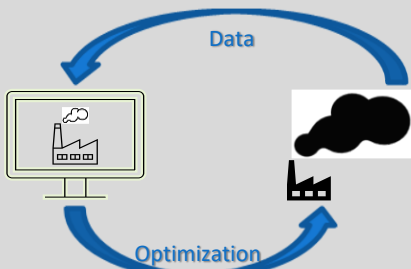


Interaction of Process Engineers and Software Tools in Machine Learning (ML)

Armin Fricke, Burcu Aker, Jan Schöneberger (Capital-Gain Consultants)

Problem: Data Quality in Optimization



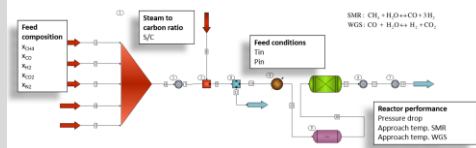
Case Study

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

Barriers to Optimization

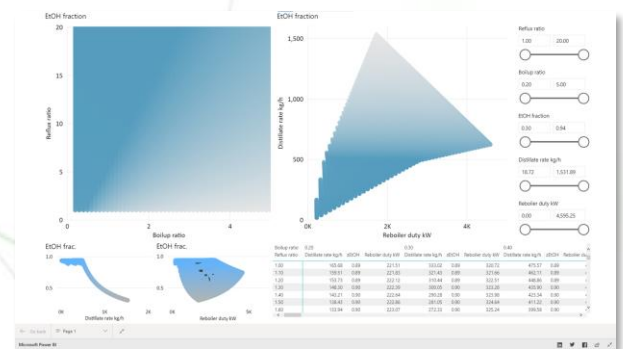
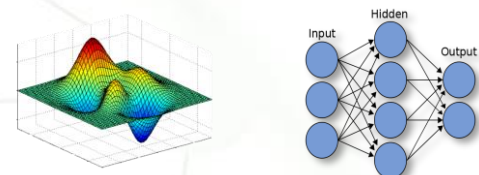
- No rigorous simulation model
- Amount and accuracy of plant data
- Combining algorithm (metaheuristic)
- ML tool stack complex or not defined
- ...

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



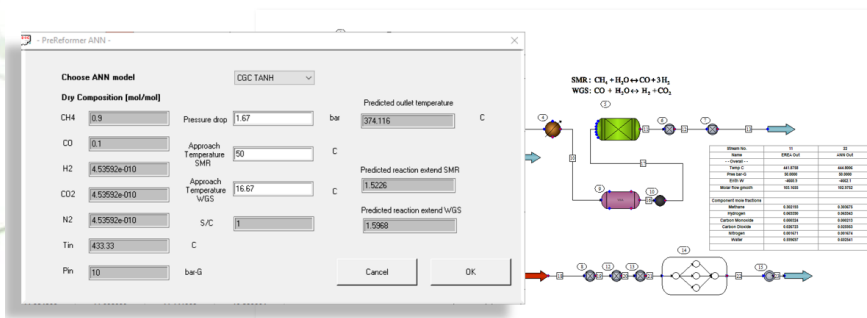
- Artificial Neural Network (ANN) for interpolation, e.g., to see isolated impacts
- Are the results consistent with rigorous simulation?

Challenge: Enhance expert knowledge with Machine Learning

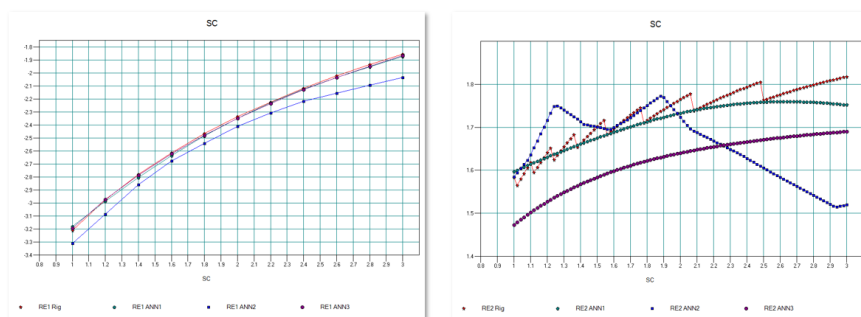


Case Study Results

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
- 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)

Solution: Tool-based engineering workflow

www.keen-platform.de

Contact

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