. Although this algorithm is highly effective for carrying out data-driven optimal control, it is limited to the availability of high-fidelity models, particularly when different interactions and experience with the environment are not practically feasible. It also struggles to guarantee the closed-loop behavior of the process near boundary conditions. In contrast, economic model predictive control solutions, like Real-Time Optimization (RTO) and Advanced-Process Control (APC), are standard tools for complex chemical processes with constraints and benefit from a rich theory to assess their closed-loop behavior. However, these solutions are limited to a valid operational range and rely on the quality of the underlying model for effectiveness. This presentation explores the use of Reinforcement Learning (RL) for optimal decision-making in a simulated CSTR. By comparing different methods such as RTO+APC and RL, the study aims to identify the most effective approach for decision-making and improving operational efficiency against disturbance variations. In fact, it compares RL with available optimal industrial solutions (RTO+APC) and examines the impact of model mismatches on their closed-loop performance. The study also investigates robustness and strict dissipativity for algorithm stability when the controllers (RL agent and RTO+APC) are designed using a low fidelity model. It should be remarked that the experimental tests and evaluations were quantitatively conducted on a CSTR case study. However, the results obtained can be generalized and serve as a guidebook for researchers and engineers interested in utilizing RTO+APC and RL techniques for process control algorithms.

Systematic selection of controlled disturbances in multi-stage model predictive control by online sensitivity analysis

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Multi-stage model predictive control (MS-MPC) is a popular approach in literature to control a system with uncertainties. The idea is to create a scenario-tree of the disturbances that can happen in the plant. These scenarios are embedded into the MS-MPC, and the controller will then ensure that the constraints of the system will not be violated if the modelled scenarios occur. The computational cost of solving the resulting optimization problem (a NLP) is high, and therefore the scenario-tree is simplified. One simplification is that we limit ourselves to incorporate only a few disturbances into the NLP, even if we know the plant is subjected to many disturbances. To the authors knowledge, there are no systematic methods on how to select which disturbances to control in the MS-MPC. Furthermore, we ask ourselves if it is reasonable that the same subset of disturbances should be used in the MS-MPC over the whole time horizon? We suspect this is not the case, especially for batch processes. As an example, when the substrate concentration is high in a bioreactor, it is reasonable to assume that disturbances/parameters relevant for the substrate are important to control. However, they might not be relevant when the substrate is depleted. We address the issue of systematically selecting the disturbance to control in MS-MPC by doing sensitivity analysis on the process model with respect to the constraints at each time step. The results on a case study with a fed-batch bioreactor show that this is a promising method to address one of the main issues with MS-MPC.

Biosolutions I: A benchmark dynamic simulation model for bio-manufacturing processes

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The growing prevalence of chronic disease, personalizing medicine, advancement in biotechnology, government support and regulatory environment and increasing patient awareness has led to increasing biopharmaceutical products and expanding research in this field. One of the most critical indicators of designing and improving biopharmaceutical processes is maintaining the quality of products along with increasing the capacity of the mentioned processes while moving towards a reduce waste and more sustainable production. Batch/fed-batch bioprocessing is currently the state of the art in the biopharmaceutical industry, and shifting from batch to continuous process is considered a solution to increase production capacity which also considered by FDA as an approach to ensure and improve the product quality (Ashely et al. 2014). Although there are some examples of continuous manufacturing at least in some steps of production the main barriers to moving from batch to continuous operation are on the one hand a stable process design incorporating up- and downstream unit operations and on the other hand to continuously monitor and control the quality and performance attributes along this integrated process. In this regard simulation models can be used to test and evaluate various process operation ranges but also, designing control systems and product quality monitoring. There has been some useful examples demonstrated for chemical industry such as Tennessee Eastman process (Downs et al. 1993) and for wastewater domain such as BSM no.1(Alex et al. 2008). However there is a lack of plant-wide benchmark process simulation platforms dedicated for biopharmaceutical domain. To address this need, Biosolutions I has been introduced as a dynamic benchmark process model in the biopharmaceutic area which already primarily introduced by Boojari et al. (Boojari et al. 2022). Here we present the production of lovastatin as an

exemplary process. The analyzed process consists of two parts, the upstream section, which includes cell culture and harvest stages, and the downstream parts, which include stages from cell separation to the final purified product. To control product quality attributes, a novel control system has been proposed. The control system has been designed based on the degree of freedom (DOF), relative gain array (RGA), and Niederlinski Index (NI). Biosolutions I benchmark model control structure and process units have been implemented into a computational simulation model, which was developed in Matlab/Simulink. Based on a stable process design and optimal operation the control system behavior was analyzed in detail. Hereby different scenarios were tested: a) a step change was applied in the lactose concentration input as a reactant, and the result has been discussed. b) In the second scenario, a pulse generator has been added to lactose concentration. In this scenario, realistic measurement delays and uncertainties gave valuable information on critical measurement points and plant behavior. The benchmark process can now be extended to more biopharmaceutical processes and used to study, test and demonstrate various control, monitoring and machine learning strategies on biopharmaceutical field.

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Real-time Moving Horizon Estimation as a Soft Sensor in fed-batch Bioprocess

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A hindrance in the development of process control and digital twins in the bioprocess industry is the scarcity of real-time direct measurements. Bacteria are used to produce a range of products within the pharmaceutical and food industry, however, they are characterized by a nonlinear time-varying dynamics, making them hard to model accurately. Combined with noisy and scarce real-time measurements, control of such continuous cultivations becomes a challenging task.

The Moving Horizon Estimaton (MHE) can address this issue by combining measurements with a process model, incorporating physical constraints to estimate states. The MHE can thereby act as a soft sensor allowing for real-time monitoring, and enabling control to improve product quality and yield. We demonstrated the first MHE use as a state estimation of a continuous cultivation of *C. glutamicum* with a limited sugar measurements. The bioreactor had online measurements of volume, cell density, and CO2, while at-line measurements of sugar were taken every hour, and offline samples of biomass cell dry weight (CDW) were taken every $\tilde{2}$-4 hours. Parameter Estimation was performed to determine parameters for the MHE, and further, the MHE tuned to the process. Two real-time runs with MHE were performed and evaluated.

The study demonstrates that real-time state estimation of sugar is possible in a *C. glutamicum* cultivation using MHE. The estimator follows the sugar dynamics with a low RMSE for the three experimental runs (two in real-time). The study highlights the importance of reliable measurements from stable and correctly calibrated equipment for optimal soft sensor performance. Suggestions for improvement include exploring alternative arrival cost updates, and conducting longer cultivation experiments to assess long-term efficiency. Future work should involve closed-loop control experiments to determine the robustness of the soft sensor for control purposes.

Data-driven modelling and predictive control solutions for pH control in microalgae-based processes

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This work presents a methodology based on neural networks and nonlinear model predictive control for pH control in raceway photobioreactors used in microalgae production. Microalgae production is a highly sustainable process with a multitude of interesting applications. However, due to its biological nature, characterizing and effectively controlling and optimizing the process poses significant challenges. In this study, recurrent neural networks were employed to emulate ARX type models, incorporating the inherent nonlinear behavior of the system. The model is developed using data acquired from a real system and validated with satisfactory results. Subsequently, a practical nonlinear model predictive control (PNMPC) strategy was proposed in order to optimize the system by maintaining the pH at its reference value while minimizing the control action required. The obtained results have been validated in semi-industrial scale installations, and demonstrate the effectiveness of the proposed methodology in optimizing pH control in raceway photobioreactors for microalgae production, contributing to the advancement of efficient and sustainable microalgae production processes.

Model-based engineering and AI for bio-based manufacturing

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In today's process industries, software tools employing state-of-the-art simulation models and advanced optimization and control algorithms are used at different stages of the project life cycle, from early stages performing scale-up and conceptual process design, front-end engineering design to retrofitting and optimization studies at the plant commissioning/operation stage. The impact of advanced process modeling and simulation, optimization and control is profound and has become mainstream in the chemical industries due to the significant economic benefits achieved. These are amongst crown achievements of the process systems engineering community in Chemical Engineering discipline. This is in particular thanks to research in modeling and simulation, mathematical programming, process synthesis and design, process control and optimization that has been performed in the past decades. Today there new paradigms in computing technologies affecting the bottom line of process industries but also universities alike namely digitalization, quantum computing, machine learning/Artificial Intelligence (AI), climate change, decarbonization, sector coupling through renewable energy, etc. These technologies open up new horizons for industry to become more efficient, to decrease CO2 footprint and to develop innovative products and services. In this talk I present our experiences with AI/machine learning in advancing the agenda for model based engineering for bioprocess industries at DTU process systems engineering lab: (1) Hybrid modeling combining artificial neural network with mechanistic models for fermentation processes at production scale, (2) Graph neural network modeling for pure-component, environment and safety related property predictions. I end the talk with a critical outlook based on a survey of digitalization on Danish life science industries and share our thoughts for the AI applications in bio-based industry.

Safe System Identification through Model-Based Design of Experiment: A Type 2 Diabetes Case Study

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A representative system model is valuable when testing and designing controllers. However, in safety-critical systems, it can be a challenge to run safe experiments to parametrize such models. Model-based design of experiment (MBDoE) offers a framework to select optimal system inputs for parameter identification under constraints. Still, when a plant-model mismatch is present, there is no guarantee that the MBDoE protocol is safe. In this work, we apply MBDoE to learn optimal excitation patterns. Instead of implementing the MBDoE protocol in open loop, we mimic the MBDoE output curve and apply it as a reference for the system. We employ a reference-tracking controller to follow the output curve and collect data for parameter estimation. In a type 2 diabetes case study, we apply the proposed method to identify three parameters in an insulin dose-response model. For 100 virtual people, we collect experimental data and identify personalized dose-response models. With the models, we can predict a safe and effective insulin dose to control blood glucose levels in each individual. In other safety-critical systems, the proposed method may offer a safer alternative to implementing a MBDoE protocol in open loop.

Enhancing Process Monitoring in Dynamic Membrane Systems for Wastewater Reclamation: A Framework for Data-Driven Fault Detection

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The increasing demand for wastewater reclamation, driven by sustainable development goals and population/industrial growth, has led to the development of dynamic membrane systems, which have shown promising results in facilitating wastewater reuse. To ensure water quality and address environmental and financial considerations, effective process monitoring is crucial. However, monitoring dynamic membrane systems in industrial settings can be difficult due to fluctuations in input conditions and disturbances (i.e. backflush and backshock). These conditions make it challenging to interpret the complex sensor signals and accurately characterize membrane fouling, ultimately leading to suboptimal system performance. In this work, a straightforward framework for fault detection is developed employing advanced signal processing techniques and different classifiers. The case study is a pilot-scale dynamic ultrafiltration for petrochemical wastewater reclamation, in which three of the 18 experiments are considered faulty. First, a feature analysis method based on wavelets is used to reveal primary characteristics of the sensor signals while minimizing the impacts of noise. To evaluate the efficiency of the features, the wavelet energy response of the measurement signals was studied along with considering statistical indices including correlation and confidence interval criteria. The obtained features are passed on to several classifiers, such as Multilayer Perceptron Neural Network (MLPNN), Support Vector Machine (SVM), and Principal Component Analysis (PCA), to determine the process conditions (i.e., undesired membrane fouling rates). The results of this study suggest that the MLPNN classifier has the highest detection accuracy of 99.7% while the PCA-based approach could detect 92% correctly. Moreover, the False Alarm Rate (FAR) of these models is less than 2%. The study demonstrates the efficient feature extraction capabilities of the proposed framework, leading to promising detection results when using commonly employed classifiers. This makes the framework well-suited for designing automated surveillance techniques for monitoring dynamic

ultrafiltration membrane processes employed in digitalization schemes.

Comparison of Different Identification Algorithms for a Closed-Loop Stirred Tank Heater System

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The accurate identification of parameters in a stirred tank heater system is crucial for ensuring its effective control design and analysis. In this paper, we address the parameter estimation problem of a stirred tank heater system in a closed-loop configuration, considering it as a stochastic system. Six different algorithms are explored, i.e., Gradient-based Iterative (GI), Multi-Innovation Gradient-based Iterative (MIGI), Generalized Projection (GP), Two-Stage GI (2S-GI), Two-Stage MIGI (2S-MIGI), and Two-Stage GP (2S-GP), to identify both linear and nonlinear models of the system. By employing these algorithms, we analyze the convergence rates and compare the resulting estimation errors. The simulation example is used to test the effectiveness of the proposed identification algorithms.

Efficient Online Identification of PID Controllers and Plant Dynamics in Feedback Control Structures using Multi-Recursive Least Squares Estimation from Closed-Loop I/O Data

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This study introduces an innovative solution for online identification of closed-loop control systems, addressing important challenges in the identification process, specifically for plants governed by PID controllers, with a focus on enhancing flexibility, real-time monitoring, and applicability in the identification process. The proposed approach utilizes hierarchical recursive least squares parameter estimation methods to estimate the dynamics of the process and controller, as well as the amplitude of the modeled measurement noise in the output. To achieve this, it leverages closed-loop input-output information and nominal controller values based on ARMAX modeling. Additionally, this approach presents new parameter identifiability conditions for each stage of the system identification protocol. These conditions are substantiated with mathematical proofs, ensuring the reliability and accuracy of the identification process. The effectiveness of the approach is demonstrated through numerical results, showcasing its capability to estimate real-time plant and controller dynamics, even in the presence of uncertainties. The simulations also highlight the approach's ability to detect sudden changes in system and controller parameters, further emphasizing its robustness. Overall, the presented approach significantly improves key aspects of the closed-loop identification process. By incorporating recursive least squares parameter estimation methods and establishing new parameter identifiability conditions, it enhances the flexibility, real-time monitoring, and applicability of the identification process.

Input estimation applied to selective catalytic reduction

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The marine sector is always under scrutiny concerning exhaust gas emissions and therefore after treatment technologies such as selective catalytic reduction (SCR) are constantly optimized to achieve less emissions with a lower cost. The SCR works that way that the NOx from the exhaust gas is reduced by adding NH3. One cannot add too much NH3, as that will lead to ammonia slip. The main practical challenge is to estimate the amount of ammonia inside the catalyst. The ammonia storage capacity of the catalyst is quite large, but if we are close to either limit, a small disturbance will lead to quickly rising concentrations of either NOx or NH3. State-estimation techniques such as Kalman filter can be used to analyze and predict the internal states and output signal of a complex dynamical system, such as the SCR unit, to make the control of that system easier. The SCR system is however nonlinear, and Kalman filters can be extended for such systems. Furthermore, standard estimation methods rely on that the input signals of a system are completely known. In reality, however, this is not always the case, and in the SCR- unit it is possible that for instance the injected ammonia is not precisely known. The NOx-emissions are not always measured either. Unknown deviation in the system inputs can lead to large deviations in the estimates, but it is possible to augment the system model with states that describe such input deviations and try to estimate these. In this work, such an input estimator is tested on simulations of a nonlinear system, and it is found that significant improvements are possible, compared to an estimator that does not take into account possible input deviations.

Estimation of absolute and distributed time delays in differential equations based on the linear chain trick

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Many dynamical processes involve time delays, and they have a significant effect on the stability and dynamics of the process. Therefore, it is important to account for them when designing an advanced process control strategy. However, identifying delays in general nonlinear differential equations is not trivial because the numerical simulation of such systems requires specialized methods. Therefore, in this presentation, we 1) describe how delays (both absolute and distributed delays) can be approximated by a distributed delay with an Erlang probability density function as kernel (also called memory function), 2) use the linear chain trick (LCT) to transform the resulting distributed delay differential equations (DDEs) to ordinary differential equations (ODEs), and 3) formulate the delay identification problem as a least-squares parameter estimation problem. We solve this problem using a single-shooting method and we compute the gradient of the objective function using a forward approach. We implement the method in Matlab, and we solve the involved optimization problem using fmincon. Furthermore, we discuss different regularization strategies for encouraging sparsity in the kernel parameters as well as an either small or large kernel derivative. Finally, we present numerical examples involving joint parameter and delay estimation in the logistic equation and in an exothermic chemical reaction in a continuous stirred tank reactor (CSTR).

A System Level Approach to Closed-Loop Best-Response Dynamics

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Modern cyber-physical systems are usually comprised of multiple subsystems operated by local self-interested decision-making agents. The inherent large-scale and distributed nature of most applications, together with information asymmetry, render the centralized approach to controller design not applicable. Dynamic game theory provides a framework for determining competitive equilibria (e.g., the Nash equilibrium [1, 2]) which provide locally optimal, yet strategically stable, operating conditions for each non-cooperative agent. However, the computation of a Nash equilibrium is a challenging task, except for specific problems [3]. In particular, potential games characterise a broad class of problems for which a Nash equilibrium can be obtained efficiently using Best-Response Dynamics (BRD) algorithms [4, 5]. In dynamical settings, BRD methods are mostly studied for computing open-loop Nash equilibria, where the strategy of each player depends only on the initial state of the game. The design of numerical routines for obtaining closed-loop equilibria, where agents react to changes in the game state, is still under active research.

In this work, we present a method towards the computation of closed-loop ε-Nash equilibria of dynamic potential games. We restrict ourselves to affine-quadratic difference games. Leveraging the recent System Level Synthesis approach (SLS, [6]), we propose a BRD algorithm in which the agents iteratively update their strategies by optimizing system responses from the other players' actions. By parameterizing all stabilizing controllers, these system responses can then be used to reconstruct a state-feedback control strategy for each player. Due to its closed-loop nature, the resulting strategy profiles allow the agents to simultaneously react to perturbations on the game state. Additionally, the method allows to enforce desirable structures to each controller (e.g., spatiotemporal information patterns), without changing the structure of the game. We demonstrate the behaviour of this method on illustrative examples.

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Analysis of potential lifetime extension through dynamic battery reconfiguration

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Growing demands for electrification result in increasingly larger battery packs. Due to factors such as cell position in the pack and variations in the manufacturing process, the packs exhibit variations in the performance of their constituent cells. Moreover, due to the fixed cell configuration, the weakest cell renders the pack highly susceptible to these variations. Reconfigurable battery pack systems, which have increased control flexibility due to additional power electronics, present a promising solution for these issues. Nevertheless, to what extent they can prolong the battery lifetime has not been investigated.

This simulation study analyzes the potential of dynamic reconfiguration for extending battery lifetime w.r.t. several parameters. Results indicate that the lifetime extension is larger for series than for parallel configurations. For the latter, the dominant factor is equivalent full cycles spread at the end of life, but resistance increase with age and the number of cells in parallel are also influential. Finally, for the former, the number of series-connected elements amplifies these effects.

Oscillating operation points in a pilot scale multiple dividing wall distillation column

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Distillation processes cover around 3% of the energy consumption in Europe. A promising way to reduce this significant amount is to use intensified processes like dividing wall columns. This contribution focuses on a dividing wall column with two walls that is suitable for the separation of a quaternary mixture in only one shell. This setup can save up to 55% of energy compared to the related conventional column sequence. However, this statement has so far only been based on theoretical calculations. In order to push the development further, the world's first multiple dividing wall column was put into operation at the end of 2021 at Ulm University in Germany. Since then several preliminary studies were performed regarding the columns start-up, stationarity behaviour and heat losses. The obtained results are considered as a proof-of-concept. Nevertheless, recently an uncommon behaviour was observed during some experiments with constant liquid split ratios: The temperatures inside the column do not reach steady-state value but oscillate in a stable manner between two levels, which are assumed to be two alternating operating points. The behaviour could be reproduced, however sometimes the exact temperature levels and oscillation periods differ. It was tested to hold only one of the two points via a temperature control of the liquid splits, which stopped the oscillation but resulted in another operating point with different temperatures inside the column. To the best of the authors knowledge this behaviour has not yet been described in literature. Thus, the aim of this contribution is to first introduce the pilot column and then present the experimental results from the plant showing the oscillating behaviour in detail. The authors hope on fruitful discussions regarding possible reasons for this behaviour and ideas regarding its control.

Implementation and evaluation of model-based control of copper flotation

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When producing metals, flotation is used to separate copper from waste rock, to increase the concentration of mineral. Flotation utilizes differences in surface properties to make the desired minerals attach to air bubbles rising through a tank cell. On top, a mineral froth–the product–is formed, and it is collected as it flows over the edge of the cell. Therefore, good level control is essential to receive good recovery.

Level control in Boliden's Aitik concentrator, near Gällivare, Sweden, was targeted and different traditional controllers, as well as a reinforcement-learning based controller, were evaluated in a simulation environment. This showed that model-based controllers, such as linear quadratic (LQ) controllers or model predictive controllers, show potential to improve the performance compared to the cascaded PI-structure used in the plant. The model-based controllers, and especially the LQ-controller, show good robustness towards model errors.

This led us to implement the LQ-controller in the plant, with pleasing results. The main benefits are seen when big abrupt changes in the inflow to the flotation process occurs. The level deviation caused by the disturbance was, in the first flotation cell, reduced from 28cm with the PI-controllers to 6cm with the LQ-controller. The implementation further confirms the robustness of the controller with respect to model errors. As an example, the control signals relation to the flow through the valves is non-linear in the real process, while in the simulation it is assumed to be linear. Despite this, the LQ-controller shows stable performance when operating the real process with a control law designed with the linear simulation model.

In this presentation we walk through the process of modeling, simulating, designing, implementing, and finally evaluating a new controller at the Aitik plant. We put a particular emphasis on encountered real-world challenges and how they were met.

Control issues in solar furnaces

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This work presents some control challenges in solar furnaces. Solar furnaces are facilities used to perform thermal treatments of materials using solar energy. A solar furnace is a system that is of great interest both for research purposes and as a benchmark for students, since the main source of energy for the process is also a main disturbance (this being a feature of most of the systems that make use of solar energy). Solar furnaces have very interesting characteristics from the modelling point of view, since they have a non-linear behaviour in which the dynamics change with the operating point and are different depending on the kind of sample to be tested, presence of uncertainties in the characteristics of the materials being tested, influence of disturbances in the energy source and non-linearities in the actuation systems, among others. From the control point of view, it is a SISO system subjected to disturbances, which makes it a suitable candidate to apply concepts of linearisation, PID+antiwindup control, feedforward, feedback linearisation, etc. This work shows the application of some of these techniques to the solar furnace of the Plataforma Solar de Almería (Spain).

Applicability of Ammonia Reactor Types for Power-to-Ammonia

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Ammonia reactors can on a general level be categorised into three different types: Internal direct cooled reactor (IDCR), Adiabatic indirect cooled reactor (AICR), and Adiabatic quench cooled reactor (AQCR). The AQCR configuration was originally most common due to its simple design, but the industry is contin-uously replacing AQCRs and building new plants with IDCR and AICR reactors (Inamuddin et al., 2020). The IDCR and AICR reactor yields a higher conversion per reactor volume but also involves a more com-plicated design with integrated heat exchange. Previous comparison of ammonia reactors has been based on conventional operation with reliable reac-tant supply from steam-methane reforming (Khademi & Sabbaghi, 2017). However, the emerging market for Power-to-Ammonia (P2A) defines an entirely new flexible operating regime with fluctuating energy supply from intermittent renewable sources. In this work, we investigate the applicability of the three types of ammonia reactors for Power-2-Ammonia. We formulate a steady-state and transient model for all three reactor types. Based on the steady-state model, the optimum reactor conditions are identified, and the reactant conversion is com-pared between the reactor types. The robustness of the reactors for operating with fluctuation reactant supply is evaluated through eigenvalue stability analysis and transient step disturbance simulations as performed for an AQCR (Rosbo et al., 2023). The stability analysis identified unstable steady states and extinction points of the reactors, which we later verified in transient simulations. This revealed significant differences between the transient behaviour of the ammonia reactors as the AQCR configuration dis-played server oscillatory transients while the IDCR and AICR showed little to no oscillations.

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Posters

Control-oriented 2D thermal modeling of battery cells for optimal tab and surface cooling

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Tab cooling offers homogenous cooling of the cell leading to a significant reduction in temperature gradients, thus prolonging battery lifetime. However, surface cooling is more effective at removing heat due to the larger surface area of batteries, leading to a lower average temperature and temperature rise. The trade-off between a cooling method's ability to minimize thermal gradients within the cell and to maintain a low average temperature necessitates the need to combine tab and surface cooling methods to take advantage of their individual strengths. This paper presents a two dimensional (2D) battery thermal model that allows independent control signals for the tab and surface cooling channels, making it ideal for optimizing thermal performance by effectively manipulating the cooling channels. The model is based on the Chebyshev Spectral-Galerkin (CSG) method and has the potential to predict the spatially resolved full temperature distribution throughout the cell with a similar computational efficiency to that of thermal equivalent circuits. The model is validated for a typical large format cylindrical lithium-ion battery through comparison with a high-fidelity CSG model with 100 states under the Worldwide Harmonised Light Vehicle Test Procedure. Results showed that the proposed model with only 2 states can faithfully capture the evolution of 2D temperature field. In aggressive cooling scenarios, a model order of 9 states can improve accuracy by 2.5%. Results also showed that cooling all sides of the cell resulted in the lowest average temperature and temperature rise, and cooling the top and bottom sides only, resulted in the lowest thermal gradient in the radial direction. Finally, results from perturbing the cell dimensions indicate that having a larger cell radius relative to the length is favorable for better thermal performance.

Applying control at molecular level: A reinforcement learning framework for optimally controlled natural flavor design

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The flavor is the focal point in the flavor industry, which follows social tendencies and behaviors. In this field, the research and development of new flavoring agents and molecules are of utmost importance. Notably, the development of natural flavors holds significant relevance in modern society. Considering this, the present work proposes a novel framework based on scientific machine learning to undertake an emerging problem in flavor engineering and industry. A combining system composed of generative and reinforcement learning models is proposed. The reinforcement learning technique serves as a data-driven control method, enabling us to discover the optimal policy for optimizing specific molecule designs. This innovative methodology facilitates the creation of novel flavors. The molecules evaluation takes into consideration synthetic accessibility, the number of atoms, and the likeness to a natural or pseudo-natural product. This work brings as contributions the implementation of a web scraper coded to sample a flavors database and the integration of two scientific machine learning techniques in a complex system as a framework. Additionally, the molecule design is guided by a reinforcement learning policy, similar to the operation of a controller in a control

system. The complex system implementation instead of the generative model by itself obtained 10% more molecules within the optimal results. The designed molecules obtained as an output of the reinforcement learning model's generation were assessed regarding their existence, or not, in the market and whether they are already used in the flavor industry or not. Through this analysis, we validate the framework's potential for discovering molecules that can be utilized in the development of flavor-based products. Furthermore, our work highlights the efficacy of reinforcement learning in chemical processes as a data-driven control approach. Overall, the proposed novel framework offers an effective solution to the exploration of flavor molecules.

A Real-time model predictive control for the microbial bioprocess production of Pediocin

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It was shown that the production of the commercial antimicorbial Pediocin PA-1 could be achieve by the workhorse cell factories *Corynebacterium glutamicum.* This antimicrobial is natively produce by pediococci families of bacteria that optimally grow and produce at acidic pH environments. Industrial cell factories however grow and produce at higher pH levels. Furthermore, being aerobic, these producers need high oxygen rates to grow but these rates the pediocin loses its bioactivity due to oxidation. Thus, the efficient production of this valuable antimicrobial requires a careful scrutiny of the conditions and poses an appealing optimization problem.

We implemented a nonlinear model predictive control (MPC) approach to optimally address this trade-off problem between microbial growth and Pediocin production by industrial cell factories. For that, we developed a nonlinear state space model that takes into account the effect of the pH on the growth and on the Pediocin production rates. We calibrated the model parameters with real-time experiments in our laboratories. We then developed and simulated a nonlinear MPC in a range of fed-batch and continuous process conditions, calculating the optimal trade-off between the pH needed for optimal growth and the pH needed for optimal Pediocin production. The NMPC managed to keep the set-point tracking values of the microbial biomass and of the glucose. It successfully adjusted the pH values of the process in order to maximize Pediocin production while satisfying the strict pH constraints of $pH_{min}= 5$ and $pH_{max}= 7.2$, the critical survival values of the cells. We found that the levels of production were highly dependent on the ratios between the weights of biomass formation, product formation and on the set-points tracking in the objective function. We successfully implemented the real-time continuous NMPC in *C. glutamicum* to maintain the glucose set-point levels during the growth phase. Finally, we concluded that NMPC is an excellent tool to solve such trade-off problems in industrial biotechnology that can arise from transferring production between bacterial hosts.

Closed loop optimisation of uncertainty aware economic control policies

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Economic nonlinear model predictive control (NMPC) is a control strategy that aims to optimise the economic performance of a plant while respecting operating constraints. In doing so, an optimization problem has to be solved at every sample time. This can be computationally expensive, especially when explicitly considering uncertainty in the problem formulation. We demonstrate a method to find a neural network control policy off-line that under mild assumptions, provides the optimal control policy for the uncertain problem. This method does not require off-line solutions of the NMPC problem, and instead directly optimises the desired closed loop performance.

In the proposed approach the neural network policy is optimised in closed loop by embedding it in the dynamic optimisation problem. With this formulation we are able to explicitly include uncertainty in the form, e.g. chance constraints and expectations in the optimisation problem. Although this optimisation is expensive, it is performed off-line and can be parallelised.

A plantwide control structure for improved flexible production of green Hydrogen

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Rising environmental awareness has recently revived interest in using Hydrogen as an energy vector for renewable electricity through water electrolysis. However, the question of how to operate the electrolysis process safely and efficiently in the face of renewable power uncertainty is still largely unanswered. In the case of reduced power, the Hydrogen-to-Oxygen ratio (HTO) at the anode is known to increase, posing a security risk which can force the plant to be shut down. At high powers, the heat generated by the electrochemical reactions can surpass the cooling capacity of the plant, again posing a threat to its safety. Considering the uncertainty in the supply of renewable energy, a control strategy for a green Hydrogen plant must therefore be able to efficiently cope with the safety constraints at disparate ends of the power supply profile.

In our work we propose a simple control strategy which extends the feasible operating range using standard advanced control elements. The control configuration is found using systematic procedures for plantwide control and tested against scenarios based on historical weather data. The model has recently been presented by Cammann et al. and is analyzed according to the "Top-Down, Bottom-Up" procedure of Skogestad for control structure design.

We find that the proposed structure gives near optimal performance for different power load scenarios. As such, it incurs close to zero steady-state loss and inherently considers the trade-offs between various performance relevant variables and safety constraints. The proposed structure is further easier to implement than a Model-Predictive Controller and can be implemented in the fast-acting regulatory control layer, offering an important extension to current efforts towards flexible green Hydrogen production.

Digital Twin Framework for Optimal and Autonomous Decision-Making in Cyber-Physical Systems: Enhancing Reliability and Adaptability in the Oil and Gas Industry

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The Cyber-Physical Systems offers a myriad of opportunities for real-time evaluations and continuous learning. This groundbreaking approach has gained substantial traction across various industries. However, implementing AI models, particularly in scenarios requiring real-time information exchange, poses computational challenges. This study introduces a novel framework for digital twinning, specifically tailored to optimize decision-making in the gas-lift process of the oil and gas industry. The primary focus of this framework is to enhance the adaptability and resilience of the digital twin. The proposed framework integrates techniques as, including Bayesian inference, Monte Carlo simulations, transfer learning, online learning, and other innovative strategies. These techniques empower the digital twin with cognitive capabilities, such as hyperdimensional model reduction and cognitive adherence. As a result, an efficient and dependable digital twin identification framework was developed. This approach effectively addresses existing gaps in the literature by amalgamating diverse learning techniques and proficiently managing uncertainties within digital twin strategies. The ultimate objective of this digital twin framework is to establish a reliable and efficient system that can adapt to dynamic environments while accounting for prediction uncertainties. By doing so, it significantly enhances decision-making in complex real-world scenarios. Moreover, this work lays a robust foundation for future advancements in digital twinning within process systems engineering. Its potential impact transcends the boundaries of the oil and gas industry, promising groundbreaking breakthroughs and applications across a broad spectrum of industrial sectors.

Integration of urban planning and design of energy systems using optimization-based control as an aid for decision-making

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In process control, it is mostly assumed that that the process is already built, and possible to observe and control. It makes sense – you cannot control something that doesn't exist. However, many of the methods developed within the control community are applicable outside of pure process control. Moreover, if the control aspect is considered in an early stage, it can heavily affect the outcome of the project, e.g., by showing ways forward that might not have been obvious without the control perspective. A residential area in Luleå in an early stage of the planning process is used as a case study to show how model-based control can be employed as a decision-making tool, integrating urban planning with modeling and design of energy systems, throughout different stages of the project. The foundation is a flexible model-based framework that allows the complexity of the model to increase as more information becomes available, combined with optimization-based control under large uncertainties.

Novel Framework for Simulated Moving Bed Reactor Optimization Based on Deep Neural Network Models and Metaheuristic Optimizers: An Approach with Optimality Guarantee

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Optimization of Simulated Moving Bed Reactors (SMBRs) necessitates robust solvers and substantial computational power. In response, surrogate models have emerged as a favored solution for such computation-intensive optimization tasks. Notably, Artificial Neural Networks (ANNs) have been deployed for modeling Simulated Moving Bed (SMB) units, although their utility for Reactive SMB (SMBR) remains uninvestigated. Despite the high accuracy of ANNs, it is imperative to evaluate their capability in accurately representing the optimization landscape. The absence of a consistent method for optimality evaluation via surrogate models in extant literature complicates this task. This study presents two significant contributions: SMBR optimization through Deep Recurrent Neural Networks (DRNNs), and the delineation of the feasible operation region, achieved by reusing data points from a metaheuristic technique for optimality evaluation. Empirical findings substantiate that DRNN-based optimization can effectively manage intricate optimization tasks, while concurrently achieving optimality, offering a novel approach to this computationally challenging endeavor.

Model Predictive Control for bioreactors based on *Escherichia coli* core metabolic network model

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Optimal control of processes is important to ensure efficient and safe plant operations. The growing popularity and use of Dynamic Flux Balance Analysis (dFBA) models have paved the way to implement more advanced control structures for bioreactors, such as Model Predictive Control (MPC). As the dFBA consists of a set of dynamic mass balance equations and an optimization that calculates the cell's metabolic fluxes, a bi-level optimization problem arises when MPC is applied. The bi-level optimization problem can be solved by reformulating the inner optimization to a set of algebraic expressions utilizing the duality theory and Karush–Kuhn–Tucker (KKT) optimality conditions.

In this work we first propose reformulations of the dFBA model for batch and continuous stirred tank (CSTR) bioreactors that would make the dFBA feasible to MPC applications. The ODE-system is discretized using the orthogonal collocation approach for finite elements and we implement an adaptive mesh strategy to place the elements. A penalization method for the optimality conditions is also utilized, as too many hard constraints may lead to convergence error and infeasible problems. We evaluate this methodology in a case study of the *Escherichia coli* core metabolism, emphasizing the accuracy and efficiency of the different dFBA reformulations. Finally, we apply MPC to our CSTR dFBA models, where we tested the controller's ability to handle changes in the setpoint, glucose feed concentration and maximal glucose uptake to the cells. The goal was to compare the KKT and duality theory reformulations of the dFBA model regarding computational time and reliability.

Virtual Reality for training hands-on operations of pilot plant – a digital educational tool.

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The Department of Chemical and Biochemical Engineering at DTU manages a large portfolio of pilot plant equipment for teaching and research activities. For educational purposes at all levels, dedicated setups focus on conventional unit operations such as distillation, absorption, extraction, crystallisation, filtration and dry-ing as well as dedicated setups for investigating aeration, mixing, heat-exchange, hygienic design, among other. The objectives are to demonstrate theoretical aspects and caveats in technical calculations in practice as well as to provide hands-on experience operating large-scale equipment.

Most practical courses offered to students in the pilot facilities consist of execution of several experiments on selected units followed by theoretical analysis and reporting of the findings. Students prepare for the exercises by reading a written manual and then perform the experiment at a fixed and limited time under supervision. This poses some challenges as it takes time for students to familiarise themselves with the physical setups before the exercise can begin and may also require frequent intervention by teachers to sup-port students during operation. The significance of the challenge depends on the individual student and his/her experience level but also the complexity of the unit operation.

Recently we have developed and deployed a virtual reality tool for six unit operations. Students can get a visual impression of the equipment and a guided virtual tour through the experimental procedure and chem-ical analysis before running the experiment. The tool is device-independent (phone, tablet, PC, 3D headset) and very user-friendly.

After one year, our experience is that through the VR tool, our students turn up with an enhanced compre-hension of the equipment and tasks. This leads to more independence and less load on teachers for onside supervision. The overall feedback from students is very positive as they perceive the VR tool as both instruc-tive and fun to use.

Discrete-to-Continuous Dynamics Reconstruction for Bilinear Systems in Process Control

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Most dynamical systems are nonlinear in nature. However, capturing the complete nonlinearities of a system in dynamical modelling is often overly complicated, especially for systems that involve strong nonlinearities. While linearization is commonly used in system modelling, the linear approximation is local, hence might not be adequate to capture the important dynamics of the system especially for a wide range of operation. Despite having similar structure to linear state-space systems, bilinear systems have the capability to better approximate some nonlinear dynamics and can hence be used in many cases where linear models are not adequate. In this work, we study the reconstruction of continuous-time models from discrete-time models of bilinear systems that belong to some common classes of nonlinear systems. While most systems evolve continuously in time, due to the use of digital sensors for data acquisition, system identification methods typically rely on sampled data and yield a discrete-time model. On the other hand, the use of continuous-time models are preferable especially in model-based control design. However, linking such a discrete-time model to its equivalent continuous-time dynamics is nontrivial. Therefore we propose a discrete-to-continuous dynamics reconstruction method for discrete-time models of some classes of bilinear systems obtained by system identification. We show that for bilinear systems we can reconstruct the continuous-time model that is consistent with the sampled measurement data. We focus on some classes of systems that are commonly found in process control applications and show that systematic reconstruction can be done for these classes of systems. Some examples are provided to illustrate the reconstruction process.

A Robust Learning Methodology for Uncertainty-Aware Scientific Machine Learning Models

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The study focuses on enhancing robust learning, an essential aspect of Scientific Machine Learning (SciML). It presents a comprehensive methodology for assessing the multifaceted uncertainties intrinsic to SciML model identification, including the lack of theory, causal models, sensitivity to imperfect data, and computational effort. The methodology ensures that SciML models are adequately uncertainty-aware. This approach is significant as the rise in Machine Learning (ML) applications and its resultant field, SciML, has necessitated the development of robust models that consider the unique characteristics of different domains and account for potential uncertainties. The uncertainties may stem from corrupted data, measurement noise, and instrument inaccuracies, leading to suboptimal performance of ML tools if not duly considered. The methodology put forth addresses this gap in the literature, considering both epistemic and aleatory uncertainties associated with the training data and the models. The approach includes building the nonlinear model parameter probability distribution (PDF) through Bayesian inference and assessing the ML model's uncertainty via Monte Carlo simulations. The methodology is corroborated by developing a robust soft sensor for a polymerization reactor. The results demonstrate the methodology's effectiveness in handling uncertainties, thereby enhancing the robustness and dependability of SciML tools.

Recirculated gas-lift optimization using Self-optimizing Control

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Optimizing subsea oil production systems utilizing recirculated gas lift and limited produced gas treatment capacity presents challenges. Real-time optimization (RTO) is a used method for optimizing such systems, but it is restricted by the lack of reliable sensors and the high cost of developing and updating models. As a result, the RTO is typically executed infrequently, and the optimal set points are not updated in real time, leading to suboptimal plant performance over extended periods. This study implements self-optimizing control (SOC) techniques as an alternative solution that can handle frequent disturbances and drive the plant towards near-optimal performance without requiring frequent model updates or solver use. It compares different SOC structures in recirculated gas-lifted oil production optimization, their advantages, and disadvantages. The study concludes that SOC structures are an effective and suitable alternative to RTO, particularly in large and complex systems with limited measurement capabilities, given sufficient process system knowledge is considered for SOC design. This conclusion reinforces previous research, but with a more realistic case study.

Simulation of ion-exchange chromatography for teaching purpose using Bioprocess Library for Modelica

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An important process step in the biopharmaceutical industry is ion-exchange chromatography. It is used to separate the protein product from other proteins and various impurities in the starting material.

The ion-exchange chromatography step is a mature technology and here is modelling done with different complexities. Here we use a simplified model based on basic binding reaction between a protein and the resin and we use a series of compartments to model the column convection, taken from the literature. Further, the model is extended with an empirical proportional relation between the difference between isoelectric point and pH-resin, and the binding strength.

Despite the model simplicity it captures in a qualitative way several operational situations well, and useful for educational purpose. Examples are:

- Separation of proteins with different isoelectric points
- Impact of slope of the desorption gradient
- Impact of salt concentration in the incoming sample of material
- Impact of change of binding strength due to pH
- Impact of column binding capacity on break-through curves

The modelling is done in Modelica with use of Bioprocess Library and compiled model in the form of an FMU is simulated in a Python environment using Jupyter notebook. The simulations are done using package PyFMI, or alternatively with FMPy, with a simplified common command line interface FMU-explore.

The Jupyter notebooks combine explaining text with code snippets and results in diagrams. It is easy for the students to go back and change parameters and see what happens. Students can also continue the notebook in an explorative way.

In a teaching situation it is of interest to minimise installation requirements. We have experience of using Google Colab virtual machines to run these notebooks from a web-browser and requires no installation. You need a gmail-address though. The simulations can be run from any computer, chrome-book, tablet or even a smartphone.

Sensor bias detection, isolation, and estimation in a gas-lifted oil well network

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Process monitoring, control and optimization are popular and spread among the chemical and petrochemical industry. These tools are usually applied online to obtain a fast response from a disturbance, equipment, or sensor fault. In order to do that, those methods rely on the data that continuously come from the sensors located in the plant. However, the sensor data comes with random noise and are subject to gross errors. This corrupted information can damage the performance of the methods. One solution is to either re-calibrate or replace the faulty sensors. However, this solution is not always available. Subsea oil and gas operations are located in a harsh environment, and the replacements of these sensors are costly and time-consuming. One example of a subsea system is the gas-lift operation, where gas is injected into the wells to increase production. Two things are needed: identify the faulty sensor for replacement, and try to correct that signal, if possible, before this replacement. This work proposes a method combining fault detection and isolation, state estimation and observability analysis. The idea is to provide information on the faulty sensors and, by doing an observability analysis, decide if the bias/drift can be tracked using the state estimator. The method was evaluated by numerical simulations on a gas-lifted oil well network model.

Realistic Fault Simulation Platform for Testing Monitoring Strategies in Wastewater Treatment Plants

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Instrumentation, control and automation for industrial chemical and biochemical processes to attain cost-effective and safe process operation are highly dependent on reliability of the real-time measurements. Despite considerable development of online sensors during the past decades, their dependability is still impaired due to various fouling and failing issues. Despite a large number of available signals, data reconciliation and validation for online instrumentation has remained a largely unexplored field with a lack of standardized approaches. Most data are stored unstructured, with lots of gaps, repetition, ambiguity and uncertainty. This has led to "data-rich, information-poor" situations in which data sets are often too large and complex for processing and analysis to be used for decision-making. To turn raw data into useful and actionable information, data need to be validated. This can be achieved through a fault detection procedure.

The aim of this study is to extend an existing benchmark simulation tool for wastewater treatment processes by including "realistically" different sensor/actuator and process faults which are compatible and unified with the previous developments (influent generator, process models, sensor and actuator models, simulation procedure, evaluation criteria). Different sensor/actuator and process faults were modelled using a Markov-chain approach, given the probability of fault occurrence and probability of transitions from one state to another. The output includes different scenarios which is suitable to test univariate/multivariate statistical monitoring methods as well as fault-tolerant control strategies. Using this platform, one can test the performance of a fault detection method. To demonstrate this in an example, an adaptive-dynamic fault detection was tested using dynamic principal component analysis (dPCA) with a moving window. The model and the database are both freely available online, and we are extending an invitation to people to test their fault detection methods on our provided dataset, which also includes labels.

Online optimization of froth flotation processes

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Froth flotation is a widespread method in mineral processing, The process consists of suspending ground ore in a water tank and floating the desired mineral to the surface by means of air bubbles, this works due to the hydrophobic and hydrophilic properties of materials. In this paper, the online optimization of froth flotation is explored. The model used in this paper is based upon a model by D.J. Oozthusien implemented in Simulink. Optimizing a froth flotation process usually revolves around two critical operational points, froth stability, and pulp level. In this context, froth stability is generally measured by the amount of air recovered at the end of the process. Due to its relation to the performance of the cell, it is treated as the variable to maximize. To drive the system to an optimum while maintaining a pulp level, this paper proposes the use of a geometrically constrained extremum-seeking controller that uses an extended Kalman filter to estimate the gradient of the system and then uses geometrical constraints to keep the system operating as close to the optimum as possible while maintaining the appropriate pulp level. The controller was tested in a simulated environment, first whit a single-cell model and then a flotation circuit of 4 cells. The controller successfully drove the air recovery to a maximum while keeping a constant pulp level in both cases. It could successfully handle disturbances of both operational parameters and feed. These results show a promising start for further work, either in developing a multi-objective approach to optimize more aspects of the process or developing a centralized controller for comparison.

DEDS-Systems and Workflows

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Computational engineering defines workflows. They are designed to solve multi-scale, multi-disciplinary simulations. The users generate models for the different parts. For example, the MoDeNa project simulated the formation and properties of polyurethane foams. It connected quantum mechanic computations for reactions, molecular modelling for properties, intermediate scale components providing the behaviour of bubbles in viscosity-changing fluids, polymerisation and forming of mechanical struts frameworks of the foam, and molecular modelling for mechanical properties of the final product. Workflows are controlled networks of computational tasks. It has the nature of a job shop. Plan, allocate, start, stop, and handle exceptions. The programs executing such complex computational tasks are called orchestrators. MoDeNa project had as a product an orchestrator based on a framework called FireWorks, which implements the facilities necessary to perform computations on facilities available via the networks, thus distributed computing. We shall discuss workflows from the system's theoretical viewpoint, namely hybrid systems. Event detection is a key issue. In the case of physical subprocesses, events are generated by hardware devices directly or from algorithms implemented on the digital side, thus after the sampling. In the case of computational tasks, events are either time events, sampling events or timer running out, state events, exceptions, or external requests such as users asking for information or changing behaviour. We generate ontologies capturing workflows. In applications, one mainly meets two domains: the business level and the scientific simulation. The main difference is that business people are not interested in the details but the logical connections, thus in one-word logistics, while science simulations are all about details. The two, therefore, differ by the business level hiding the data operations, while for science applications, the data are in the foreground. The objective is to generate ontologies that capture both. Also, one is interested in a minimal ontology that can capture all different implementations of workflow description languages, intending to enable the transfer of workflows between applications.

DEDS-Control and Desired State Orchestration in Cloud Computing Systems

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Distributed computing faces significant challenges in resource allocation and exception handling. A scheduler automaton orchestrates the execution of programs on multiple automata across distributed computing environments. This coordination ensures efficient resource allocation, effective exception handling, and the implementation of feedback control mechanisms to optimize system performance.

The advancements in cloud computing and containerisation have drastically changed how software systems are deployed, managed, and scaled. Kubernetes is a top platform in this area and has become the standard for container orchestration due to its flexibility, scalability, and resilience. The container orchestrators use discrete-event dynamic system (DEDS) based control principles to manage computing systems that rely on asynchronous discrete events.

Kubernetes uses a feedback control loop to maintain a desired system state, continuously monitoring and updating the state to align with user-defined configurations and behaviors. It also has self-healing abilities to handle system failures, including container restarts and auto-scaling based on policies and thresholds. It helps maintain system stability and robustness.

State prediction in the Kubernetes ecosystem involves leveraging predictive models to anticipate future system states. By analyzing historical data and considering factors like workload patterns and resource usage, predictive algorithms can forecast potential states. These predictions enable proactive resource allocation and informed decision-making, optimizing efficiency and adaptability in the distributed computing environment.

By combining the power of desired state orchestration capabilities with DEDS-control principles, cloud computing systems can further be augmented with sophisticated control strategies that optimize resource allocation, workload management, and system performance in distributed cloud computing ecosystems.

Receding-horizon control of full-scale wastewater treatment plants as water resource recovery facilities with energetic constraints

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The arising paradigm of perceiving wastewater as a sustainable source of water, nutrients, and the production of electricity, is pressuring solutions for operating treatment plants as water resource recovery facilities (WRRF) [1, 2]. A treatment facility should control its effluent quality to match external demands, while recovering energy from sludge, thus ensuring a balanced water-energy nexus. Common to most urban areas, biological treatment through activated sludge processes is an important platform for recovering resources from wastewater. The optimal operation of wastewater treatment plants (WWTPs) is extensively studied thanks to support tools that provide a simulation protocol for real-world facilities: The Benchmark Simulation Model no. 2 (BSM2, [3]), specifically, provides a reference platform for controlling the wastewater and sludge treatment in WWTPs subjected to typical municipal influents. Despite the existence of numerous control strategies for satisfying regulatory constraints, the operation of BSM2-like plants for resource and energy recovery is still an active area of research.

We research control solutions to operate WWTPs as energy self-sufficient WRRFs [4, 5, 6]. Towards this goal, we present an output model predictive controller that operates WWTPs to produce effluents of specified quality on demand. The controller ensures that the energy needed for this operation can be recovered from disposed sludge through biogas production. Our controller solves state-feedback model predictive control (MPC) problems in which the current process state and disturbances are determined by moving horizon estimation (MHE) [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 illustrate the controller's behaviour when operating a large-scale plant to produce water of varying quality while ensuring energetic self-sufficiency. Given the generality of the approach, this controller can be configured to achieve alternative goals and/or relaxed energetic requirements.

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Mesoscopic thermodynamics of single-particle enzymatic reactions

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In this work, we consider the framework of mesoscopic non-equilibrium thermodynamics [4, 3, 5] to evaluate the stochastic energetics of enzymatic reactions described in terms of classic Michaelis-Menten/Briggs-Haldane theories. We consider a system comprising of a single enzyme which can exist in one of two states, either in free form or complexed with the substrate, and that the formation of product is reversible. Moreover,we assume that the kinetics of the reaction network can be expressed using elementary reactions and that the system is coupled to a heat reservoir. Because the interactions with the heat bath are assumed to be uncontrolled and intrinsically stochastic, each reaction will be described as a random event characterised by a single parameter, the rate constant. It is thus expected that a different evolution of the system is observed each time the experiment is repeated. Such a description leads to model the system as a continuous-time Markov process with discrete state-space, a Markovian jump process.

The resulting stochastic kinetics are represented with two complementary formulations of the dynamics: either in terms of the fluctuating number of molecular species that follow the Gillespie algorithm [1], or in terms of the probability distribution that satisfies the chemical master equation [2]. We discuss how thermodynamic observables of relevance, like the stochastic heat and the stochastic work, are defined at the level of single trajectories and compute their value for this system. We establish the stochastic counterpart of the first and second law of thermodynamics and we establish the fundamental fluctuation relations. The energetic analysis relies on the irreversible nature of non-equilibrium processes and the definition of non-equilibrium entropy and entropy production. Free energy is computed as the quantity proportional to the Kullback-Leibler divergence between the system's probability distribution and its equilibrium distribution

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Approximate Model Predictive Control of Hybrid Systems using Multitask Deep Neural Networks

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Hybrid dynamical systems are a class of dynamical systems that exhibit both continuous and discrete behaviors, often involving the interaction of dynamics and logic components. They are used to model complex engineering systems in different application areas including power electronics, automotive applications, robotics, etc. The traditional approach to MPC design for hybrid systems involves solving mixed integer programs online. However, the inherent combinatorial nature of these problems often leads to substantial computational time, limiting their implementation in real-time scenarios.

In this work, we study the design of an approximate model predictive control for a class of linear hybrid systems. We leverage the insights from explicit hybrid MPC and propose to use multitask deep neural networks to approximate the solution of MPC for hybrid systems. A mixed integer linear encoding of the closed loop system is provided to compute the reachable sets for the closed loop systems that helps to analyze the safety and stability properties of the hybrid system under the influence of the multitask deep neural networks controller. Once trained offline, the resulting controller results in a solver-free approach that is highly suitable for implementation on embedded hardware with limited resources. Several illustrative examples will be presented to show the efficacy of the proposed.
