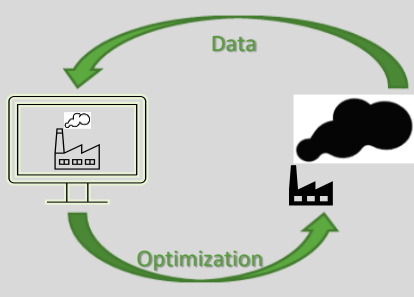


Interaction of Process Engineers and Software in Machine Learning

Armin Fricke, Burcu Aker, Jan C. Schöneberger
CGC Capital-Gain Consultants GmbH

Work with Flowsheets, smarter

Problem: Data Quality in Optimization



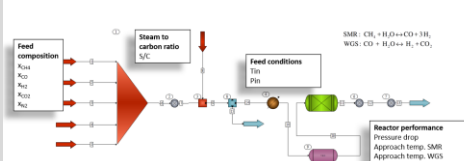
Case Study

- Latin Hypercube Sampling fills 11D input space
- Linear analysis and linear regression not sufficient to correlate the variables

Barriers to Optimization

- No rigorous simulation model
- Amount and accuracy of plant data
- Combining algorithm (metaheuristic)
- ML tool stack complex or not defined
- ...

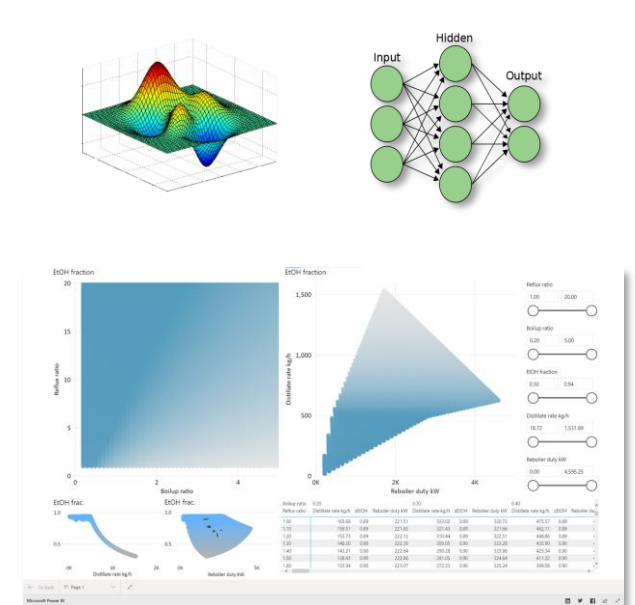
WHICH PARAMETERS AFFECT THE PERFORMANCE OF A PRE-REFORMER REACTOR MOST?



Artificial Neural Network (ANN) for interpolation, e.g., to see isolated impacts

- Are the results consistent with rigorous simulation?

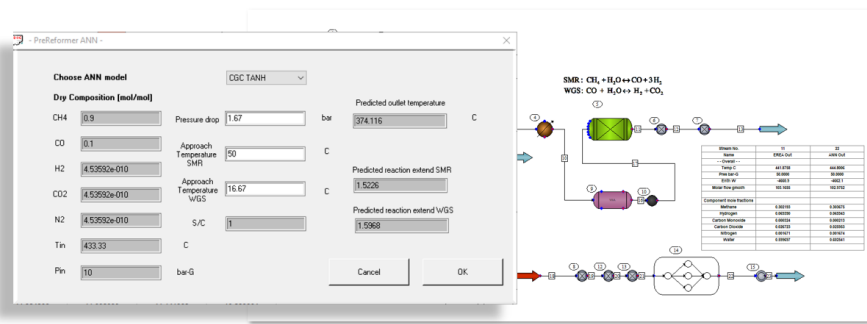
Challenge: Enhance expert knowledge with Machine Learning

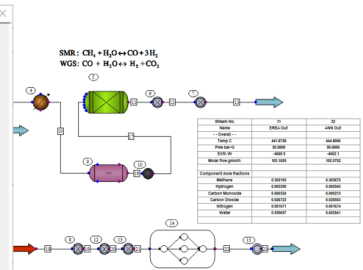


Solution: Tool-based engineering workflow

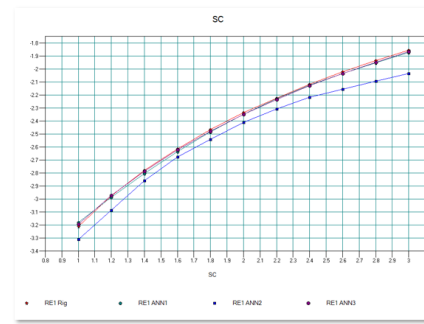
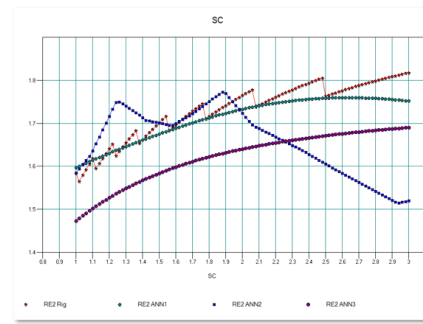
Case Study Results

WE USE SENSITIVITY STUDIES TO COMPARE THE ANN PREDICTIONS WITH RIGOROUS CHEMCAD CALCULATIONS





TRENDS SHOW WHEN THE ANN MEETS THE UNDERLYING (SIMULATED) PHYSICS PRECISELY ENOUGH

Process Engineering Requirements
Software Engineering Requirements

↔
Interactive workflow

- Understand parameter dependencies and process non-linearities
- Reduce dimensionality
- Update (retrain) Surrogate Model
- Create Surrogate Model for interpolation

↑
Interactive workflow
↓

- Visualize solution space and space-filling, and navigate parameters (sliders)
- Calculate test data set
- Calculate additional points (training data)
- Script in R/Py (use DoE and graphics libraries)

↓
Surrogate Model (SM)

