Analytical Sciences

Incremental Model Identification using the Concept of Extents

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Kinetic models contribute greatly to cost reduction during the process development phase and are also helpful for process monitoring and control purposes. Kinetic models describe the underlying reactions, mass transport and operating conditions of the reactor. In the typical one-step *simultaneous method* of identification, one postulates a dynamic model encompassing the effects of all phenomena at stake, and model parameters are estimated by comparing measured data with model predictions. Simultaneous identification can be computationally costly and exhibit convergence issues in case of poor initial guesses. Furthermore, this method is characterized by high correlation between parameters, which can lead to structural mismatch.

In contrast, the *extent-based incremental method* of identification is a two-step approach, in which measured data are first transformed into extents, each one representing the effect of a particular phenomenon [1-3]. Then, for each phenomenon individually, a model is postulated and the corresponding parameters estimated by comparing the simulated and measured extents. Since each extent, and thus each effect, is handled individually, the correlation between model parameters is considerably reduced.

This presentation will give an overview of the extent-based incremental identification and will describe the procedure to analyze homogeneous and gas-liquid systems. The performance of simultaneous and incremental methods of identification will be compared via simulated examples.

[1] Bhatt et al, Ind. & Eng. Chem. Res. 50, 12960-12974, **2011**
[2] Srinivasan et al, Chem. Eng. J. 208, 785-793, **2012**
[3] Billeter et al, Anal. Chim. Acta 767, 21-34, **2013**