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Mechanistic modelling of industrial crystallization processes –Challenges and opportunities at the initial solution stage

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Crystallization processes are important and widely used unit operations in the pharmaceutical industry and there is a need to understand and improve the performance of these processes in terms of e.g. yield and batch time as well as the performance of downstream processes affected by crystal size and shape e.g. yields and processing times of subsequent centrifugation, filtration and drying steps. The non-linear, dynamic nature of the process along with the high number of operational degrees of freedom makes experimental improvement and optimization of such processes a complex task. However, the process can be described mathematically using mechanistic models coupling the mass, energy, and population balances of the system allowing for advanced process understanding, targeted experiments, optimization, etc. The development of such models becomes increasingly challenging with the complexity of the phenomena involved (e.g. non-linearity, large number of phenomena, coupling, etc.) [1]. In this work, a mechanistic model for an industrial crystallization has been developed using a systematic framework with selection of numerical method and model complexity based on phenomena identified from available data and observations. The model has at the initial solution stage been applied to e.g. explain observations in production, design space exploration, and performing what-if analyses for risk evaluation. Next, the goal is to estimate the model parameters to apply the model for process optimization. However, with limited data availability and a high number of phenomena/parameters, an appropriate experimental strategy is needed to generate the required data to estimate the parameters of the individual but simultaneously occurring phenomena.

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