Local vs global estimability analysis of population balance models for crystallization processes

[Abstract]

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Local vs Global Estimability Analysis of mono-dimensional Population Balance Models for Crystallization Processes

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ABSTRACT

The population balance framework has been accepted as the most fundamental approach for modelling population entities whose properties are distributed [1]. While the functional form of the population balance model (PBM) is based on first principles, identification of several empirical kinetic parameters is often required, in order to develop a robust tool for modelling, control and optimization. However, due to a number of factors (e.g. limited experiments, the correlation between the model parameters or between their effects with respect to the outputs and the structure of the mathematical model) the PBM model may contain more parameters than can be accurately identified from the available experimental data [2]. This particular challenge can be solved by identifying the subset of most influential parameters and estimating their values accurately from the measurements, while the parameters with the least estimability potential are fixed at certain nominal values [3]. This approach has been applied to a one-dimensional PBM model that describes the dynamic evolution of the crystal size distribution as one of the critical quality attributes (CQA) for a batch cooling crystallization process. Hybrid non-convex optimization model-based approaches have been utilized for the identification of the crystallization kinetics by minimizing the maximum likelihood criterion. The results were validated by using experimental online and offline process analytical tools (PAT) for the determination of the evolution of the crystal size distribution (CSD) and the solution concentration. Then the optimum subset of parameters was determined based on two different approaches: (1) a sequential orthogonalization of the sensitivity matrix and (2) a variance-based global sensitivity analysis approach. The results of the investigation showed that the most influential and least correlated parameters could be identified more reliably, providing enhanced prediction capabilities of the overall dynamics of the studied crystallization process, which agreed well with independent experimental runs.

References