

# Efficient and purpose based model development for process plants

## Abstract:

Modelling is a necessary step for understanding and optimizing a process. The purpose of the model strongly influences which model type and which model design to use and as such determines the time and resources required for model development. To give an example, for planning purposes a simple regression model might suffice, whereas for simulation, when detailed information about the composition of an individual stream is required, a rigorous model involving thermodynamics or a data driven model will be necessary. In industrial projects, model development is a bottleneck and for many projects not attempted, especially, as the model development effort increases with modeling depth.

The aim of this thesis is to understand and describe the effort required for modeling a plant at different modelling depths, using data-driven models (surrogate models). For a small section of the plant, the effort needed to develop a rigorous model has to be compared with that to develop a regression model. The work will be done using a real example in cooperation with INEOS in Köln. The results of this work will be used in the development of a methodology for finding the optimal model type and level of detail.

This thesis includes the following steps:

- Development of a structural model for the plant under study (see Fig. 1)
- Identification of the relevant measurements and their values in each level
- Building surrogate models on different structural layers (similar to the method in Cozad, A., Sahinidis, N. V., & Miller, D. C. (2014))
- Development of a criterion that reflects both the improvement of the model fit and the increase in model complexity as conflicting objectives
- Using the criterion to determine a stopping level and a choice towards a change in model type, if required a rigorous physical model.

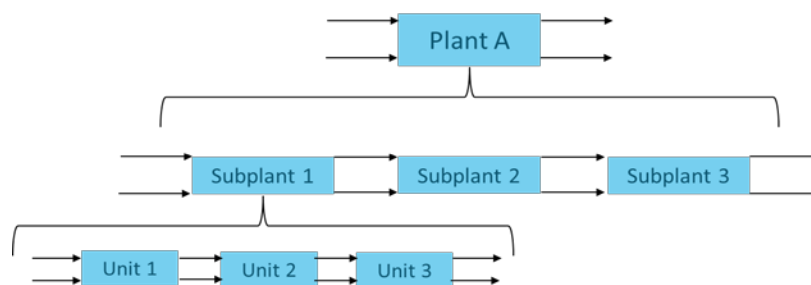


Fig. 1. Structural model and its different layers.

**Literature:**

- Cozad, Alison, Nikolaos V. Sahinidis, and David C. Miller. "Learning surrogate models for simulation-based optimization." *AIChE Journal* 60.6 (2014): 2211-2227.
- Lohmann, B., and W. Marquardt. "On the systematization of the process of model development." *Computers & chemical engineering* 20 (1996): S213-S218.
- Marquardt, Wolfgang. "Trends in computer-aided process modeling." *Computers & Chemical Engineering* 20.6-7 (1996): 591-609.

**Prerequisites:**

- Programming skills in MATLAB
- Knowledge in mathematical modeling
- Interest in data analysis of chemical plants

**Begin and duration:**

Immediately, 6 month full time

**Remarks:**

The thesis will be done on-site at INEOS Köln.

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