Model Reliability of Multi−dimensional Population Balance Models for Crystallization

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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. While the functional form of the population balance model (PBM) is based on first principles, identification of several kinetic parameters is required, in order for a robust tool for modelling, control and optimization to be developed. However, due to potential lack of measurements, correlations among the effects that parameters may have on the outputs and the mathematical model structure, the PBM model may contain more parameters than could be accurately identified from the available experimental data. This particular challenge could be solved by selecting the subset with the most influential parameters that could be estimated accurately from the measurements while the unselected ones would be fixed in certain nominal values. This approach has been applied to the multi-dimensional, multi-impurity adsorption PBM model that accounts the combined effects of different crystal growth modifiers (CGM) on the crystal size and shape distribution of needle like crystals for a batch crystallization process. Hybrid nonconvex optimization model based approaches are utilized for the identification of the crystallization kinetics by minimizing the maximum likelihood criterion.