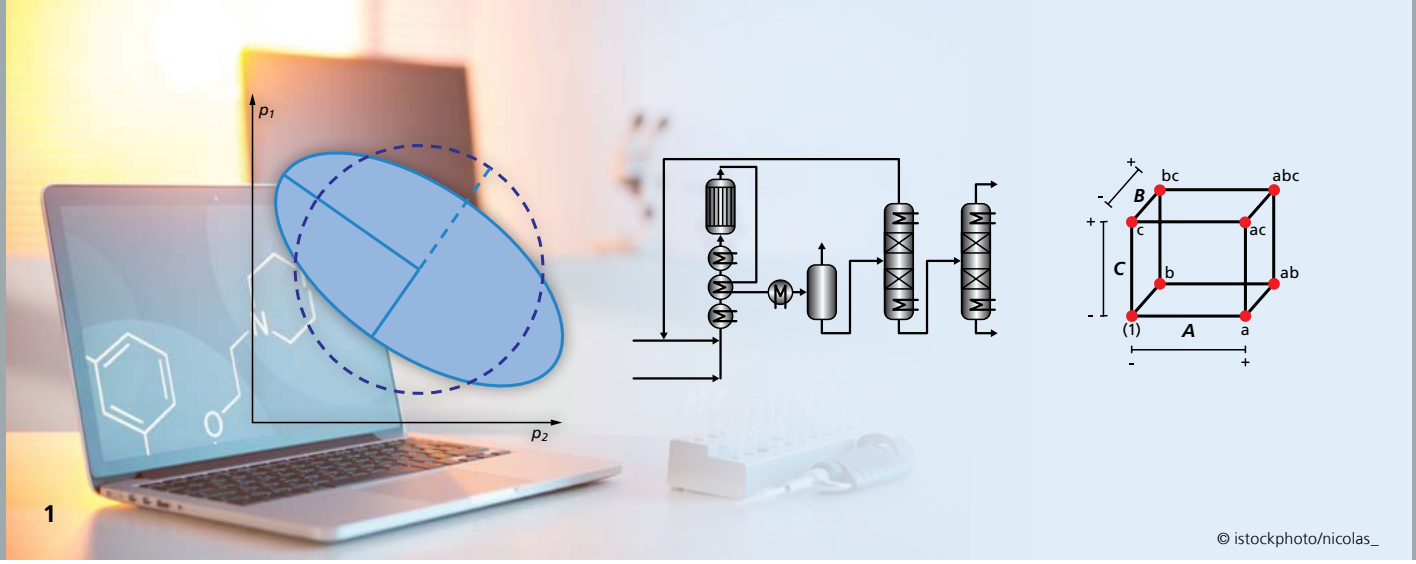

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MODEL-BASED EXPERIMENTAL DESIGN IN PROCESS ENGINEERING

In chemical process engineering, data are collected in experiments in order to calibrate physically motivated models. These experiments are always time- and cost-intensive. Therefore, their planning is about deriving as reliable models as possible from as few experiments as possible. In a cooperative project with BASF, we develop and implement methods that support this.

1 *Left: Scheme of a covariance ellipsoid to illustrate the confidence region of adjusted model paramaters*

Center: Scheme of a mini-plant with one tubular reactor and two distillation columns

Right: Statistical design of experiments for a linear model with three inputs

The reliability of model calibrations is influenced in two ways: On the one hand, the error bars of the estimated parameters, but also the prediction errors of the model are directly proportional to the measurement accuracy in the experiments. In other words, the more accurate the sensors, the more reliable the model prediction.

On the other hand, in order to calibrate successfully, it is crucial to consider correlations in the sensitivity of the models – especially with regard to the model parameters at the measurement points. This is illustrated in the following example.

Catalyst: Aging versus Temperature

Chemical reactions are generally faster at higher temperatures than at lower ones - this is why, for example, foods are cooled to prolong their shelf life. In chemical reactors, catalysts are often used to accelerate reactions. These catalysts age, so their effect decreases over time. Therefore, the reaction temperature is increased with increasing catalyst age in order to guarantee a constant quality of the reaction product. In this way, catalyst age and reaction temperature are closely related. It is not possible to calculate the separate effects of temperature and catalyst age on the end product. The experimental design proposes to run the reactor once at low temperatures and high catalyst age, and once at high temperatures and low catalyst age. With these two additional operating conditions, the effects can be separated and independently quantified.

The aim of the cooperation project with BASF is to transfer the concepts described above to complex models of pilot plants (Fig. 1). These are then calibrated to model parameters on the basis of their sensitivities, uncertainties are estimated (Fig. 2) and the corresponding experiments are planned. To this end, we solve large nonlinear optimization problems and make their results usable on interactive user interfaces.