Is AI now controlling our plants?

Lessons learnt from the KEEN project

KEEN
Künstlich**E** Int**E**lligenz **IN**kubator Labore in der Prozessindustrie
AI Incubator Labs in the Process Industry

Dr. Kai Dadhe, Evonik

Prof. Dr. Sebastian Engell, TU Dortmund

Or to put it in another way:

- Is AI ready to control our plants?
- Is AI able to control our plants?
- Do we want AI to control our plants?
- Where are the benefits when AI controls our plants?
- Do we have to forget everything we learnt when AI is controlling our plants?

Source: https://scherlund.blogspot.com/2019/01/call-to-reimagine-artificial.html licensed under CC BY

1. The KEEN Project

2. AI Applications in Process Operations in KEEN
   - Detection of phases of batch processes from recorded data
   - Optimization of operating points
   - Model-based control

3. Embedding the use of AI into the enterprise

NAMUR

01

The KEEN Project

This project has been supported by the Federal Ministry of Economics and Climate Protection (BMWK) under grant number 01MK20014T

The KEEN philosophy:
AI as „Cognitive Amplifier“ expanding our toolbox

Lab / Plant

Process Control

DCS

Assisting Systems

Interaction with AI

Process Identification & Modelling

Additional Insight

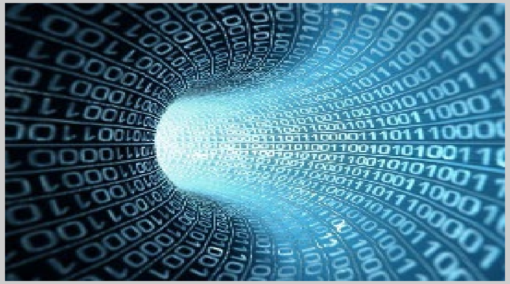
Machine Learning
Pattern Recognition
Time Series Analyses

Process, Equipment and Plant Technology, System Theory

Better Foresight

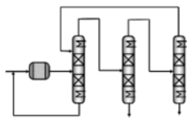
AI-based Optimization
Graph Based Inference
Hybrid Models

Virtual World



Modelling & Simulation

Mechanistic



AI Models

Fill Gaps or Reduce Complexity

Insight / Foresight / Exploration

KEEN addressed AI along the full Asset Life Cycle

NAMUR

AI based modeling	Computation of thermodynamic properties, flowsheets with AI models
AI based engineering	Support for Hazop, P&ID development
AI enabling technologies	Sensor data collection, MTP for camera, embedding of AI algorithms
AI based monitoring	AI-based image processing, analysis of recorded data
AI based control	Real-time optimization, model-based control

KEEN connected all the necessary players

NAMUR

Innovative Owner/Operators

Established Technology Providers

Associated Partners

Experienced Scientists

Agile SMC / Startups

Facts and figures

- Sponsored by BMWK
- Only project related to the Process Industry
- Budget ~ 17 M€
- More than 20 partners
- Apr 2020 – Sep 2023

NAMUR

02

AI Applications in Process Operations

Applications of AI in Process Operations

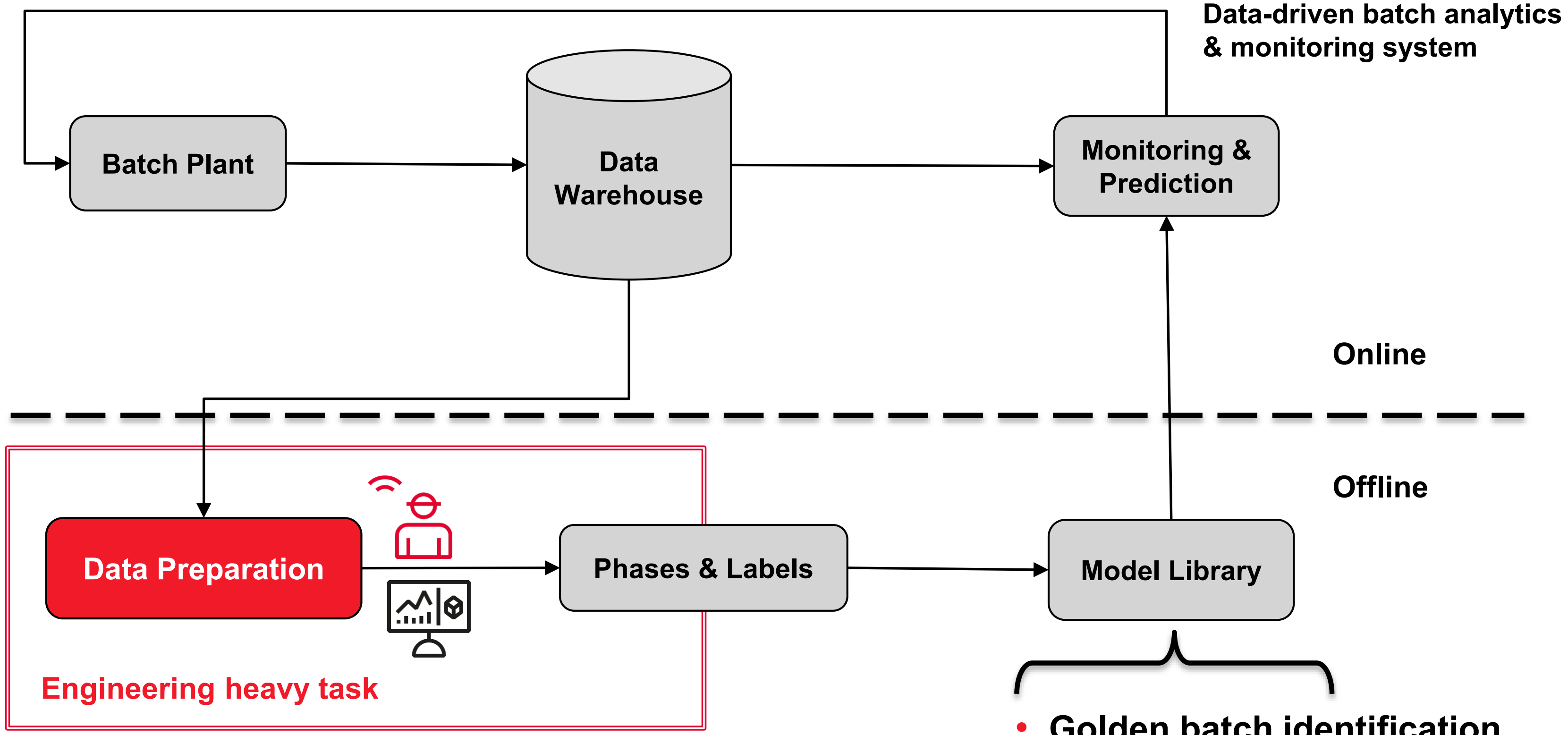
Goal: Progress towards self-optimizing plants

Main topics:

- Data analysis and monitoring
  → **Detection of the batch phases in batch process data**
- Optimal operation (real-time optimization, RTO)
  → **Industrial case**
- Model-based monitoring and control with AI (machine learning) models
  → **How to generate trust in AI models**

Support for batch process analysis and monitoring

Can AI support batch phase labeling without intensive human effort?



- **Time series segmentation**
- **Batch phase labeling**

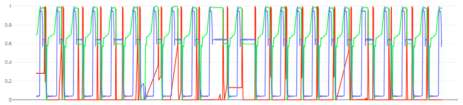
- **Golden batch identification or construction**
- **Root-cause analysis**
- **Anomaly detection**
- **Quality assessment**

Challenges

- Efficient methods for batch analysis rely on the detection of batch phases.
- Information about batch steps is not always accessible.
- Data preparation remains an engineering heavy task.
- Domain knowledge is extremely important but is only held by few experts.
- Automatic phase extraction and labeling can expedite model deployment and continuous improvement.

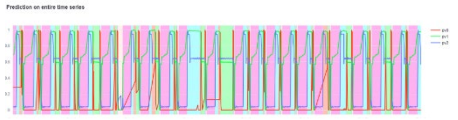
AI-supported batch phase extraction toolbox

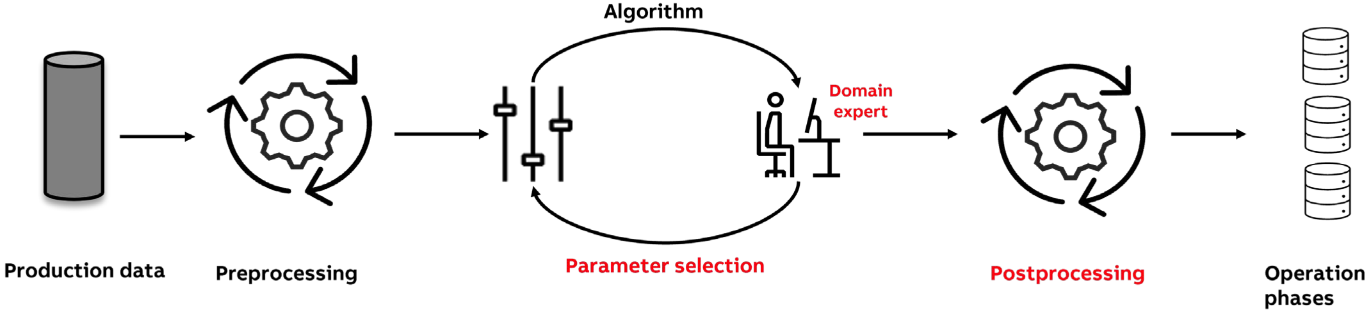
- **Input**
  - Batch process time series
- **User Interaction**
  - Selection of a single batch
  - Marking of the batch phases



- **Output**
  - Segmented batch phases of input data
  - Labelling of the extracted
  - Statistical analytics of the results
- **Features**
  - AI supported segmentation & labeling
  - Active learning framework with user interaction
  - Only labeling of one batch
  - No ML knowledge required, semi-automatic parameter tuning

Will be integrated into ABB BatchInsight

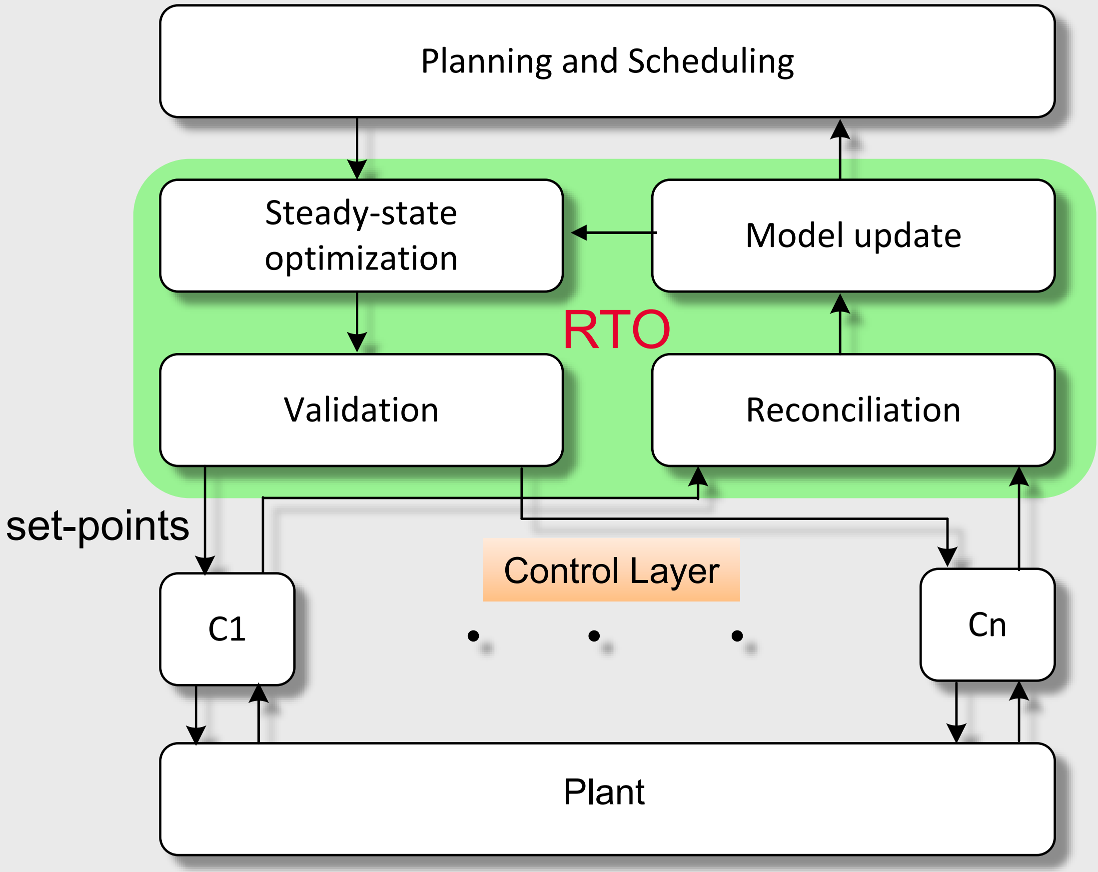




Toolbox Architecture

Iterative real-time optimization using ANNs

Real-time optimization



- Computation of optimal set-points for varying conditions
- Usually based on rigorous nonlinear models
- Areas of application: Large plants, refineries, crackers, …

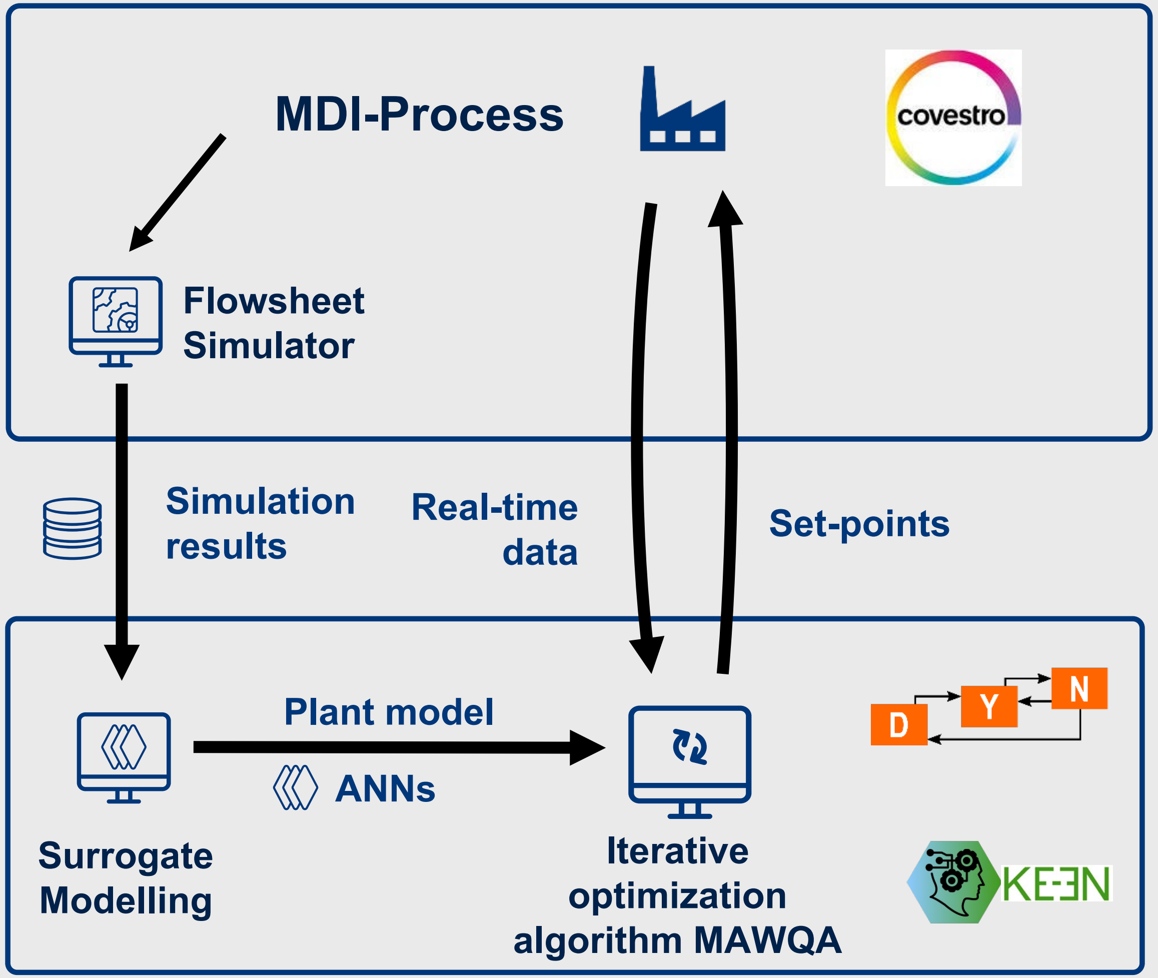
Challenges:

- Modeling comes with a large effort
- Models and real plants behave differently

Solution:

- ✓ Use an existing flowsheet simulator
- ✓ Replace the model by fast executable **ANNs**
- ✓ Cope with model errors by „***modifier adaptation***“

Application to the MDI-Process



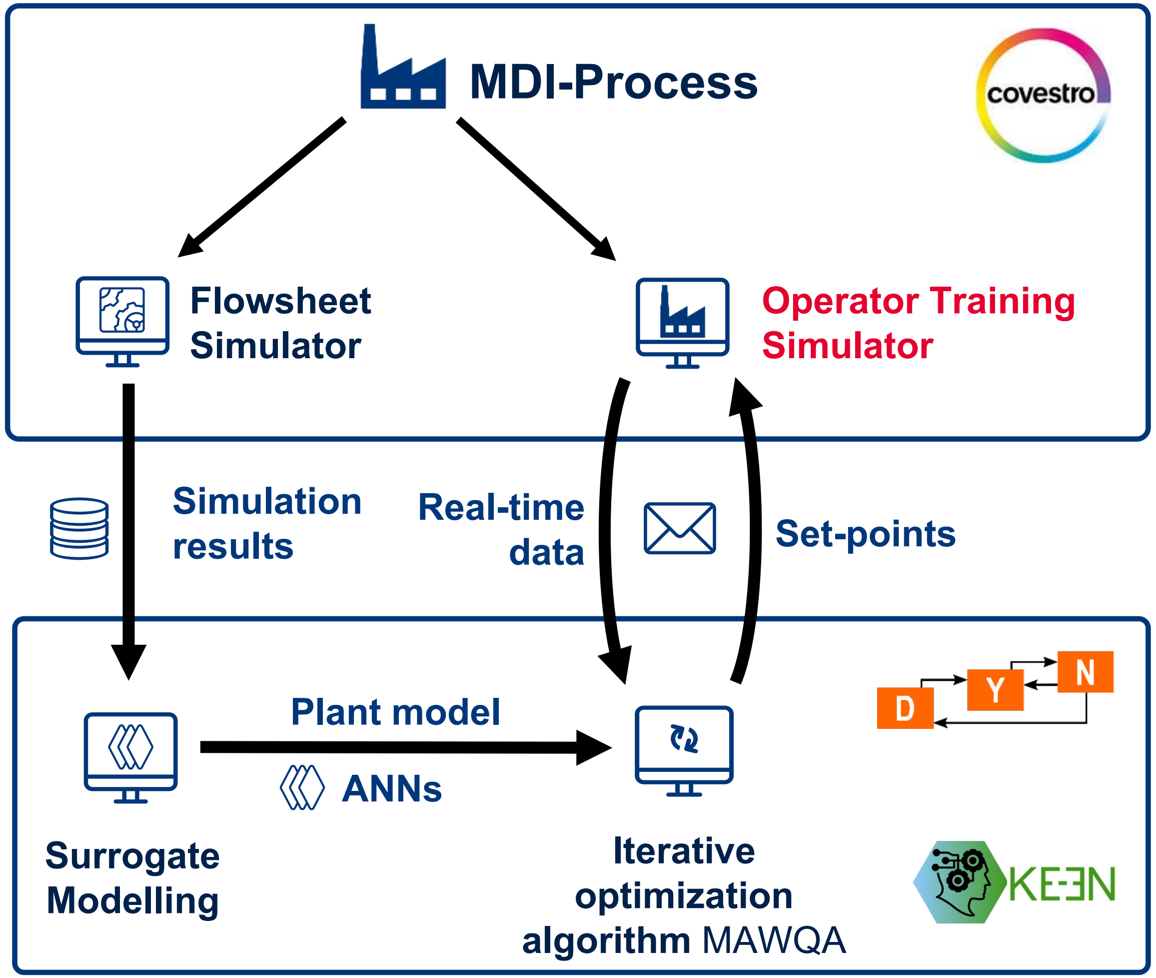
Goal:

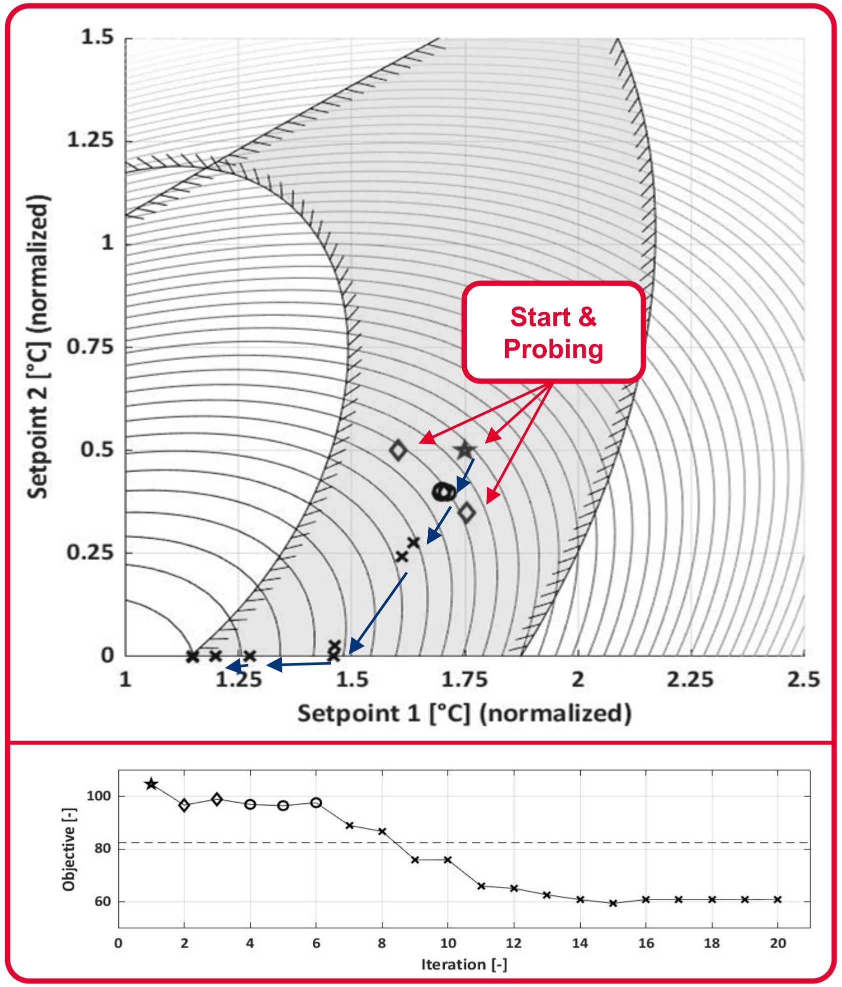
Reduction of fouling by optimization of the distribution of steam to different units

Ehlhardt, J., Ahmad, A., Wolf, I., Engell, S., 2023. *Real-Time Optimization Using Machine Learning Models Applied to the 4,4'-Diphenylmethane Diisocyanate Production Process*. Chemie Ing. Tech. 95, 1096–1103.

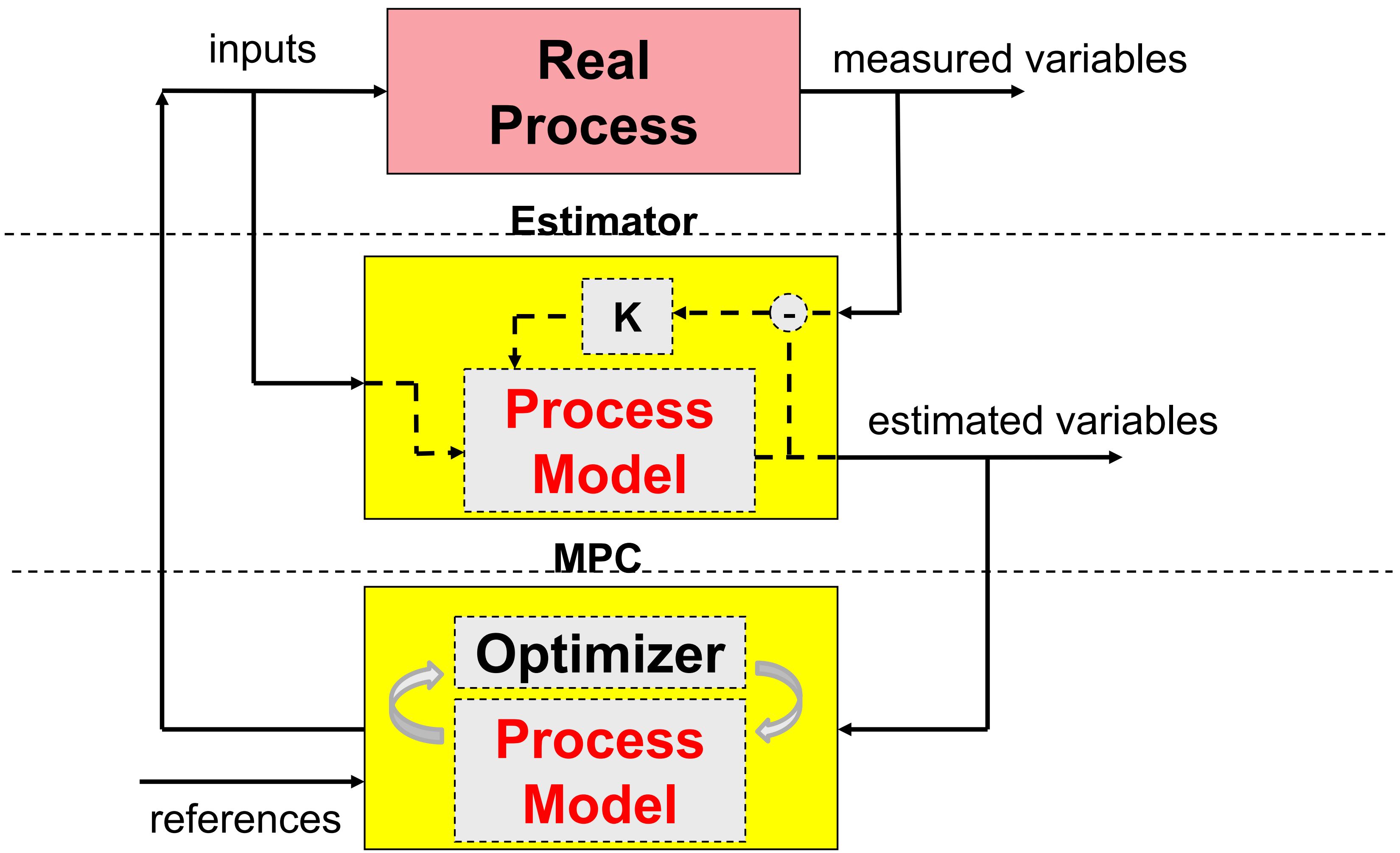
Engell, S., Ahmad, A., Ehlhardt, J., Wolf, I., 2022. Method for controlling a distributed control system. EP 22209645.5.

Application to the MDI-Process





AI in model-based control (MPC)



- The model is the central element!
- Modelling requires a significant effort.
- Model errors can lead to negative consequences which are hard to predict.

Idea:

- Reduce the modelling effort by the use of data-based (machine-learning) models!
- Not completely new …

Model-based control with neural net models was a hot topic already 1995

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

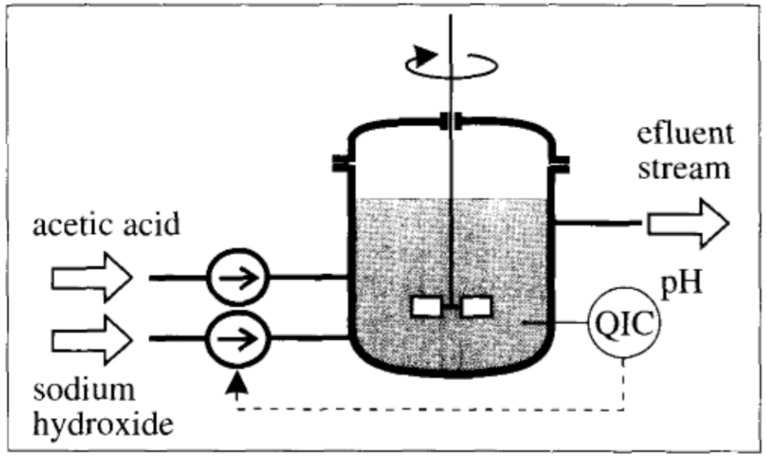


Fig. 1. Neutralization plant.

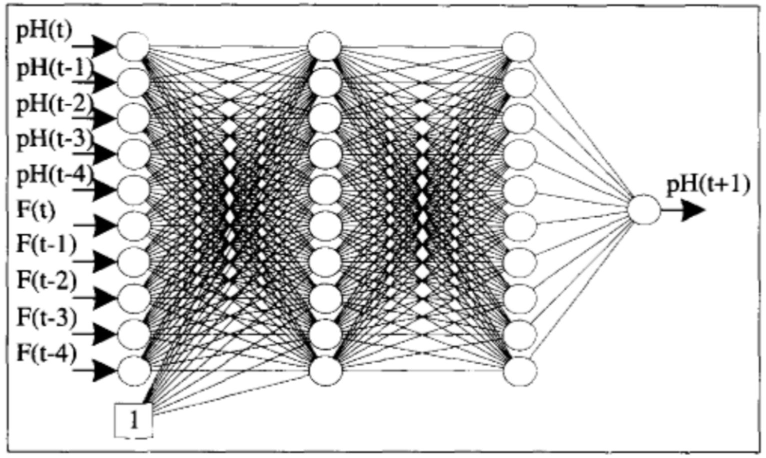
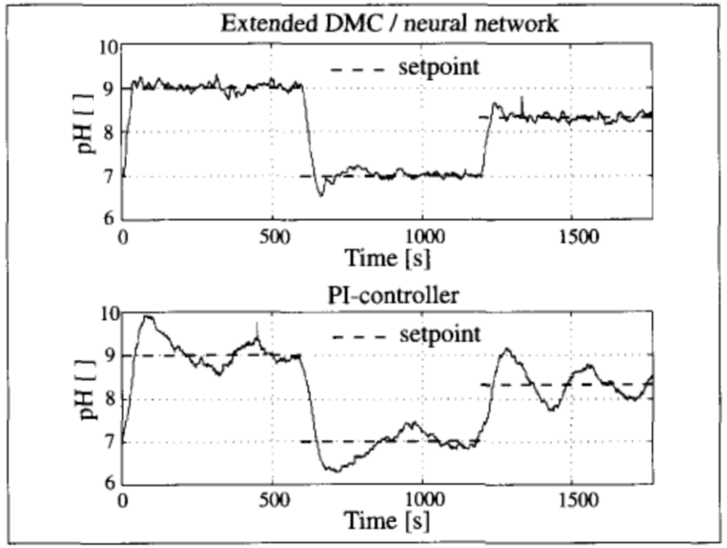


Fig. 3. Topology of the neural network.



The euphoria however decayed

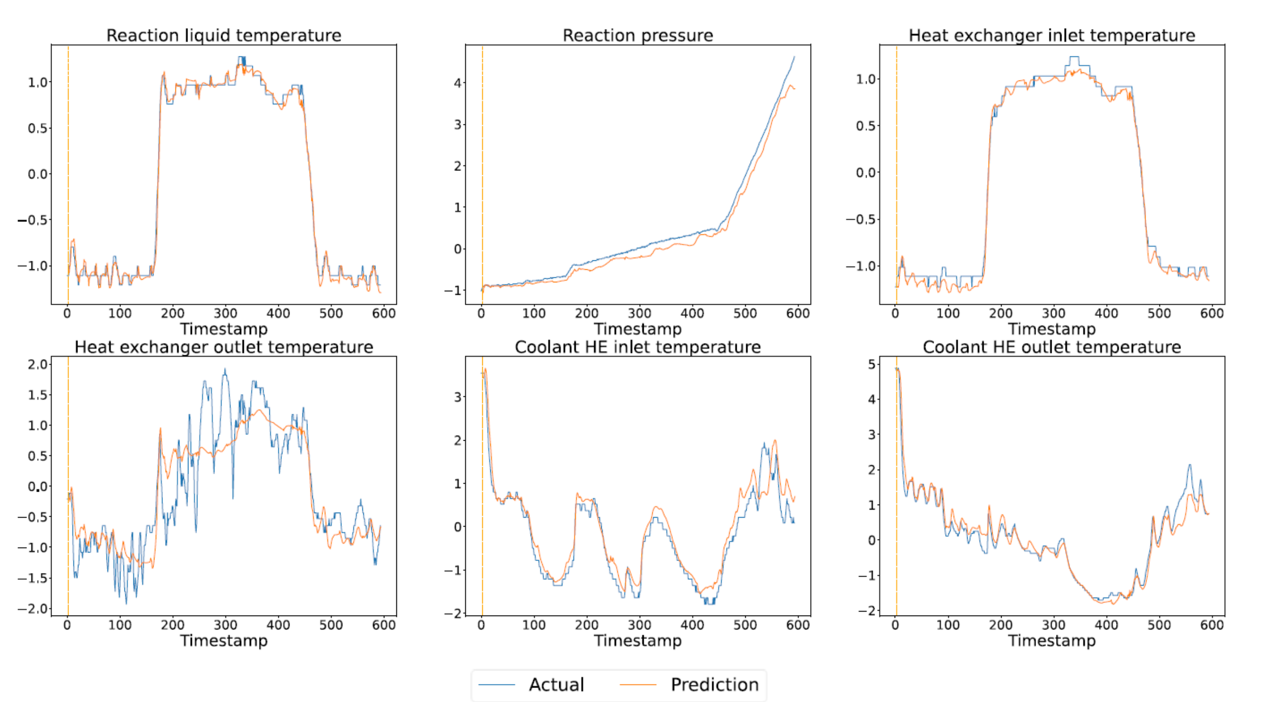
- Not accepted in industry, „black-box“- models were not welcome
- Problem to quantify the accuracy of a model and to rule out that it is not used when it is not valid

Results of the Master Thesis by Maria Paola Galvis supervised by Balazs Bordas

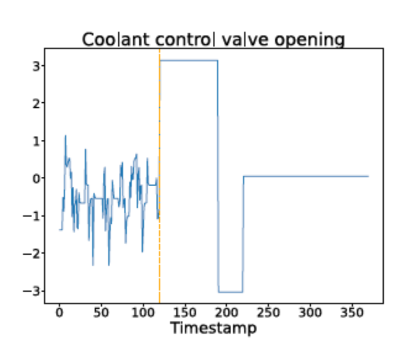
Modelling of a semi-batch production reactor

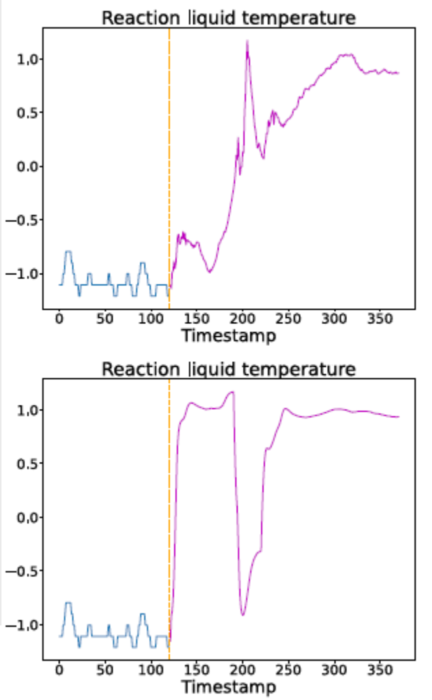
460 batches, 600 data points of all variables per batch

Careful tuning of the training algorithms for different dynamic NN models



- The models represent the data almost perfectly.
- But they are qualitatively wrong – the effect of the opening of the cooling valve is in the wrong direction.
- The models „learned“ correlations, not causal relationships.





Trust in models is key in online applications!

NAMUR

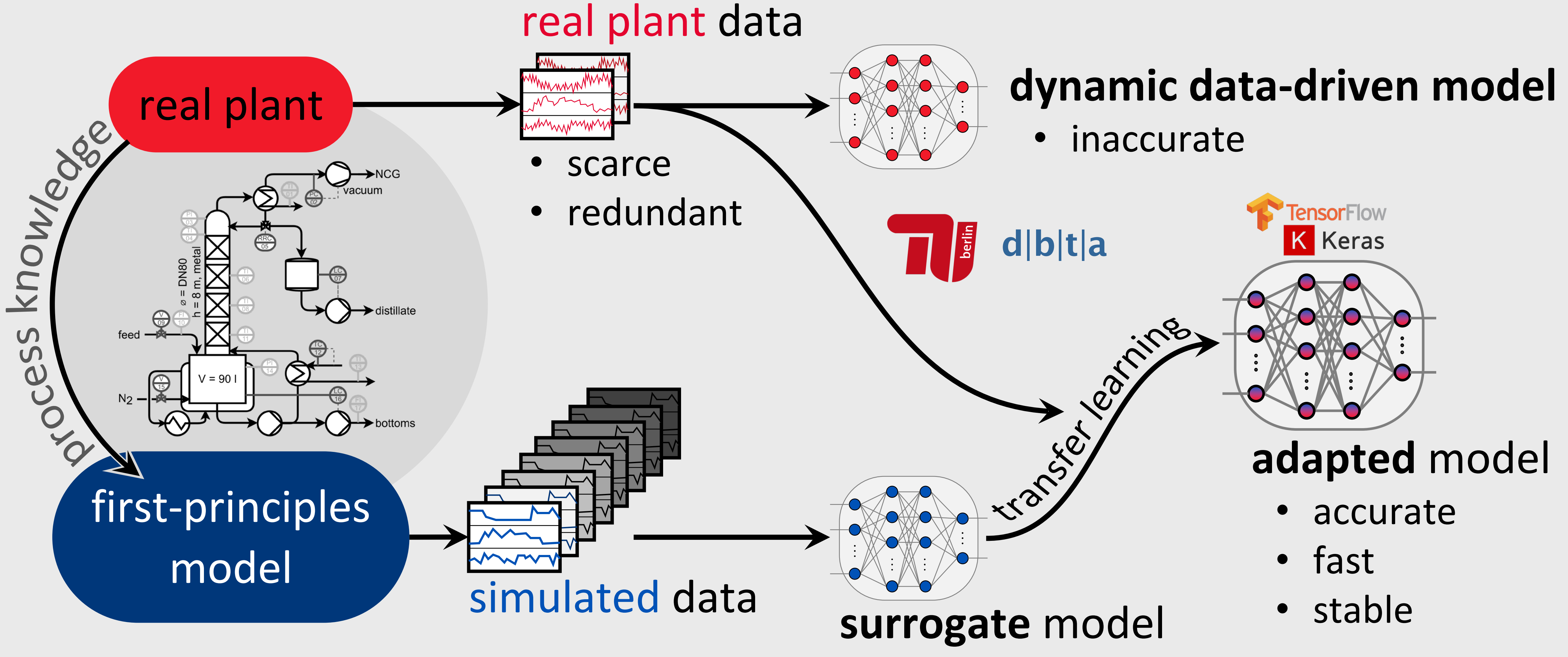
Data-based models can only predict what they have seen!

A dog or a bagel?

Solutions investigated in KEEN

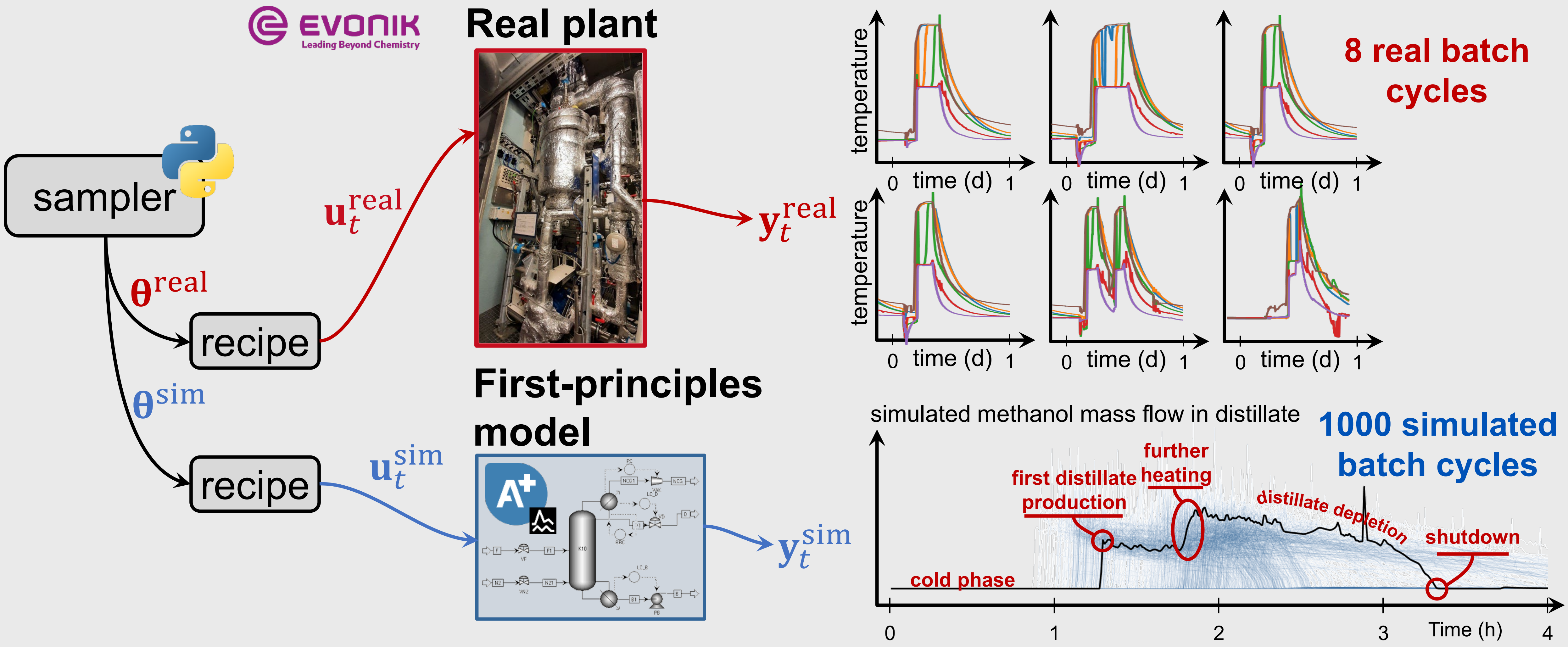
- **Transfer leaning if not enough plant data is available**
  - ➢ Pre-train models using simulations → sufficient data over a broad range
  - ➢ Adapt to real plant data to improve the prediction accuracy
- **„Hybrid“ or gray-box models with mechanistic and data-based elements**
  - ➢ Only corrections or embedded relationships must be learned
  - ➢ The qualitative behaviour is correct
- **Monitor whether AI models are used in their domain of validity**

Fine-tuning an inaccurate model by transfer learning



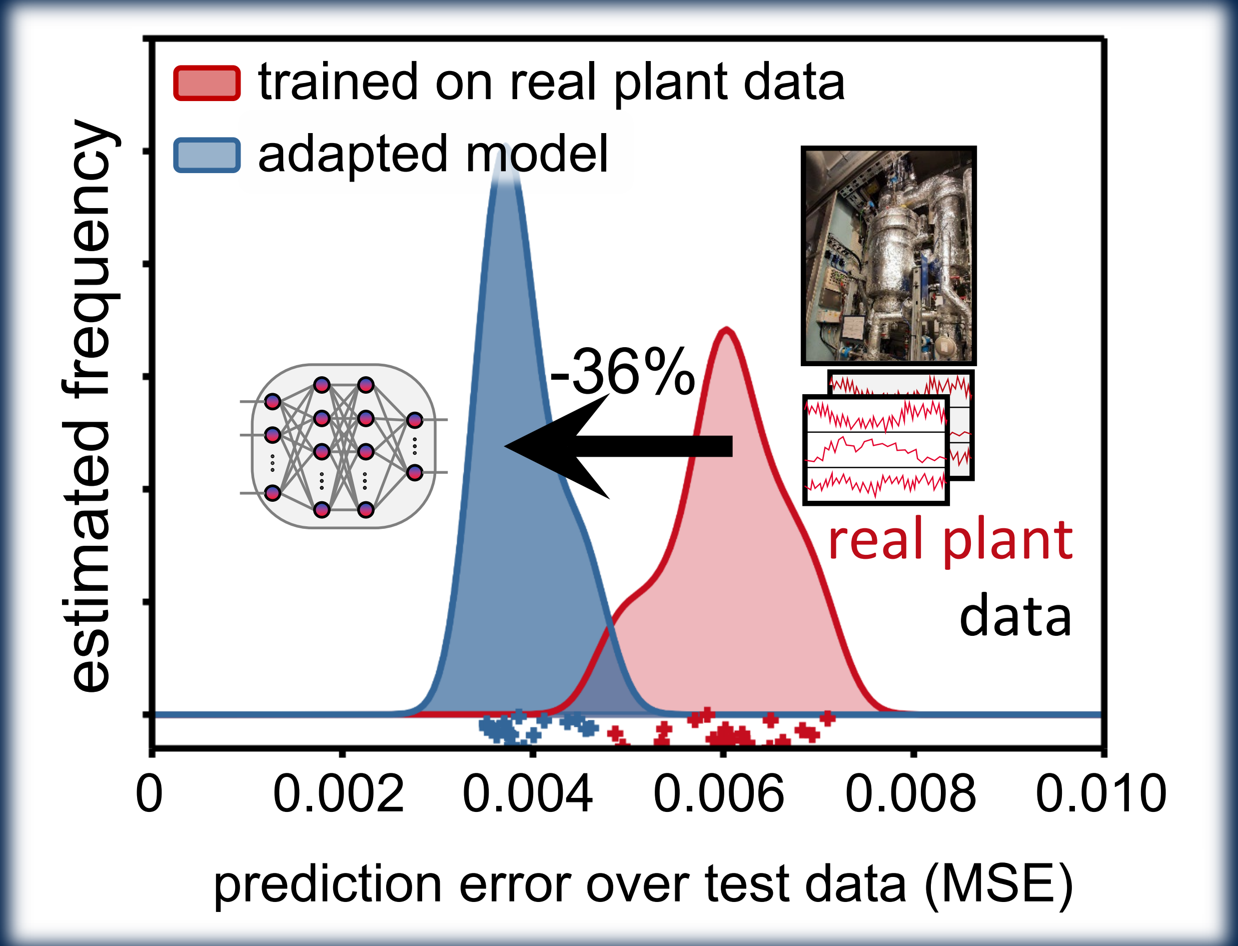
Brand Rihm, G. *et al.*, 2023. Adaptation of Dynamic Data-Driven Models for Real-Time Applications: From Simulated to Real Batch Distillation Trajectories by Transfer Learning. Chem Ing Tech.

Data acquisition – case study: batch distillation



Brand Rihm, G. *et al.*, 2023. Adaptation of Dynamic Data-Driven Models for Real-Time Applications: From Simulated to Real Batch Distillation Trajectories by Transfer Learning. Chem Ing Tech.

Transfer learning – case study: batch distillation



Transfer learning from simulation to real (*sim2real*) provides accurate, fast and trustable models.

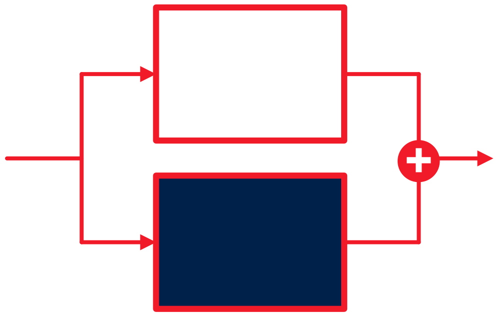
Brand Rihm, G. *et al.*, 2023. Adaptation of Dynamic Data-Driven Models for Real-Time Applications: From Simulated to Real Batch Distillation Trajectories by Transfer Learning. Chem Ing Tech.

Gray-box modeling

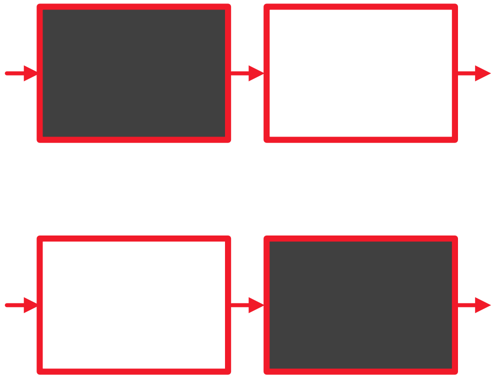
NAMUR

White-box model	Gray-box model	Black-box model
Equations from first principles and correlations	Combination of both	Data based models (Neural networks, Gaussian process, etc.)

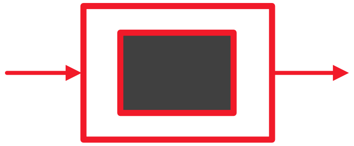
Parallel structure



Serial structures



Embedded structure



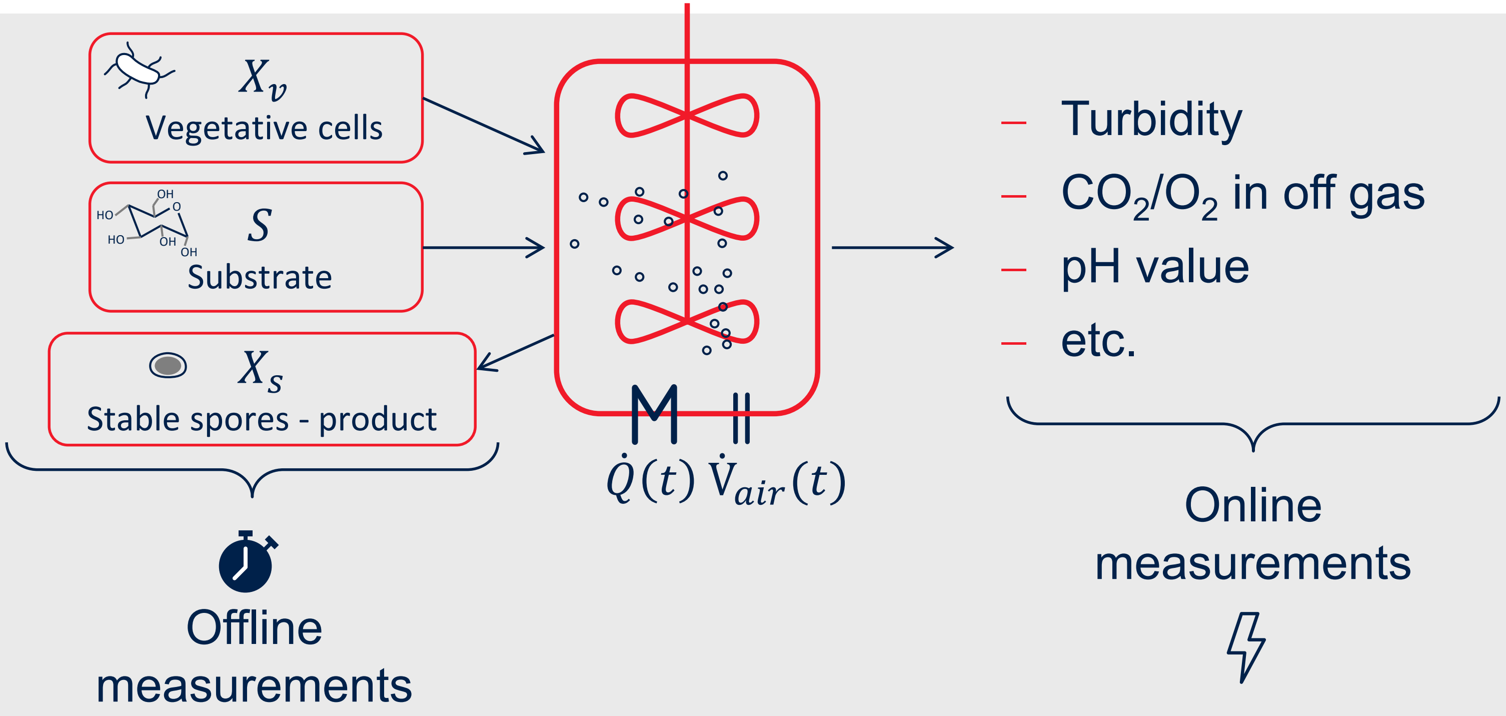
- Mechanistic models are qualitatively accurate over a large range of conditions
- Some phenomena are difficult model mechanistically, but data is available

Combine mechanistic (white box) models with black-box models to exploit existing data for simplified modeling and a higher accuracy!

Example: Fermentation process

Process: Fermentation of sporulating bacterium

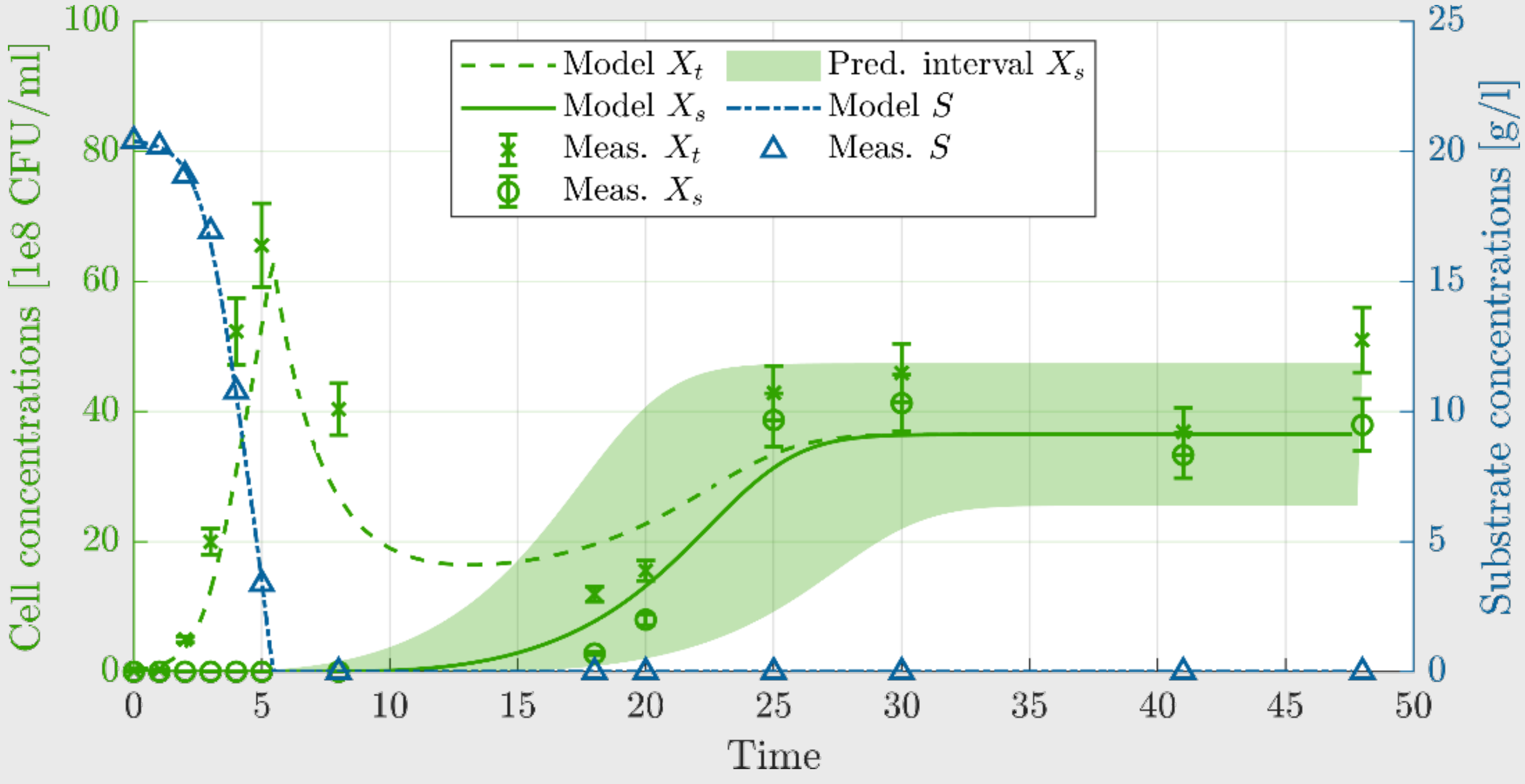
- Growth of biomass
- Conversion of vegetative cells with substrate to stable endospores
- Batch time: ~48h
- Lack of understanding of the sporulation process
- Limited batch reproducibility
- Relatively large data base: > 60 batches with different input patterns



Dynamic gray-box modelling with embedded ML models

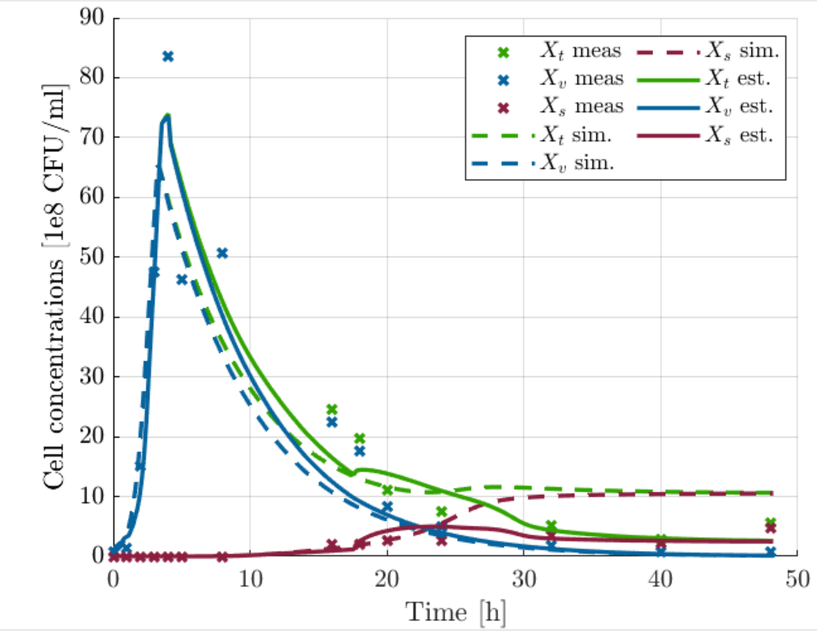
J. Winz, F. Fromme, S. Engell, Overcoming the modeling bottleneck: A methodology for dynamic gray-box modeling with optimized training data, Journal of Process Control. 130 (2023) 103089.

Application of gray-box modeling to the fermentation process



Prediction quality of the gray box model

Use for process monitoring using a state estimator

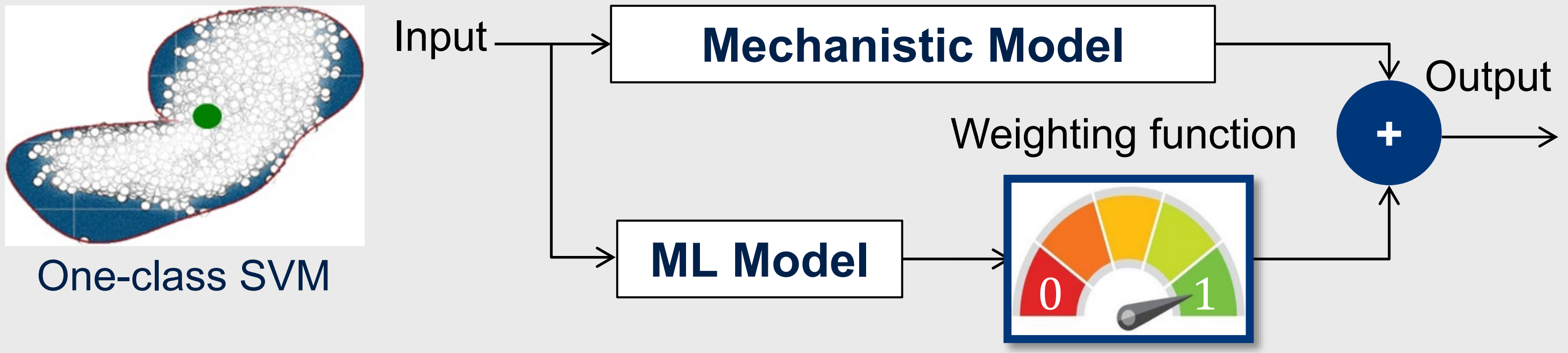


J. Winz, S. Assawajaruwan, S. Engell: Development of a Dynamic Gray-Box Model of a Fermentation Process for Spore Production, Chemie Ingenieur Technik. 95 (2023) 1154–1164.

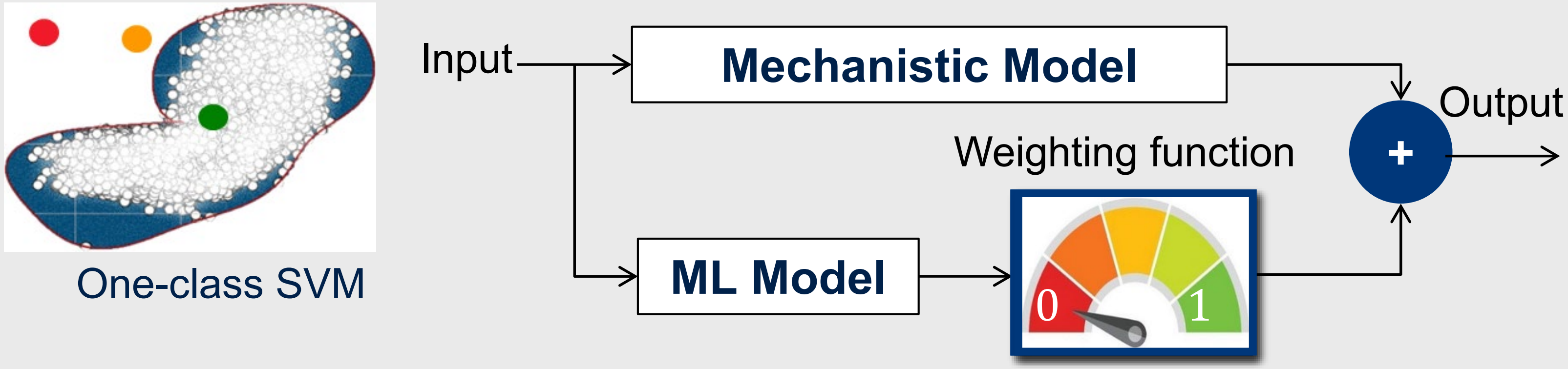
Monitoring of the reliability of ML models

Hybrid model with error correction by an AI model

- Use the ML model inside its **domain of validity**



- Fade out the contribution of the ML model **outside** its domain of validity



- **Prevents wrong model predictions when there was no data to train the model.**
- **Improves the prediction quality when enough data was available.**
- **The domain of validity can be adapted online.**
- **Succesfully tested in simulations of a distillation column together with Bayer.**

M. Elsheikh, et al. (2023), Control of an Industrial Distillation Column Using a Hybrid Model with Adaptation of the Range of Validity and an ANN-based Soft Sensor. CIT, 95: 1114-1124

KEEN Learnings related to process operations

NAMUR

- The application of AI was investigated beyond image processing and detection of degradation / faults
- AI / machine learning has the potential to
  - Improve the classification of data
  - Lead to better models faster
- AI methods need significant amounts of high quality data
- The closer to online application, the more critical becomes the aspect of trust in the monitoring and control algorithms
- Models that fit the data well may be qualitatively wrong
- Safety nets are indispensable

Hardening of AI-based solutions remains a challenge!

03

Embedding AI into Enterprise Operations

Embedding AI into Operations needs to consider two major dimensions with their own challenges!

PEOPLE

TECHNOLOGY

It’s all about setting expectations and delivering values

NAMUR

PEOPLE

- Upper management expectations have to meet with technological capabilities
  - And yes: AI needs good quality data!
- Language makes a difference
  - “AI takes over plant control.” vs
  - “You are supported by AI based decision systems.”
- If AI technology works and simplifies plant personnel’s life, they will love it!
  - Data infrastructure, automation systems, and additional measurements installed for AI applications provide additional value even w/o AI

Robustness and ease of deployment and maintenance

TECHNOLOGY

- Industry-ready and proven AI deployment and runtime systems
  - Still a lot of homemade python coding
- Mature service management processes for AI applications
  - Problem, change and incident management
  - Even software and applications need maintenance budget
- Collaboration of IT, OT and data science teams
  - Automatic data preparation, evergreening, and sanitation is a fundamental must-have for efficiency.

Conclusion and take-home messages

NAMUR

1. Is AI now controlling our plants?
   Not today, not fully, maybe even not tomorrow!
2. Is AI ready to control our plants?
   It depends on us!
3. Is AI able to control our plants?
   We have learnt during this presentation!
4. Do we want AI to control our plants?
   No! Instead, we want AI to help and support us in optimal plant operation!
5. Where are the benefits when AI controls our plants?
   They are there. But the problem at hand determines the applied technology!
6. Do we have to forget everything we learnt when AI is controlling our plants?
   A clear No!

Many thanks to the contributors to this presentation:

Martin. W. Hoffmann and Chen Song
ABB Research Germany

Gerardo Brand Rihm
TU Berlin, Dynamik und Betrieb technischer Anlagen

Jens Ehlhardt, Mohamed Elsheikh, and Joschka Winz
TU Dortmund, Systemdynamik und Prozessführung

and to the whole KEEN team for a great collaboration!


Juli 2023
95. Jahrgang
CITAH 95 (7)
961–1184 (2023)
ISSN 0009-286 X
www.CIT-journal.com

Chemie Ingenieur Technik

Verfahrenstechnik · Technische Chemie · Apparatewesen · Biotechnologie

7 | 2023

Themenheft:
KEEN – Artificial Intelligence Incubator Labs in the Process Industry

Gastherausgeber:
Norbert Kockmann
Thorsten Schindler
Leon Urbas

Herausgeber:
DECHEMA
GDCh
VDI-GVC

WILEY-VCH

D 2048
© Luis Augusto Weber Mercado

See CIT special edition on KEEN project results

NAMUR

Dadhe, Engell: Is AI now controlling our plants?

Thank you!