Crystallization Kinetics Identification within a Generic Modeling Framework

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Crystallization serves as an efficient separation process for compounds, which are solid in their pure form at the given separation conditions. Crystallization is an essential step in the production of many pharmaceutical products as the active pharmaceutical ingredients (APIs) are often separated efficiently through this operation. The monitoring and analysis of crystallization operations has recently received increased attention due to the growing need to control the final crystal size distribution (CSD) in a relatively narrow range as well as to measure and monitor the final product characteristics.

The objective of this work is to provide the ability to establish the kinetics of a crystallization operation systematically and efficiently. Initially an operational scenario is defined for which the specific balance equations are set up. The constitutive parameters are available, it can be used for simulation of the corresponding crystallization operations. If an established model can be handled through the modeling framework are continuously being expanded to accept more data types with different kinetics. A full representation of a crystallizer requires models for all these kinetic phenomena and saturation rate of dissolution. Growth of the crystals occurs in multiple dimensions and the growth rates of the facets determine the shape of the crystals. The size distribution is obtained because of different competing phenomena such as nucleation and growth, each with different kinetics. A full representation of a crystallizer requires models for all these kinetic phenomena and saturation descriptions (constitutive equations) coupled with descriptions of the equipment and an operational policy. Such a description is possible within a generic framework where the models can be combined, reused and identified. This framework has been established for crystallization operations in combination with monitoring tools will be presented using case studies involving different scenarios for crystallization operations.

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 different scenarios for crystallization operations.

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