Population Balance Modelling of Continuous Crystallization Processes

D.Fysikopoulos[1,*], **Q.Su**[1], **A. Trybala**[1], **B.Benyahia**[1], **Z.K. Nagy**[1, 2], **C.D. Rielly**[1]

[1] *Department of Chemical Engineering, Loughborough University,* [2]*School of Chemical Engineering, Purdue University*

*D.Fysikopoulos@lboro.ac.uk

Abstract

The population balance framework has been accepted as the most fundamental approach for modelling population entities whose properties are distributed. The present work is associated with the development of a study mainly focused on the theoretical prediction of the dynamic evolution of the Crystal Size and Shape Distribution (CSSD) in continuous crystallization systems. A continuous 2-stage MSMPR cascade system is modelled, when cooling is applied as a driving force for crystallization. A multi-dimensional model, which constitutes the tool for modelling crystal shape distribution, is developed for a single-stage MSMPR crystallizer in order to study the dynamic evolution of the CSSD of high aspect ratio crystals. The trajectory of the mean sizes of the different facets and the mean aspect ratio is illustrated by taking into account the nucleation and growth of two characteristic crystal facets and random binary breakage phenomena. The results indicate that the applied model-based approaches can describe accurately the crystal size and shape distribution.

Optimization model based-approaches are also utilized for the identification of the crystallization kinetics. The parameters are obtained by applying the maximum-likelihood method. Due to the fact that 1-D models are used for determination of the kinetics, uncertainties in the CSD may relate to the non-spherical and non-uniform crystal shape for the laser diffraction measurement. The estimated parameters sufficiently illustrate the experimental outputs.