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Publication date:
2011

Document Version
Publisher's PDF, also known as Version of record

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Citation (APA):
Meisler, K. T., Abdul Samad, N. A. F., Gernaey, K., von Solms, N., & Gani, R. (2011). *Generic Model and Data Based Framework for Analysis and Development of Crystallization Processes*. Abstract from 2011 AIChE Annual Meeting, Minneapolis, MN, United States. <http://aiche.confex.com/aiche/2011/webprogram/Paper226484.html>

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Generic Model and Data Based Framework for Analysis and Development of Crystallization Processes

Monday, October 17, 2011: 12:30 PM

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Crystallization is an efficient process for separation of compounds, which are solid in their pure form at the given separation conditions. Crystallization is often applied in the production of salts and active pharmaceutical ingredients (API), where the crystallization step is an essential part of the manufacturing process for many pharmaceutical products. In recent years the monitoring and analysis of crystallization operations has received increased attention due to the growing need to control more sophisticated production lines as well as the increased possibilities of monitoring such processes with the advance of measurement techniques. This presentation addresses the need for a generic model and data based framework for the generation of population balance based models for crystallization operations in one to three dimensions with the analysis of data-driven crystallization kinetic models. The crystallization models are valid for batch as well as continuous operations.

A generic multi-dimensional model-based system for use in crystallization modeling (for cooling as well as solvent and/or anti-solvent based operation) has been set up and its use to study a wide range of chemical (crystallization) systems as well as different crystallizer operation phases (scenarios) has been demonstrated previously (1). This system has now been combined and extended with systematic methods for collection of data and model-based analysis of known crystallization kinetic models and their use in simulating crystallization operations. This combination provides a framework for monitoring, analysis and optimization of crystallization operations. Measurements can be taken and used for offline analysis and parameter regression. With an established kinetic model it is possible to translate the predicted model results into a form, which is directly comparable (and visualized) to the data for evaluation of the model. Furthermore, if there is model – data mismatch, the measured data can be used for online parameter estimation.

The models used for the crystallization usually include several phenomena such as growth, nucleation, agglomeration and breakage in order to give a satisfactory description of the crystallization operation. The generic framework handles population balances for these phenomena and has been expanded into covering multiple dimensions accounting for temperature and concentration gradients in the crystallization operation.

The expanded model framework combined with the systematic approach to establish the kinetic models for use in general crystallization operations in combination with monitoring tools will be presented using case studies involving API crystallization.

Works Cited

1. *A generic multi-dimensional model-based system for batch cooling*. Noor Asma Fazli Abdul Samad, Ravendra Singh, Gürkan Sin, Krist V. Gernaey, Rafiqul Gani. 2011, Computers and Chemical Engineering, Vol. 35, pp. 828–843.

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