Design of experiments, design of simulations: Using model knowledge to improve the information content of data

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Hybrid modelling – that is the integration of data- and knowledge-driven approaches - can enhance both the value of data and models, especially in situations where the acquisition of data is costly and physical or chemical expert knowledge is available. In this contribution, special attention is paid on two use cases of data acquisition: Building a machine-learning based surrogate model for a heavy-load simulation and setting up an experimental plan to discriminate between models and identify parameters within one model as reliably as possible.

The first use case is demonstrated for a stationary simulator of chemical production processes. With such a simulator, flowsheet simulations were performed with three goals: i) the discrimination of feasible regions, which is accomplished by identifying the range of free design variables in which meaningful solutions exist; ii) the training of surrogate models within the feasible region, where different process-related objectives, such as product purities, operating costs or environmental impacts, reach the most favorable values; and iii) the assurance of small uncertainty in the prediction of the short-cut model [1]

The second use case addresses model-based design of experiments, where both the optimal number and the experimental designs are identified. Here, we focus on mini-plant experiments, where the underlying model comprises a large amount of variables with nonlinear dependencies. We present novel techniques that tackle this challenge, and illustrate the procedure for a Cumene process.

[1] Raoul Heese, Michał Walczak, Tobias Seidel, Norbert Asprion, Michael Bortz, *Comp. Chem. Eng.*, **2019**, *124*, 326-342.

[2] Charlie Vanaret, Philipp Seufert, Jan Schwientek, Gleb Karpov, Gleb Ryzhakov, Ivan Oseledets, Norbert Asprion, Michael Bortz, *EasyChair*, **2020**, 2518 (submitted to Comp. Chem. Eng.)