The current challenges in the process industries and how optimization and control contribute to meeting them

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Content of the talk

1. A bit of biography and on drivers or KPIs
2. Priority themes on the Strategic Research and Innovation Agenda of Processes4Planet
3. Optimal operation of electrified processes (demand side management)
4. Examples of using RTO and MPC for the improvement of energy efficiency
5. The modelling bottleneck - is AI the solution?
6. Final remarks

1. A bit of biography and on drivers or KPIs

The beginning

- **1977** Started to work on the **control of multivariable systems** using Rosenbrock‘s method
  - How to compute optimal approximate decouplers that achieve diagonal dominance?
  - Learned how to design controllers in the frequency domain
- **1979** Switch of topic for my PhD*:* Relationship between information theory and filtering
  - Developed a ***theory for the transformation of information in real time***, PhD thesis 1981

IEEE TRANSACTIONS ON INFORMATION THEORY, VOL. IT-33, NO. 2, MARCH 1987

New Results on the Real-Time Transmission Problem

SEBASTIAN ENGELL, MEMBER, IEEE

Abstract—A new concept is presented for the treatment of real-time transmission problems. It basically consists of a modification of the flow of information. The resulting quantity, which we call the forward flow of information, is smaller than the flow of information according to the usual definition except for special cases. We derive various negative coding theorems in which the forward flow of information is used. These bounds are sharper than those previously known for transmission with finite delay.

  - Took 5 years to write the paper in the required jargon of information theory and to get it published.
  - At the time of publication there was no interest in the topic, few citations 20 years later.
- **1982 – 1984**
  - Work on a broad range of topics from frequency domain controller design over decentralized control and estimation (matrix pencil theory) to the information-theoretic analysis of feedback systems

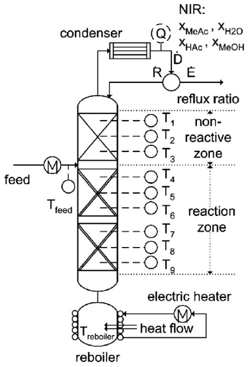
Bio - continued

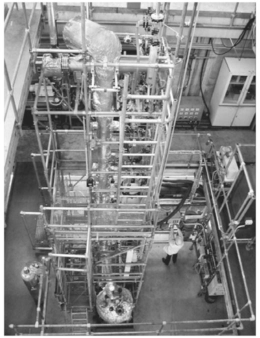
- **1984** Ambition of my **Habilitation project**: A complete theory of the limitations of feedback control from the point of view of the available information as well as dynamic limitations
  - E.g. “An information-theoretical approach to regulation”, Int. Journal of Control, 41 (2), pp. 557 – 573, 1985
  - However the results using information theory were not really useful, despite the fact that feedback obviously uses information.
  - Especially the analysis of the role of models was completely missing in information theory.
  - Therefore I concentrated on dynamic limitations based on the theory initiated by *George Zames* „IH^{∞}“

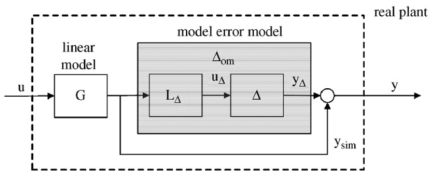
- **1986 - 1990 Group leader at Fraunhofer IITB** for Process Automation
  - Managed a broad range of industrial projects, sensing technology, CIM of the production of synthetic fibres
  - First „real“ controller design
  - Started to work on scheduling assuming that it could be treated as a feedback control problem
  - Realized the importance of logic controllers and the difficulties of designing them

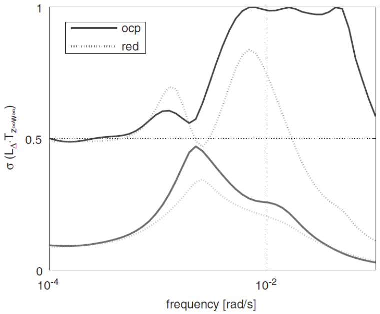
Bio - continued

- **1990** Appointed as a Full Professor in Chemical Engineering at TU Dortmund
  - Started to learn about chemical and later biochemical processes
- **Research topics in the first 10 years:**
  - **Frequency-domain controller design**
    - Computation of optimal robust linear controllers, Jorge Trierweiler‘s Robust Performance Number
    - **Highlight:** M. Völker M., C. Sonntag, S. Engell: Control of integrated processes: A case study on reactive distillation in a medium-scale pilot plant. Control Engineering Practice, 15 (7), 2007, 863 – 881









Initial research topics (ct‘d)

- Nonlinear control, gain scheduling („Klatt-Engell reactor“)
- „AI-based“ controllers:
  - Control using Takagi-Sugeno Fuzzy models
  - MPC with NN models

Model Predictive Control Using Neural Networks

Andreas Draeger, Sebastian Engell, and Horst Ranke

IEEE Control Systems Magazine 15 (1995), 61-66
>160 citations in Scopus, reprinted 2020

Real experimental data

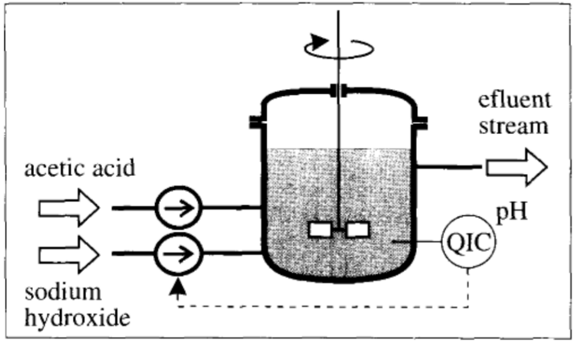


Fig. 1. Neutralization plant.

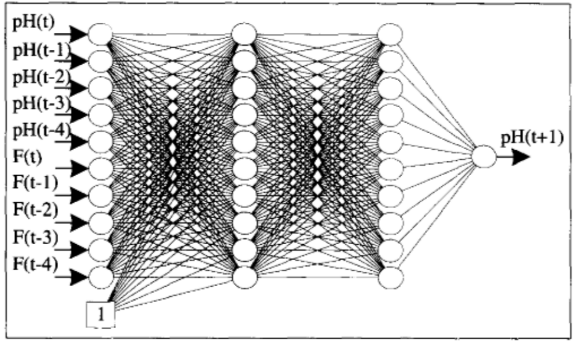
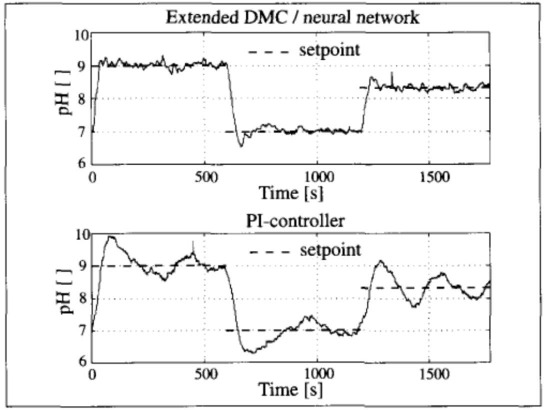


Fig. 3. Topology of the neural network.



Initial research topics (ct'd)

- **Hybrid systems and design of logic controllers**
  - Successful in terms of funding, PhD theses, publications that are still cited today
  - No breakthrough, problems of the complexity encountered in reality cannot be tacked rigorously
  - No tools of value developed

- **Simulation of the recipe-driven operation of batch processes**
- **Scheduling of batch processes**

- **Modeling, trajectory optimization, and control of polymerization processes**
  - PET, later emulsion polymerisation
  - Reached the limit of what can be done without measurements and good models of product properties

- **Control of chromatographic separations, in particular SMB → optimizing control, iterative RTO**
  - A. Toumi and S. Engell: Optimization-based control of a reactive simulated moving bed process for glucose isomerization, Chem. Eng. Sci. 59(18), 2004, 3777-3792
  - A perfect example of how an application drove methodological developments

What drives us? What are our KPIs?

Affection and aesthetics
Intellectual pleasure, curiosity
Understanding the world

„Beauty is the splendor of truth“

„It is such a pleasure to think and it is great that we are even paid for it“ (George Zames)

KPIs in the academic world

external and personal

Resources and funding

Try to shape it!

Personal pleasure, e.g. travel

Impact in the real world

- Can all drivers be aligned?
- Depends on your aesthetics and on the „framework conditions“

How did I achieve my KPIs before 45?

Affection and aesthetics
Intellectual pleasure ✓
Understanding the world

„Beauty is the splendor of truth“

KPIs in the academic world

external and personal

✓

Resources and funding

✓✓

Personal pleasure, e.g. travel

✓✓

Impact in the real world

?

Impact

Affection and aesthetics
Intellectual pleasure
Understanding the world

„Beauty is the splendor of truth“

KPIs in the academic world

external and personal

Resources and funding

Personal happiness, e.g. pleasure

Impact in the real world

- **Work on something that has an impact! (**Manfred Morari)
- **What is going on in the process industry ?**

2. Priority themes on the Strategic Research and Innovation Agenda of Processes4Planet

PROCESSES4PLANET

Processes4Planet: a co-programmed Partnership in Horizon Europe

PROCESSES4PLANET

ASPIRE

10 Process Industry **Sectors**

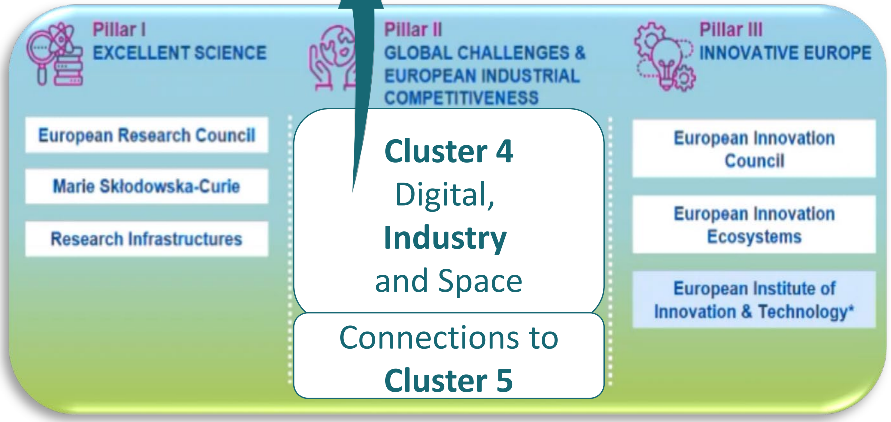
+SMEs
+ RTOs,
+ Universities
+ NGOs
+ Innovation agencies
et al…

European Commission

DG RTD
DG Grow

Co-programmed Partnership

MoU signed:
€1.3 bn exclusively for projects
27% more than in H2020



THE ASSOCIATION

A.SPIRE

General Assembly

Board of Directors
Up to 29 members + 1 SME

Executive Director
A.SPIRE Office

Advisory and Programming Group (APG)

Chair SE

- Process Innovation for Climate Neutrality
- Circularity Innovation
- Competitivene ss
- Digitalisation
- Portfolio
- Foresight
- Collaborations

A.SPIRE PWGs / Experts

- PWG1 ENERGY
- PWG2 PROCESS OPTIMIZATION & CCU
- PWG3 I-US / H4Cs
- PWG4 RESOURCES & CIRCULARITY
- PWG5 FRAMEWORK CONDITIONS
- PWG6 SOCIETAL INNOVATION
- Special WGs

THE PARTNERSHIP

PRIVATE PARTNER
A.SPIRE

Board of Directors
5 representatives

Executive Director
1 representative

APG
15 representatives
(Incl. **Ambassadors Group Leader**)

Co-chair of PB

PARTNERSHIP BOARD

PROCESSES4PLANET
- Signatories
- Commitment
- Decision making

Co-chair of PB

PUBLIC PARTNER

European Commission

***€1.3 bn** funding for projects from HEU – C4*

3. Future research and innovation priorities of Processes4Planet

- Driven by the goals of
  - **Climate** (Reduction of the CO_2-Emissions) (-55% by 2030 but -60% for EEI compared to 2005)
  - **Circularity** (Reduction of waste, assure availability of critical raw materials also affects the CO_2 footprint)
  - **Competitiveness**

- **Triple urgency**: Climate goals, de-industrialization, dependency on imports of raw materials

- **Priorities of the update of the Strategic Research and Innovation Agenda**
  - **Electrification** and **use of other carriers of energy** (hydrogen, ammonia, methanol)
  - **Energy and material efficiency**, industrial symbiosis and industrial-urban symbiosis
  - **CCU**
  - **Circular Economy** – recycling systems

Electrification

- Electrification will be a major contributor to decarbonization in the process industries
  - Core element in the planning of many European companies
- Depends on the availability of „green“ power which is strongly varying

  → **need for flexibility**

- Differerent designs of plants needed
- Much more agile operation, demand response
- Costly – unused capacity, higher CAPEX
- Currently many studies on optimal flexible peration, e.g. air separation units, electrolysers
  - Review: M. Cegla, R. Semrau, F. Tamagnini, S. Engell.: Process operation for electrified chemical plants. Current Opinion in Chemical Engineering, 39, art. no. 100898, 2023.

An example from the steel industry

- Plans of *thyssenkrupp steel Europe* for the Duisburg site
  - Direct reduction using first NG and then hydrogen from electrolysis
  - CCU to produce ammonia and methanol from CO_2 and CO (Carbon2Chem)
- From the project web site:
  - “One challenge of the transition to renewables is the sharply fluctuating availability of electricity from wind and solar power set against the need for a reliable energy supply. By using surplus electricity for the Carbon2Chem® process we are helping to keep the electricity supply in balance. Carbon2Chem® offers the opportunity to use large-scale industrial facilities like steel mills and chemical plants as energy buffers.”
  - “We then activate our chemical production when large quantities of energy are available at low prices. In this situation the steel mill gas streams are split so that part is available for steel production requirements and part for chemical production using renewables. This strategy is known as load management or demand side management. This helps stabilize the power grid and contributes toward the energy transition.”
- It is estimated to take 15 years to make the processes flexible enough and to achieve the integrated operation of the complex.

3. Optimal operation of electrified processes (demand side management)

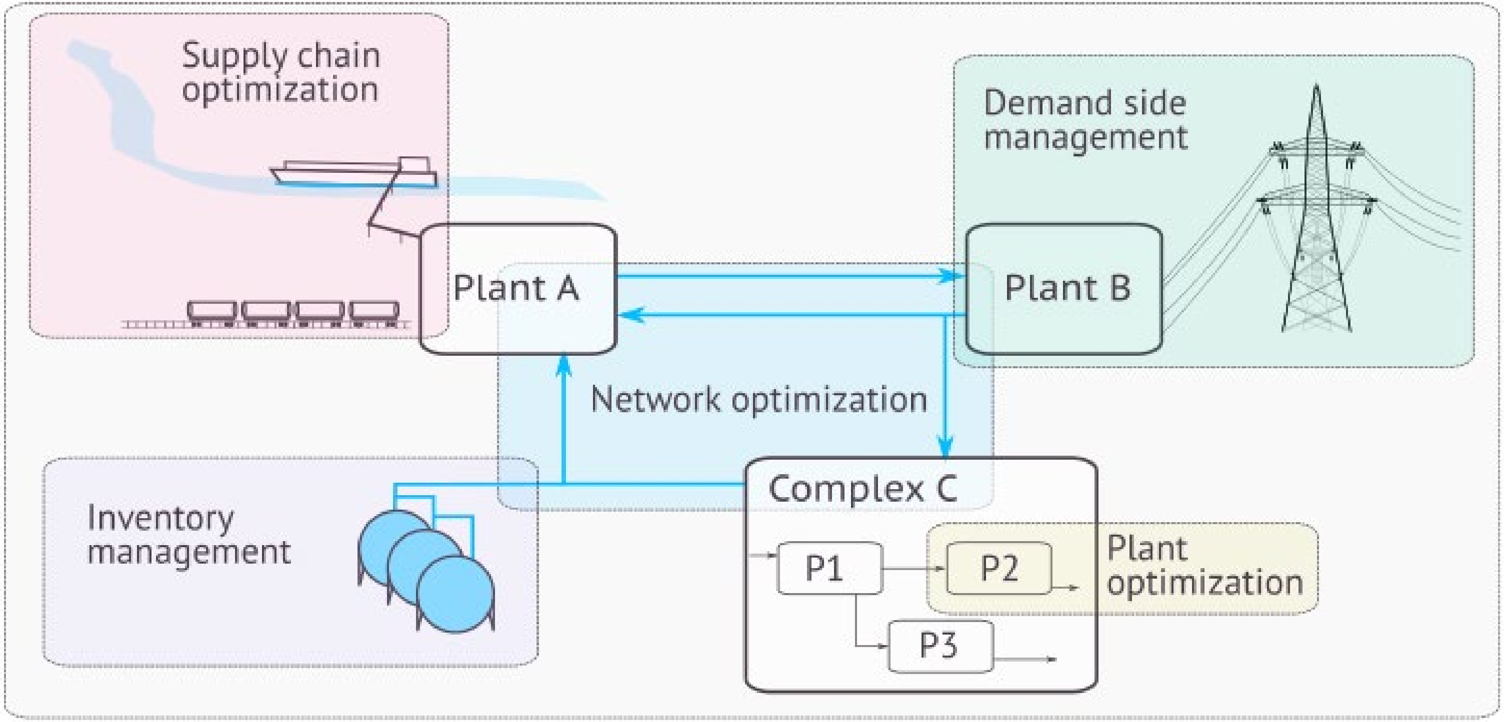
Different layers of demand response

- Planning – based upon forecasts of supply and prices of electricity and production demands
  - Rolling horizon adaptation
  - Two-stage planning
  - Bidding processes

- Dynamic optimization

- Three examples:
  - Operation of a network in a chemical site (INEOS in Cologne)
  - Stochastic short-term integrated electricity procurement and production scheduling applied to a stainless steel plant
  - Operation of a novel intensified electrified process (COBR reactor)

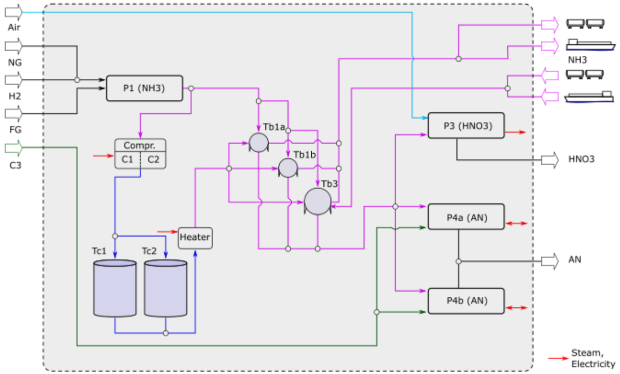
Optimisation of the operation of the ammonia network of INEOS in Cologne



Simon Wenzel et al.

S. Wenzel, Y.-N. Misz., K. Rahimi-Adli, B. Beisheim, R. Gesthuisen, S. Engell: An optimization model for site-wide scheduling of coupled production plants with an application to the ammonia network of a petrochemical site. Optimization and Engineering, 20 (4), 969 – 999, 2019

Logistics



NH_3 (and other products) can be sold to or purchased from different customers and suppliers

Logistics mainly involve barges (ships) and train vessels

Limited capacities in filling and discharging

Normal and cryogenic tanks

Planning of the logistics is incorporated into the optimisation problem

Modeling as a MILP

- Subsystem models required for:
  - Plants
  - Reactors
  - Compressors
  - Heaters
  - Storage tanks
  - Buffer tanks
  - Network topology
  - Logistic constraints
    - Ships
    - Trains
    - Pipelines

The models came from

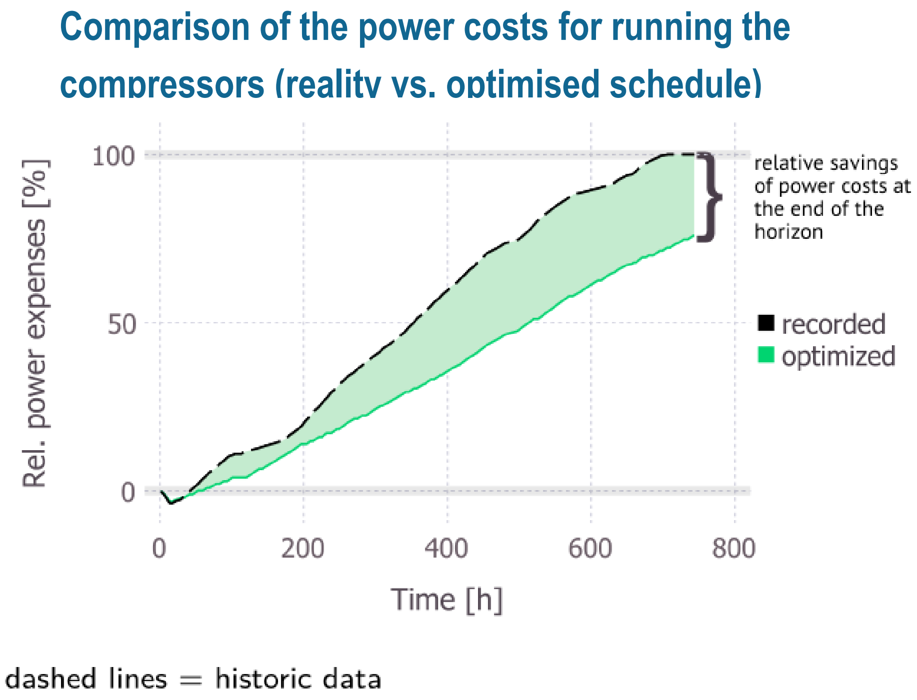
- Planning tools of INEOS in Cologne
- Data-based relations identified by TUDO
- Generic equations and constraints

Model size for a horizon of 31 days

- 282,000 variables
- approx. 180,000 binary

MIP gap after 1 h of computation time 0.04%

Saving potential in power for the compressors

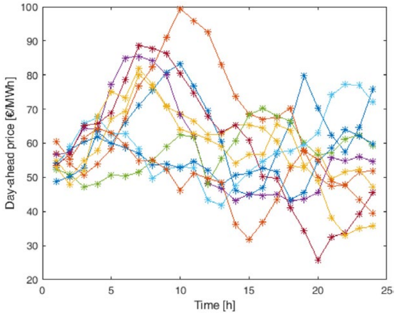


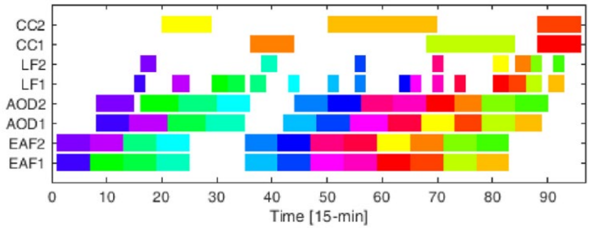
More than 20% savings!

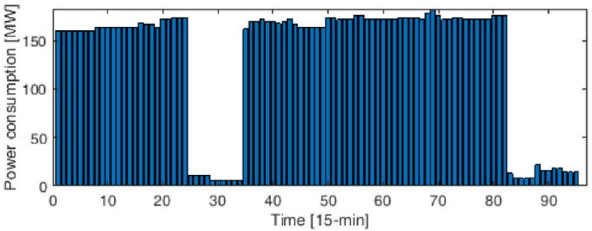
Stochastic short-term integrated electricity procurement and production scheduling (work by Egidio Leo)

PRONTO
PROCESS NETWORK OPTIMIZATION

- Reality is more complex than just buying power in a shop:
  - Large consumers must bid for electric power a day ahead
  - The resulting clearing prices are uncertain.
  - Unsatisfied power demand has to be procured at higher cost.
  - When the plant is operated, the production schedule and hence the power demand can be adapted to the realized price.
  - The bid should consider the the uncertainty in the outcome **AND** the possibility to react to both.
- Fits into the framework of *two-stage stochastic programming*
- Risk aware formulation
- Applied to a full MILP model of a stainless steel plant
  - E. Leo, G. Dalle Ave, I. Harjunkoski, S. Engell: Stochastic short-term integrated electricity procurement and production scheduling for a large consumer. Computers and Chemical Engineering, 145, art. no. 107191, 2021.





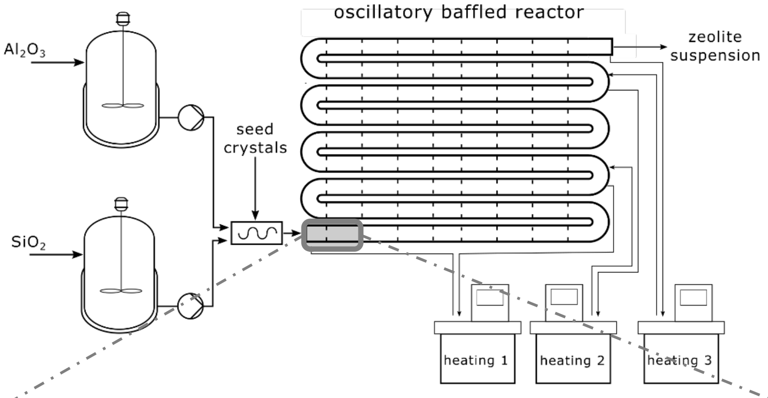


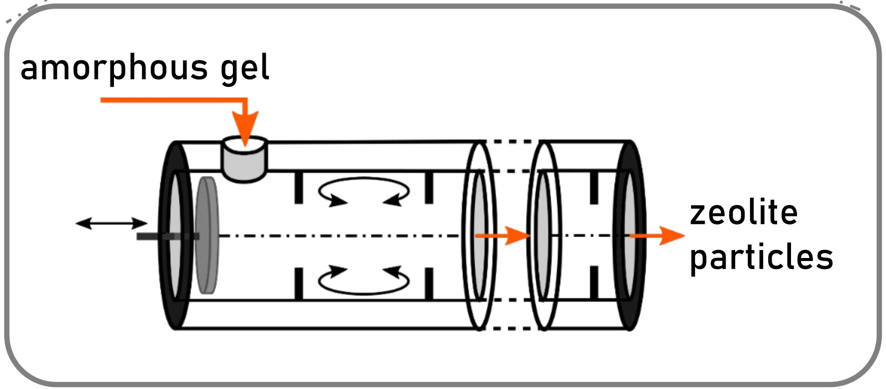
DSM in the continuous production of zeolites[1]

- Work by **Robin Semrau**
  in collaboration with ARKEMA

SIMPLIFY
SONICATION & MICROWAVE PROCESSING OF MATERIAL FEEDSTOCK

- Zeolite production
  - Hydrothermal synthesis
  - Long processing times in batch reactors
  - Elevated temperatures needed
- Continuous Oscillatory Baffled Reactor (COBR)
  - Intensified continuous process
  - Superimposed oscillating flow
    - avoids sedimentation
    - good axial mixing
  - Long residence times with high solid loadings
- Can reduce the energy input by 80%



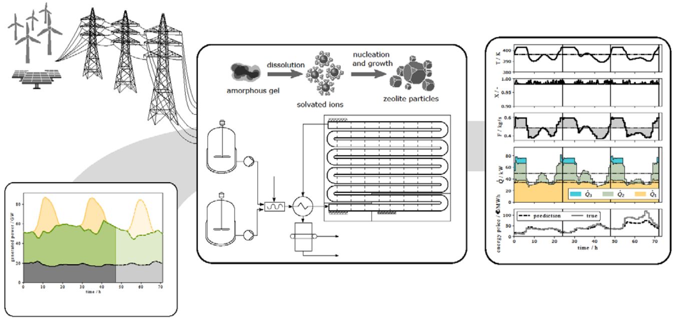


[1] Ramirez, Valdez, van Gerven, Lutz: Continuous flow synthesis of zeolite FAU in an oscillatory baffled reactor, Journal of Advanced Manufacturing and Processing 2020

Optimal dynamic operation

- Demand side management
  - Flexibly shift the production during a day
  - Ensure an average production rate
  - Use the energy at low prices & emissions

  - Manipulated variables:
    - Flowrate
    - Heat duties of the heaters
  - Constrained variables:
    - Crystallinity of the zeolites above 98%
    - Maximum temperature



R. Semrau, S, Engell: Process as a battery: Electricity price aware optimal operation of zeolite crystallization in a continuous oscillatory baffled reactor. Computers & Chemical Engineering 108143, 2023

"All in one" solution

Stage cost

Expected economic cost
- Energy consumption
- Production revenue

Time discretization

OCFE time discretization
- 2nd order polynominals
- Radau roots

Implementation

Implented in CasADi (python)
Solved with IPOPT
- 100.000 variables
- 1 h computation time

$$\min_{u,x} \int_0^{t_f} \Phi(u,\gamma)\,dt + \lambda_{ss}^{*,T} x(t_f)$$

$s.t.:$

$$\dot{x} = f(x,u),\, x(0) = x_0$$

$$u_{ub} \geq u \geq u_{lb}$$

$$T_w \leq 403.15\mathrm{K}$$

$$X \geq 0.98$$

$$F_{fix} = 1/\Delta t \int_{t_k}^{t_{k+1}} F(t)\,dt$$

Terminal cost

To avoid terminal sell-off

Model

Rigorous plant model

Input constraints

Limit of controlled variables

Quality constraints

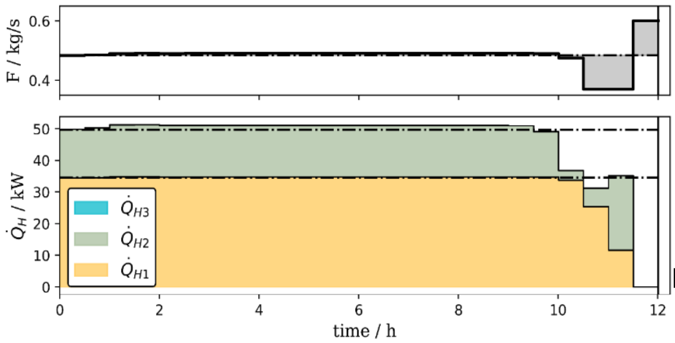
Cyristallinity

Averaging constraints

Ensures average production over a given time horizon

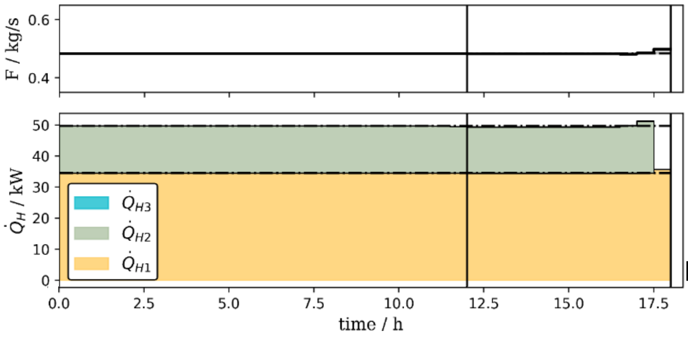
Terminal sell-off

- Terminal sell-off effects
  - Shutdown of the heater at the end of the prediction horizon
  - Effect pronounced due to the integral constraint
  - Constraint violation in the following period



[1]

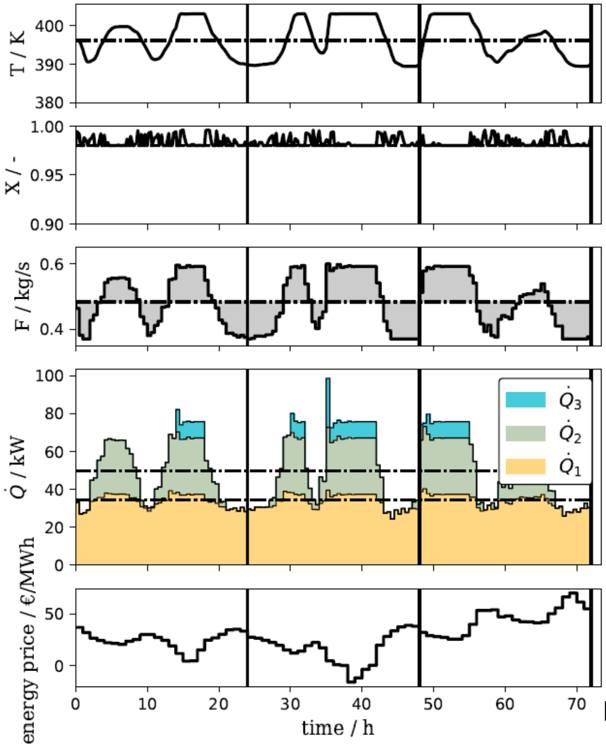
- Approach to reduce the sell-off effect
  - Second averaged horizon
  - Terminal Cost: $\lambda_{SS}^{*,T} x(t_f)$
    - Multiplier of a steady state optimization



[1]

Results

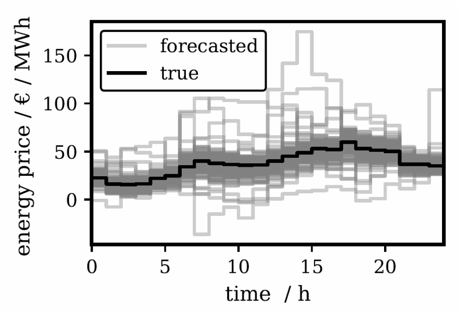
- Dynamic day-ahead production scheduling
- Knowledge about the future electric energy price assumed
- Variations taken from the energy stock market
  - 13.01.2020-15.01.2020
- Production shifted to the lower price time intervals
  - **Energy cost savings: 11.8%**
  - **Emission reduction: 3%**

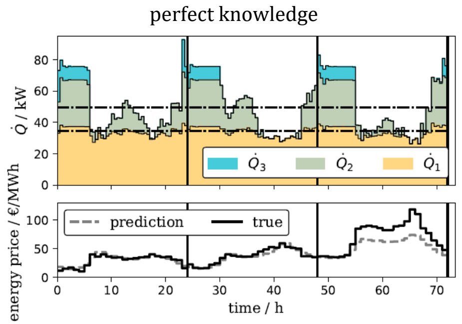


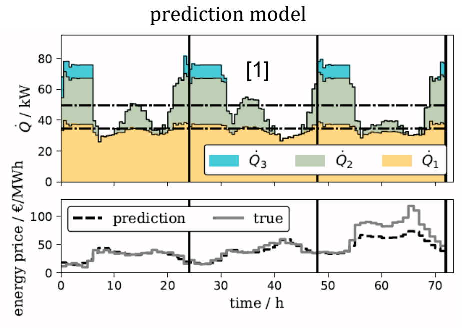
[1]

Results with uncertain prices

- Description by error scenarios for the price







- **Savings:**
  - Perfect information: 8.7 %
  - Prediction model: 7.8 %

4. Examples of using RTO and MPC for the improvement of energy efficiency

Energy and material efficiency

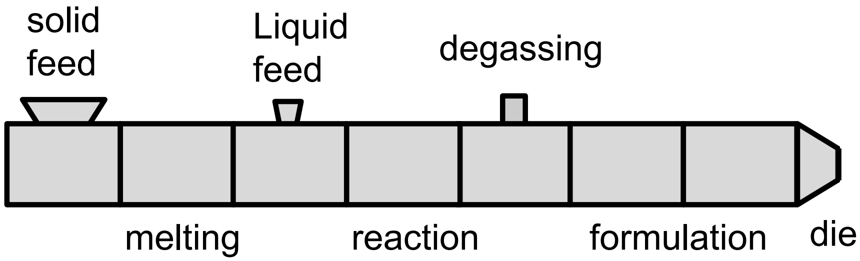
- Increasing the energy and material effiency usually happens in small steps
- For electric power from renewables, there is limited supply, high cost, and competition between sectors

- Efficiency must continously be improved also for „old“ technologies to reach the 2030 targets

Application of real-time optimization with modifier adaptation and quadratic approximation to a reactive extrusion process

Maximilian Cegla, Aleksandra Fage, Simon Kemmerling, SE, IFAC World Congress 2023

- Twin-Screw Extruders
  - Extruders with two screws, counterrotating
  - Melting of solids, Homogenization of viscous media
  - High flexibility, can be combined with reaction
  - Short residence times 1-10 min
  - Modeling is challenging



SIMPLIFY
SONICATION & MICROWAVE PROCESSING OF MATERIAL FEEDSTOCK

  - **Energy efficient electrified process compared to synthesis in stirred tank batch reactors**

Modifier Adaptation with Quadratic Approximation

Iterative optimization based on a modified model

Quadratic approximation of the outcomes

- $J_Q(u,P) = \sum_{i=1}^{n_u}\sum_{j=1}^{n_u} a_{i,j}u_iu_j + \sum_{i=1}^{n_u} b_iu_i + c$

  $$\min_P \sum_{i=1}^{n} \left(J_P(u^i) - J_Q(u^i,P)\right)^2$$
- Based on historic data points
- Differentiation yields: $\nabla J_Q, \nabla G_Q$

Solution of

$$\min_u J_m^{ad,k}(u)$$
$$\text{s.t. } G_m^{ad,k}(u) \le 0$$
$$J_m^{ad,k} = J_m(u^k) + \left(\nabla J_Q(u^k,P) - \nabla J_m(u^k)\right)^T (u-u^k)$$
$$G_m^{ad,k} = G_m(u^k) + G_Q(u^k,P) - G_m(u^k) + \left(\nabla G_Q(u^k,P) - \nabla G_m(u^k)\right)^T (u-u^k)$$

W. Gao, S. Wenzel, S. Engell: Reliable modifier-adaptation strategy for real-time optimization. Computers and Chemical Engineering 91, 318-328, 2016

MA with Quadratic Approximation – switching depending on the model accuracy

Optimization based on the modified model

$$\min_u J_m^{ad,k}(u)$$
$$\text{s.t.}\, G_m^{ad,k}(u) \le 0$$
$$J_m^{ad,k} = J_m(u^k) + \left(\nabla J_Q\left(u^k, P\right) - \nabla J_m\left(u^k\right)\right)^T \left(u - u^k\right)$$
$$G_m^{ad,k} = G_m\left(u^k\right) + G_Q\left(u^k, P\right) - G_m\left(u^k\right) + \left(\nabla G_Q\left(u^k, P\right) - \nabla G_m\left(u^k\right)\right)^T \left(u - u^k\right)$$

- Theoretical model corrected by the quadratic process model

Optimization based on the quadratic model:

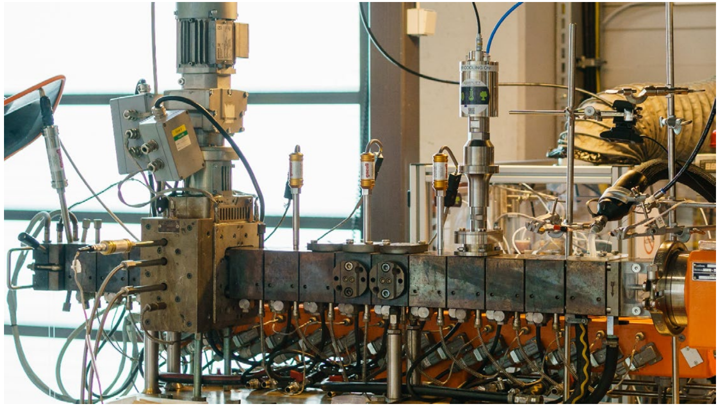
$$\min_u J_Q(u, P)$$
$$\text{s.t.}\; G_Q(u, P) \le 0$$
$$\left(u - u^k\right)' \cdot cov\left(\boldsymbol{u}^k\right) \cdot \left(u - u^k\right) \le \gamma^2$$

- Data-based quadratic model used
- Restriction of the moves

Here only the quadratic model was used → effective low-cost solution

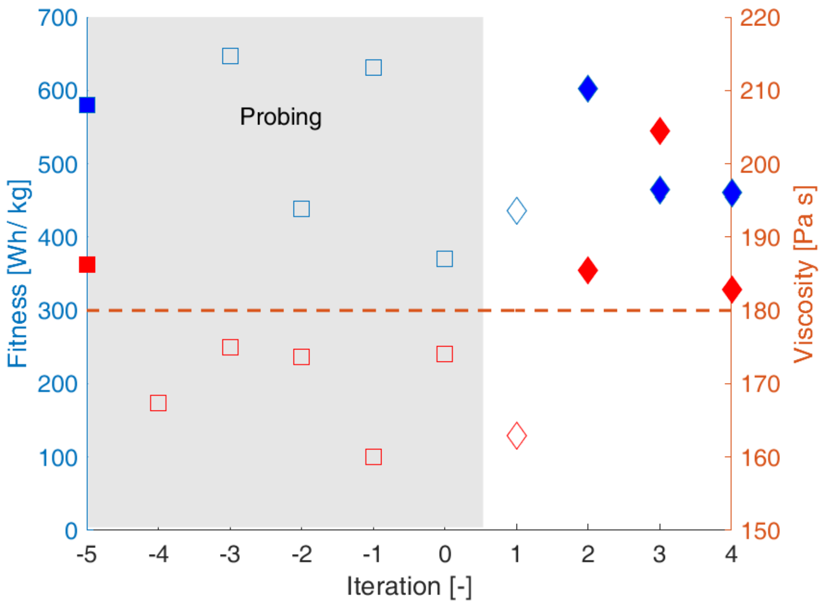
Application in pilot scale

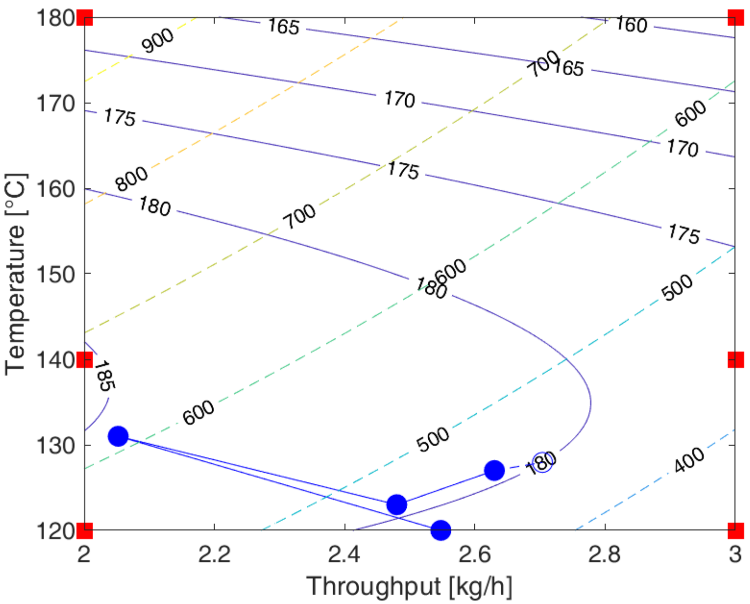
- Leistritz 18mm Maxx Extruder 60 L/D at FhG ICT
  - In-Line Viscometer
- Manipulated variables:
  - $T_{B,7}$ [120-180°C]
  - $\dot{m}$ [2-3 kg/h]
- Objective: Specific energy input
  - $J = \frac{\dot{Q}_{motor} + \dot{Q}_{heat}}{\dot{m}}$
- Constraint:
  - $\eta > 180$ Pa s → Information on M_w as the temperature is held constant



Experimental Results

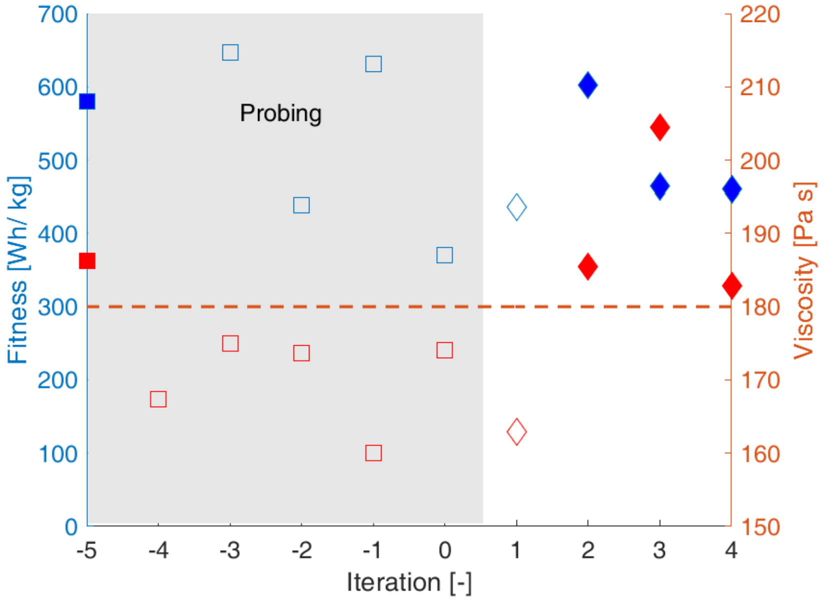
Probing
Iterations





Cost-function

Experimental Results



Satisfaction of the constraints while:

- - 20% energy consumption
- + 31,5% throughput

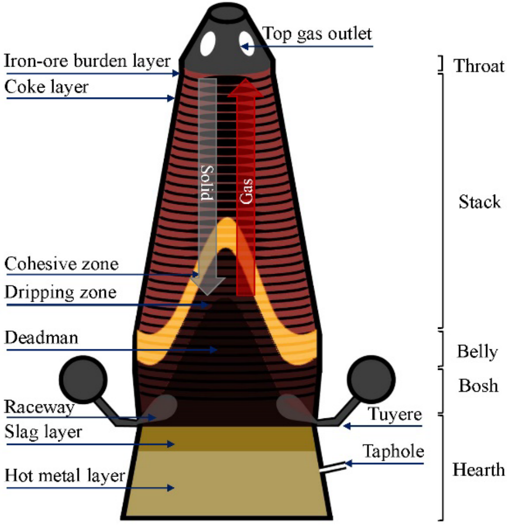
Efficient approach to achieve optimal operation even at smaller scales

Should be exploited commercially!

Improved operation of a large-scale blast furnace – Work by Pourya Azadi

- Core piece of equipment in the steel industry
  - Large energy consumption and CO_2 emissions (7 M ton p.a.)
- **Primary goals**
  - Stable, efficient, and economically viable operation
  - Automated optimal control of the internal thermal state
- **Challenges**
  - Multi-phase and multi-scale physics and chemistry
  - Nonlinear dynamics with largely different time scales
  - Presence of unmeasured disturbances
  - Absence of direct internal measurements
- **Proposed approach**
  - Optimizing model-based control scheme
  - **Based on a hybrid model**

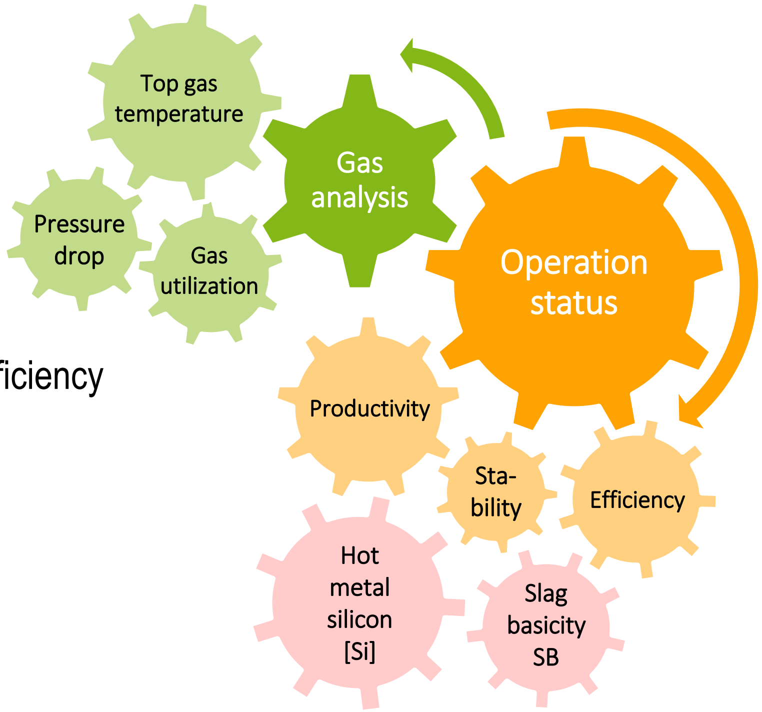
HYPRO Hybrid Process Control



Overall sketch of a blast furnace

Complex process – complex control task

- Key aspects and indicators
  - **High quality**
    - **Low [Si] → better product quality** for steelmaking
  - **High efficiency**
    - **Higher CO gas utilization:** $\eta = \frac{CO_2}{CO+CO_2}$ → **higher** CO efficiency
  - **Stability**
    - Avoid a low top gas temperature
    - **Slag basicity SB**
      - Slag fluidity



Hybrid process model

- Input set $\underline{U}$: Hot blast and solid phase variables
- Output set $\underline{Y}$: Top gas and product quality indices
- Gas dynamics: data-driven nonlinear auto-regressive model with exogeneous input (NARX)[1]

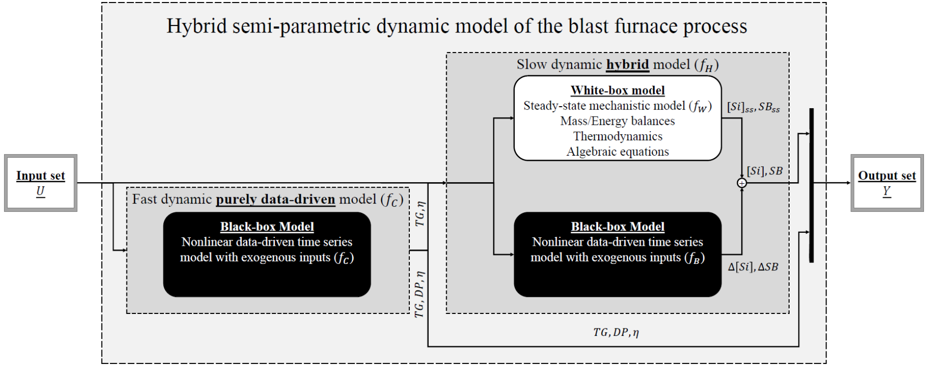
$$\underline{y_g}(t) = \underline{f_C}\left(\underline{y_g}(t-1), \ldots, \underline{y_g}\left(t-d_{y_g}\right), \underline{U}(t), \ldots, \underline{U}(t-d_u)\right)$$

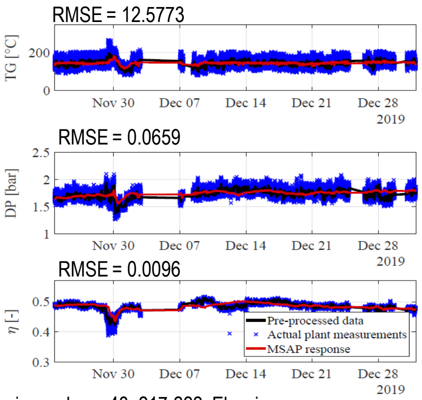
- Slow dynamics → hybrid model[2]

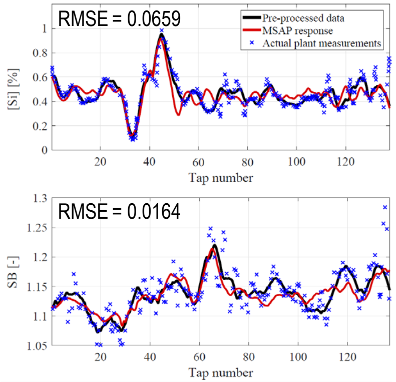
$$\underline{y_s}(t) = f_H\left(\underline{y_s}(t-1), \ldots, \underline{y_s}(t-d_{y_s}), \underline{U'}(t-\underline{d}_{u'}), \ldots, \underline{U'}(t-\overline{d}_{u'})\right)$$

With: $\underline{U'}(t) = \underline{U}(t) \cup \{TG(t), \eta(t)\}$

  - Steady-state, simplified white-box model (f_W)
    - Algebraic mass and energy balance equations
  - Data-based NARX model (f_B)





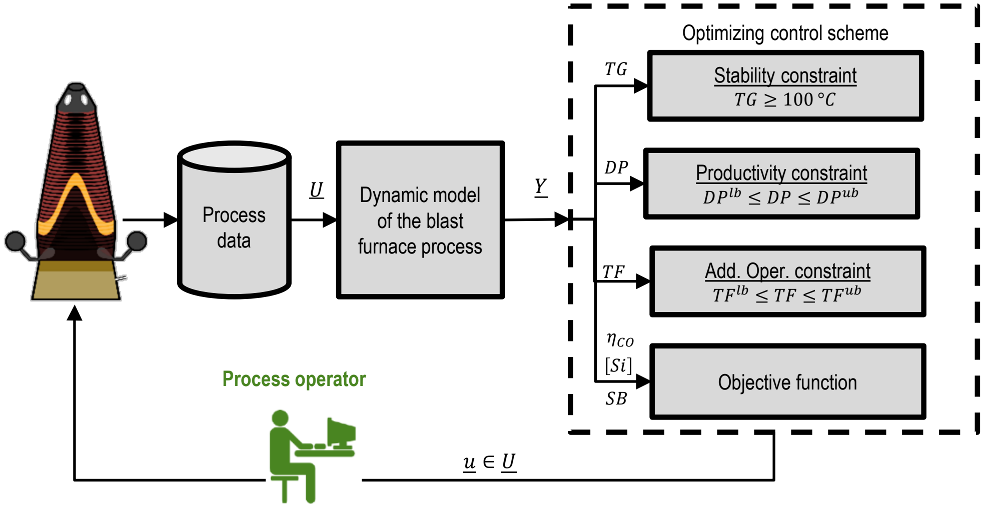


[1] Azadi, P. et al. (2020). Nonlinear prediction model of blast furnace operation status. In Computer Aided Chemical Engineering, volume 48, 217-222. Elsevier.
[2] Azadi, P., et al. (2022). A hybrid dynamic model for the prediction of molten iron and slag quality indices of a large-scale blast furnace. Computers & Chemical Engineering, 156, 107573.

Optimizing MPC

Goal: Efficient thermal control

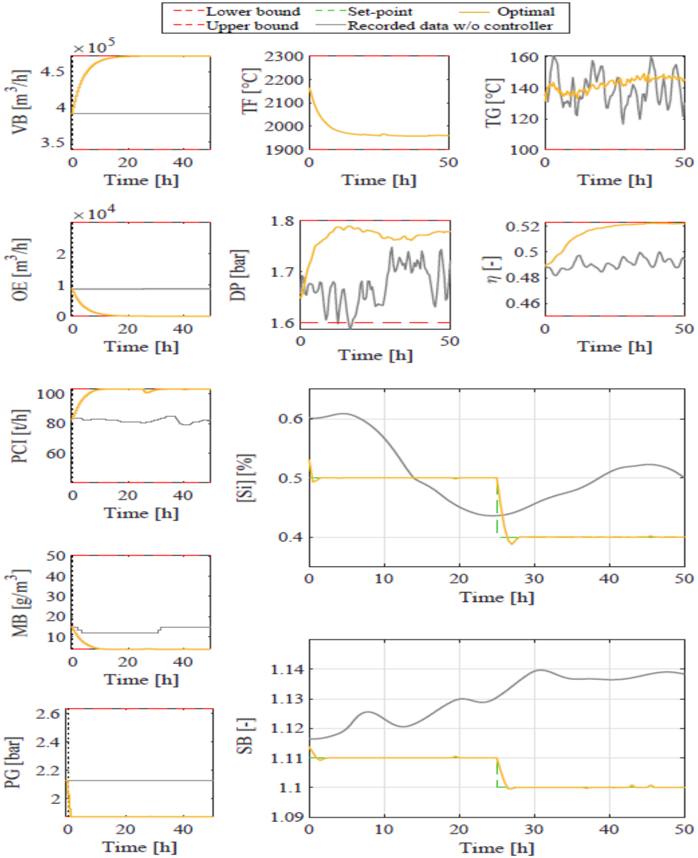
- Adjustment of the fast dynamic variables to counteract the unmeasured disturbances that are imposed by the solid feed
- Manipulated variables $\underline{u}$:
  - Blast volume, blast moisture, top pressure, oxygen enrichment, pulverized coal
- Objective function: tracking and efficiency



$$\min_{\underline{u}\in\underline{U}} w_1 \sum_{i=1}^{N_P}\sum_{k=1}^{N_y} \alpha_{k,i}(y_{k,i}-y_{ref_{k,i}})^2 - \mathrm{w}_2 \sum_{i=1}^{N_P} \eta_{CO_i} + \sum_{i=1}^{N_C}\sum_{k=1}^{N_u} \theta_{k,i}(u_{k,i}-u_{ref_{k,i}})^2 + \sum_{j=1}^{N_C}\sum_{k=1}^{N_u} \beta_{k,j}\Delta u_{k,j}^2$$

Simulation results

- Combined tracking and efficiency objective
  - Controller actions make sense from the point of view of the physics and chemistry of the process
  - Impact of the controller on productivity and fuel-saving
    - **5.4% higher production rate**
    - **2.3% fuel saving**
- **Can be used as an operator advisory**

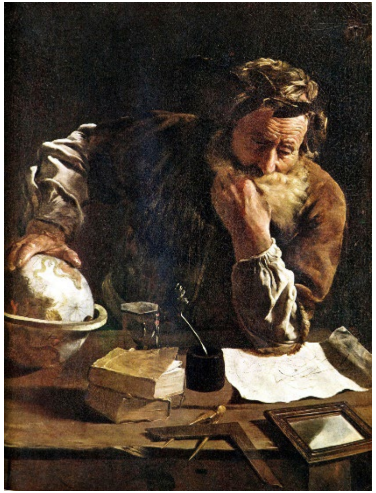


Azadi, P., et al.: Improved operation of a large-scale blast furnace using a hybrid dynamic model based optimizing control scheme. Journal of Process Control, 129, 103032., 2023

5. The modelling bottleneck - is AI the solution?

The Archimedian point of real-time optimization and control

- The term **Archimedean point** *(punctum Archimedis)* refers to the great Greek mathematician and physicist Archimedes of Syracuse (c. 287 – c. 212 BC), who supposedly claimed that he could lift the Earth off its foundation if he were given **a place to stand, one solid point, and a long enough lever**. (Wikipedia)
- Our Archimedean point are **MODELS**.
- Control theory and optimization methods provide a huge store of levers.
- But to apply (most of) them, you need the fixed point: **the model**.
- Given a good model, we can do almost everything – within the limits of fundamental restrictions due to system dynamics, actuation etc.



Wikipedia

The modelling bottleneck

- The main obstacle for the widespread application of model-based solutions is the engineering effort
  - to develop the solution
  - **to keep it alive.**
- Most of the engineering effort in the development phase goes into model development.
  - One PhD thesis for modelling of each and every process is not realistic
- Adaptation of models to changes in the plants and in the products is a major issue in the maintenance of the solution.

- For inaccurate models, the use of **measurements** (data) and **feedback** is the key to success, as it alleviates the requirements for the quality of the models.
- But the mismatch may also lead to complete failure.

- Great linear theory for this, very little for nonlinear systems

Can AI overcome the modeling bottleneck?

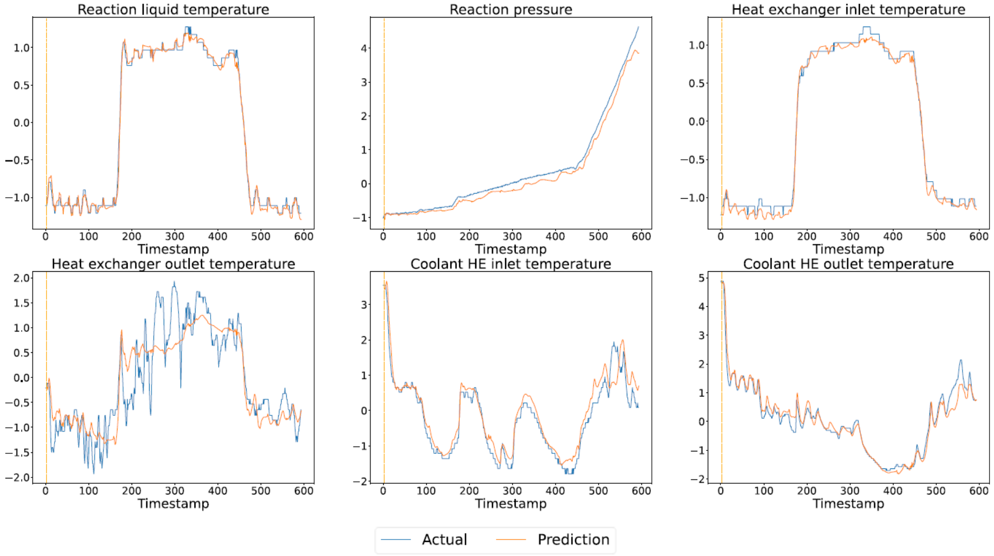
Experiences with the use of machine learning models

Based on work on several applications with industry in the KEEN project

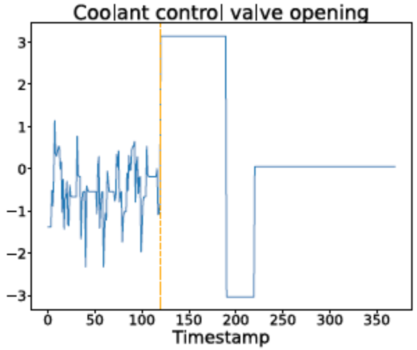
Results of a Master thesis in cooperation with Balasz Bordas at MERCK

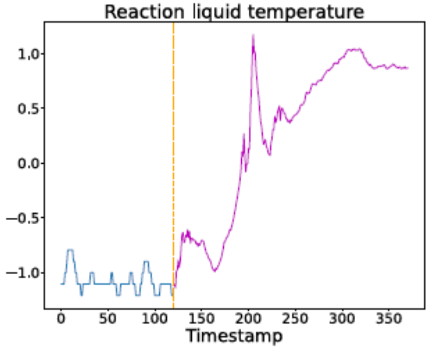
KEEN

- Modeling of a semi-batch reactor by Maria Paola Galvis
- Large data base, 460 batches, 600 samples of all variables per batch
- Training of dynamic NARX und LSTM models, careful choice of the hyperparameters
- Excellent predictions



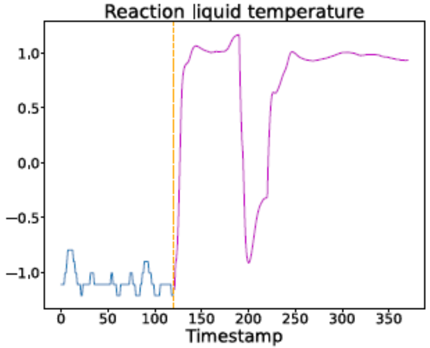
But the models were qualitatively wrong and not fit for the purpose





Model 1

Temperature rises for increased flow of coolant!



Model 2

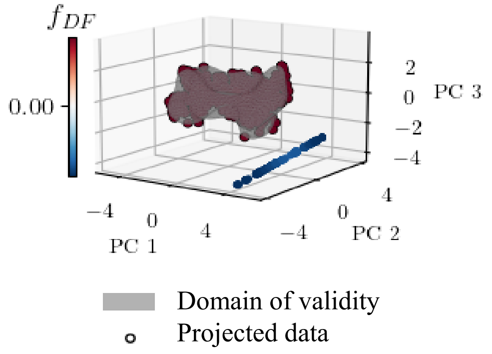
What is important for the online use of models?

- Models have to be dependable and qualitatively correct.
  - Then feedback can take care of small to medium-size deviations (in the best case)
- Model errors should be quantified!
  - Very difficult with purely data-based techniques in a global manner

- Strong preference for hybrid models
  - (Simplified) mechanistic models improved by parallel data-based error correction models
  - Mechanistic models with embedded data-based submodels for relationships that are difficult to describe

Parallel data-based models

- Intuitively convincing, but no guarantee of a qualitatively correct behaviour
- Our approach (**Mohamed Elsheikh**):
  - Monitoring of the domain of validity of the data-based model using a one-class SVM
    - A. M. Schweidtmann, et al., Obey validity limits of data-driven models through topological data analysis and one-class classification. Optimization and Engineering, 2022.

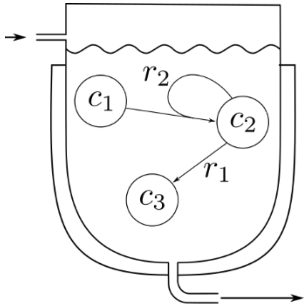


  - Fading out of the data-based element outside of the domain of validity
  - Adaptation of the domain of validity if the prediction error of the data-based model was lower than a null-hypothesis

Elsheikh M., Ortmanns Y., Hecht F., Roßmann V., Krämer S., Engell S.:
Control of an Industrial Distillation Column Using a Hybrid Model with Adaptation of the Range of Validity and an ANN-based Soft Sensor. Chemie-Ingenieur-Technik, 95 (7), 1114 - 1124, 2023

Gray-box modeling with embedded machine learning models

- Define a model structure that is based on first principles
- Use ML-submodels to describe the complex relationships of specific embedded variables to state variables and inputs
  - Typical example: reaction rates

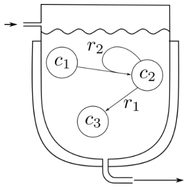


$$\overbrace{\frac{dc_3}{dt} = \frac{\dot{V}}{V}(c_{3,in} - c_3)}^{\text{Standard first principles model equations}} + \underbrace{\boldsymbol{r_1}}_{\text{embedded variable, which is supposed to be described with ML-submodel, for example an artificial neural network}}(c_2, T)$$

- Advantage: Transparency of the overall model, easier to check the ML-submodels, additional flexibility where needed
- Challenge: Finding a suitable ML-model structure and parameter values
- Approach: Estimate a static training set that can be used with any ML-Toolbox for generating good initial values of ML-parameters and a model structure

Methodology of dynamic Gray-Box Modelling (Joschka Winz)

1 Setup first principles equations



$$\frac{dc_3}{dt} = \frac{\dot{V}}{V}(c_{3,in} - c_3) + r_1$$

Formulate model as set of DAEs / ODEs

2 Specify variables with unknown submodels

$$\frac{dc_3}{dt} = \frac{\dot{V}}{V}(c_{3,in} - c_3) + \underbrace{\boldsymbol{r_1}}_{\varphi = r_1}$$

Find small set of variables for ML modelling

3 Estimate a training set for embedded variables

What values should the ML-model assume to describe the experimental data?

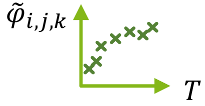
Training set:

$$\begin{bmatrix} \vdots & \vdots \\ \hat{c}_2(t_k) & T(t_k) \\ \vdots & \vdots \end{bmatrix} \qquad \begin{bmatrix} \vdots \\ \tilde{\varphi}(t_k) \\ \vdots \end{bmatrix}$$

Input from $\hat{x}, \hat{z}, u$ Output $\tilde{\varphi}$

4 Use the estimated training set for input and model selection

Correlation analysis:



Training set

ML toolbox

ML model structure + Θ_{ML}

5 Full dynamic parameter estimation

Set of input quantities, initial parameter values and ML model structure from **4**

<u>Result: Dynamic model with embedded ML submodel</u>

Application to a fermentation process

- Virtual plant with three states

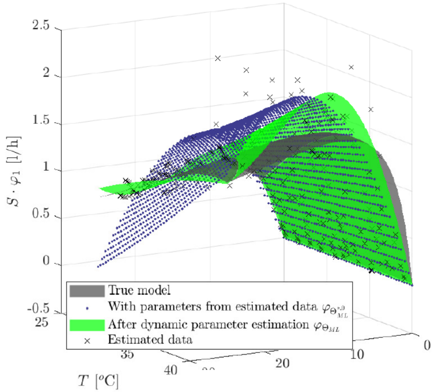
$$S \xrightarrow[\text{growth}]{r_g} X_v \xrightarrow[\text{sporulation}]{r_s} X_s.$$

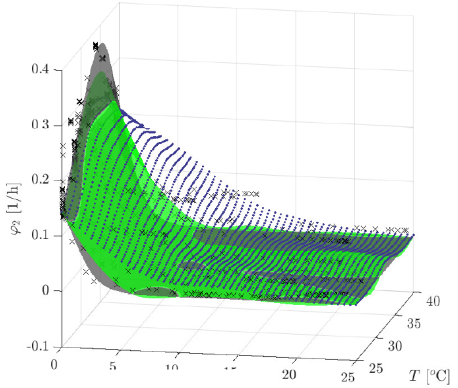
- Assumed gray-box model structure

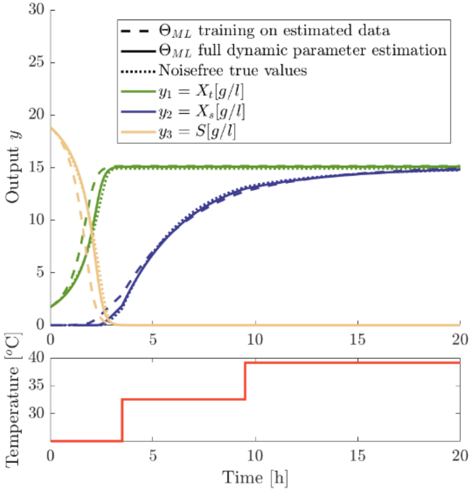
$$\dot{\hat{X}}_v = \varphi_1\, \hat{X}_v\, \hat{S} - \varphi_2\, \hat{X}_v$$

$$\dot{\hat{S}} = -\theta\, \varphi_1\, \hat{X}_v\, \hat{S}$$

$$\dot{\hat{X}}_s = \varphi_2\, \hat{X}_v$$







Conclusions

- Machine learning holds the promise to provide better models from data
  - Provided there is enough and rich enough data!
  - That there is a lot of gold in operational data is a fairy tale.
- For online applications, **dependability is key**.
- The more structured a model, the more easy it is to establish dependability.
- ML models are promising as surrogates that are trained on simulation models
  - Coverage is possible, range and dynamics!
  - But then again a simulation model is the starting point and the reference.
- Online-training of controllers (RL)?
  - Probably realistic only if most of the learning is done in simuations

6. Final remarks

Uncertainty

- All engineering activities must cope with uncertainty
- To consider and quantify uncertainties is key – between science and intuition
- In uncertain situations, an important element is **recourse** (plan B)
  - Feedback is recourse – a pre-programmed reaction to the uncertainty with often only vaguely understood consequences
- Multi-stage formulations anticipate recourse in the here-and-now decisions
  - Leads to non-conservative decisions (in contrast to always expecting the worst)
  - Can be used to include risks in the decision
  - Can be used to quantify the (best-case) effect of the uncertainties
  - Dual control can be treated rigorously

    S. Thangavel, S. Lucia, R. Paulen, S. Engell: Dual robust nonlinear model predictive control: A multi-stage approach. Journal of Process Control, 72, 2018, 39-51.

Models and feedback

- Feedback reduces the need for good models by using measurements
- But can also enhance model errors up to instability
- Model-based methods are powerful and applicable to complex real-world scale problems, cf.

  Haßkerl, D., Lindscheid, C., Subramanian, S., Markert, S., Górak, A., Engell, S.: Dynamic Performance Optimization of a Pilot-Scale Reactive Distillation Process by Economics Optimizing Control. Industrial and Engineering Chemistry Research, 57 (36), 12165-12181, 2018

- MA is great because it works with simplified models – should be commercialized!

- Hybrid models are the most promising way to apply machine learning

Drivers and KPIs

- Everybody has to find their own balance – there is a tension between the pragmatic, seeking truth and glory, and the necessities of life.
- Good to have „large themes“, e.g. for me how to deal with uncertainty

- It is very satisfactory to have an impact
  - My biggest impact was by educating great engineers

- Impact does not (only maybe even not predominantly) depend on the academic side
  - Deployment, roll-out of innovations need commercial companies that take them up
  - People and company policies are very important, see evidence in:

    S. Klessova, S. Engell, C. Thomas: The interplay between the contextual conditions and the advancement of the technological maturity in inter-organisational collaborative R&D projects: A qualitative study. R&D Management, 2023.

Thanks to my coworkers

and to our industrial cooperation partners!

Thank you very much for your attention!

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SIMPLIFY
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This research has been supported by the project "KI-Inkubator-Labore in der Prozessindustrie - KEEN", funded by the Bundesministerium für Wirtschaft und Klimaschutz (BMWK) under grant number 01MK20014T.