Parameter identification, reliability and model discrimination of population balance models for crystallization [Poster]

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Parameter Identification, Reliability & Model Discrimination of Population Balance Models for Crystallization

**Overview**

- Population Balance Modelling (PBM) framework has been accepted as the most fundamental approach for dynamic modelling of numerous particulate processes.
- The functional form of the model (PBM) is well – established but kinetic parameters need to be estimated from experimental data [1].
- The PBM model may contain more parameters that can be accurately identified from the available experimental data (e.g. limited experimental data, correlation between parameters or between their effects with respect to the outputs, structure of the mathematical model) [2].
- This 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 nominal values [2].
- This approach has been applied to a multi-dimensional, multi-impurity adsorption (MIAM) PBM model that accounts for the combined effects of crystal growth modifiers (CGM) on the crystal size and shape distribution (CSSD) of needle-like crystals [1].

**Conclusions & Future Work**

- Both local and global estimability & identifiability concepts has been applied to the MIAM PBM model that accounts for the combined effects of different crystal growth modifiers on the crystal size and shape distribution (CSSD) of needle-like crystals.
- Although noisy data were used, the most influential and the least correlated parameters while the others are parametrically fixed at initial guesses.
- The 4 last parameters could be neglected or fixed at certain nominal values without compromising the accuracy of the model.

**References**


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