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

  ![Abstract](image)

  *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
  - 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

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![Diagram of a chemical process](image1.png)

![Image of a reactive distillation system](image2.png)

![Graph of frequency response](image3.png)
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

>160 citations in Scopus, reprinted 2020

Real experimental data
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,
  - 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)

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

KPIs in the academic world
- External and personal
- Personal pleasure, e.g. travel

Resources and funding
- Try to shape it!

Impact in the real world
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

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

- 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

- Beauty is the splendor of truth

- Resources and funding

- External and personal
2. Priority themes on the Strategic Research and Innovation Agenda of Processes4Planet
Processes4Planet: a co-programmed Partnership in Horizon Europe

Co-programmed Partnership

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

Cluster 4
Digital, Industry and Space
Connections to Cluster 5
**Public Partner**

- **Board of Directors**
  - Up to 29 members + 1 SME

**Private Partner**

- **Board of Directors**
  - 5 representatives
- **Executive Director**
  - 1 representative
- **APG**
  - 15 representatives (incl. Ambassadors Group Leader)

**Advisory and Programming Group (APG)**

- **Executive Director**
  - A.SPIRE Office

**A.SPIRE PWGs / Experts**

- **Executive Director**
  - A.SPIRE Office

**PARTNERSHIP BOARD**

- **Processes4Planet**
  - Signatories
  - Commitment
  - Decision making

**ASYNC**

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

**THE ASSOCIATION**

- **Board of Directors**
  - 5 representatives
- **Executive Director**
  - 1 representative
- **APG**
  - 15 representatives (incl. Ambassadors Group Leader)

**Co-chair of PB**

**Co-chair of PB**

**THE PARTNERSHIP**

**Public Partner**

- **Chair SE**
3. Future research and innovation priorities of Processes4Planet

- Driven by the goals of
  - **Climate** (Reduction of the CO₂-Emissions) (-55% by 2030 but -60% for EEI compared to 2005)
  - **Circularity** (Reduction of waste, assure availability of critical raw materials also affects the CO₂ 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
  \( \rightarrow \) need for flexibility

- Different designs of plants needed
- Much more agile operation, demand response
- Costly – unused capacity, higher CAPEX
- Currently many studies on optimal flexible operation, e.g. air separation units, electrolysers
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 CO₂ 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

NH₃ (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

Comparison of the power costs for running the compressors (reality vs. optimised schedule)

More than 20% savings!
Stochastic short-term integrated electricity procurement and production scheduling (work by Egidio Leo)

- 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 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
DSM in the continuous production of zeolites\cite{1}

- Work by Robin Semrau in collaboration with ARKEMA
- 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%

\cite{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
  - 2\textsuperscript{nd} order polynomials
  - Radau roots

Implementation
- Implemented in CasADi (python)
- Solved with IPOPT
- 100,000 variables
- 1 h computation time

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

\[ \min_{u,x} \int_0^{t_f} \Phi(u, \gamma) \, dt + \lambda^*_s T x(t_f) \]
\[ \text{s.t.:} \]
\[ \dot{x} = f(x, u), x(0) = x_0 \]
\[ u_{ub} \geq u \geq u_{lb} \]
\[ T_w \leq 403.15K \]
\[ X \geq 0.98 \]
\[ F_{fix} = 1/\Delta t \int_{t_k}^{t_{k+1}} F(t) \, dt \]
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

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

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[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%
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 efficiency usually happens in small steps
- For electric power from renewables, there is limited supply, high cost, and competition between sectors
- Efficiency must continuously 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

- 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

- $J_Q(u, P) = \sum_{i=1}^{n_u} \sum_{j=1}^{n_u} a_{i,j} u_i u_j + \sum_{i=1}^{n_u} b_i u_i + c$
- $\min_p \sum_{i=1}^{n} (J_P(u^i) - J_Q(u^i, P))^2$

Based on historic data points

- Differentiation yields: $\nabla J_Q, \nabla G_Q$

Solution of

$\min_{u} J_m^{ad,k}(u)$

s. t. $G_m^{ad,k}(u) \leq 0$

$J_m^{ad,k} = J_m(u^k) + (\nabla J_Q(u^k, P) - \nabla J_m(u^k))^T (u - u^k)$

$G_m^{ad,k} = G_m(u^k) + G_Q(u^k, P) - G_m(u^k)$

$+ (\nabla G_Q(u^k, P) - \nabla G_m(u^k))^T (u - u^k)$

MA with Quadratic Approximation – switching depending on the model accuracy

Optimization based on the modified model:

\[
\begin{align*}
\min \limits_u J_{m, k}^{ad}(u) \\
\text{s. t. } G_{m, k}^{ad}(u) \leq 0
\end{align*}
\]

\[
J_{m, k}^{ad} = J_m(u^k) + \left( \nabla J_Q(u^k, P) - \nabla J_m(u^k) \right)^T (u - u^k)
\]

\[
G_{m, k}^{ad} = G_m(u^k) + G_Q(u^k, P) - G_m(u^k) + \left( \nabla G_Q(u^k, P) - \nabla G_m(u^k) \right)^T (u - u^k)
\]

- Theoretical model corrected by the quadratic process model

Optimization based on the quadratic model:

\[
\begin{align*}
\min \limits_u J_Q(u, P) \\
\text{s. t. } G_Q(u, P) \leq 0
\end{align*}
\]

\[
(u - u^k)' \cdot \text{cov}(u^k) \cdot (u - u^k) \leq \gamma^2
\]

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

Here only the quadratic model was used \(\rightarrow\) 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 $\rightarrow$ Information on $M_w$ as the temperature is held constant
Experimental Results

- Fitness [Wh/kg]
- Probing
- Iterations
- Temperature [°C]
- Throughput [kg/h]
- Viscosity [Pas]

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 CO₂ 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 $U$: Hot blast and solid phase variables
- Output set $Y$: Top gas and product quality indices
- Gas dynamics: data-driven nonlinear auto-regressive model with exogeneous input (NARX)\(^1\)
  \[
  y_g(t) = f_C \left( y_g(t-1), \ldots, y_g(t-d_y), U(t), \ldots, U(t-d_u) \right)
  \]
- Slow dynamics → hybrid model\(^2\)
  \[
  y_s(t) = f_H \left( y_s(t-1), \ldots, y_s(t-d_y), U'(t-d_u), \ldots, U'(t-d_u') \right)
  \]
  With: $U'(t) = U(t) \cup \{TG(t), \eta(t)\}$
  - Steady-state, simplified white-box model ($f_W$)
  - Algebraic mass and energy balance equations
  - Data-based NARX model ($f_B$)

RMSE = 12.5773
RMSE = 0.0659
RMSE = 0.0096

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 $u$:
  - Blast volume, blast moisture, top pressure, oxygen enrichment, pulverized coal
- Objective function: tracking and efficiency

$$\min_{u \in U} w_1 \sum_{i=1}^{N_P} \sum_{k=1}^{N_Y} \alpha_{k,i} (y_{k,i} - y_{ref,k,i})^2 - w_2 \sum_{i=1}^{N_P} \sum_{k=1}^{N_Y} \eta_{CO_i} + \sum_{i=1}^{N_C} \sum_{k=1}^{N_u} \theta_{k,i} (u_{k,i} - u_{ref,k,i})^2 + \sum_{j=1}^{N_C} \sum_{k=1}^{N_u} \beta_{k,j} \Delta u_{k,j}^2$$

Diagram:
- Process data
- Dynamic model of the blast furnace process
- Optimizing control scheme
- Stability constraint $TG \geq 100^\circ C$
- Productivity constraint $DP^{lb} \leq DP \leq DP^{ub}$
- Add. Oper. constraint $TF^{lb} \leq TF \leq TF^{ub}$
- Objective function
- Productivity constraint $DP^{lb} \leq DP \leq DP^{ub}$
- Add. Oper. constraint $TF^{lb} \leq TF \leq TF^{ub}$
- Objective function
- Process operator
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

5. The modelling bottleneck - is AI the solution?
The Archimedian point of real-time optimization and control

- The term **Archimedian 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 Archimedian 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.
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 KE-EN

- 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
  - 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
- 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

\[ \frac{dc_3}{dt} = \frac{\dot{V}}{V} (c_{3,in} - c_3) + r_1(c_2,T) \]
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
   \[
   \frac{dc_3}{dt} = \frac{\dot{V}}{V} (c_{3,in} - c_3) + r_1
   \]
   \[\varphi = r_1\]
   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:
   \[
   \begin{bmatrix}
   \hat{c}_2(t_k) & T(t_k) \\
   \vdots & \vdots \\
   \hat{\phi}(t_k)
   \end{bmatrix}
   \]
   Input from \(\hat{x}, \hat{z}, u\)  Output \(\hat{\phi}\)

4. Use the estimated training set for input and model selection
   Correlation analysis:
   \[\hat{\varphi}_{i,j,k}\]
   Training set
   ML toolbox
   ML model structure + \(\Theta_{ML}\)

5. Full dynamic parameter estimation
   Set of input quantities, initial parameter values and ML model structure from 4
   Result: Dynamic model with embedded ML submodel
Application to a fermentation process

- Virtual plant with three states

\[ S \xrightarrow{r_g} X_v \xrightarrow{r_s} X_s. \]

- Assumed gray-box model structure

\[
\dot{X}_v = \varphi_1 \dot{X}_v \dot{S} - \varphi_2 \dot{X}_v \\
\dot{S} = -\theta \varphi_1 \dot{X}_v \dot{S} \\
\dot{X}_s = \varphi_2 \dot{X}_v
\]
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 simulations
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

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.
- 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:

Thanks to my coworkers

and to our industrial cooperation partners!
Thank you very much for your attention!

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