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Systematic Modeling and Crystal Size Distribution Control for Batch Cooling Crystallization Processes

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Crystallization processes form an important class of separation methods that are frequently used in the chemical, the pharmaceutical and the food industry. The specifications of the crystal product are usually given in terms of crystal size, shape and purity. In order to predict the desired crystal morphology by means of model-based approaches, appropriate models covering the effects of the various operational parameters on the behavior of the crystals are necessary. Usually the main difficulty in batch crystallization is to accomplish a uniform CSD. There are many ways to enhance the control of CSD such as to use supersaturation control which drives the process within the metastable zone or by determining the amount and size of seeds that should be added into a crystallizer through seed recipe design approach. Therefore, there is a need for a generic crystallization model that can provide a better understanding of crystallization operations and from which a large number of specific models for different crystallization processes can be generated. Furthermore, to control and monitor the crystallization operations and to ensure that the desired CSD is achieved, an appropriate Process Analytical Technology (PAT) system needs to be available. That is, the design of process control and product monitoring system that will obtain the desired end-product properties is also needed.

The generic multi-dimensional model-based framework of batch cooling crystallization processes has been developed covering a wide range of crystallization models and operational scenarios. The use of the generic model will be illustrated, in this paper, through the ICAS-PAT software for design of process monitoring and control system. ICAS-PAT consists of a model library and a knowledge base that allows the user to design/validate PAT systems through a systematic computer aided framework. The generic crystallizer model has been implemented in the ICAS-PAT model library. The application of the model-based framework will be highlighted through a batch cooling crystallization processes where the objective is to obtain a desired CSD. In order to predict the desired CSD at the end of the batch, an analytical CSD estimator based on the assumption of the constant supersaturation will be employed. Through this estimator, supersaturation set-point can be identified indicating that by maintaining the supersaturation at its set-point will result into achieving the specified CSD consistently. Thus using the ICAS-PAT, the crystallization operations can be monitored and controlled according to the required set-point during the batch run. For this purpose, the generation of the needed crystallization model will illustrated together with its use in the ICAS-PAT software.

Keywords: multidimensional, crystal size distribution, crystal shape

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