243g Design of Industrial-Scale Crystallizers to Include the Effects of Macromixing and Micromixing on the Crystal Size Distribution

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The systematic design of particle nucleation and growth processes that includes the effects of hydrodynamics has been of academic and industrial interest since the 1960s (Hulburt and Katz, 1964). These effects can be especially important in industrial-scale crystallizers, which are prevalent in the agricultural, pharmaceutical, and specialty chemical industries (Hill and Ng, 2002; Wibowo et al., 2001). A major bottleneck to the systematic design of such crystallizers has been the lack of computationally-feasible methods for simulating the evolution of the crystal size distribution (CSD) in industrial-scale crystallizers. Simulating the high-Reynolds number turbulent fluid dynamics by Direct Numerical Simulation (Chakrabarti et al., 1995; Moody and Collins, 2003) while simultaneously solving population balance equations for the crystals is not computationally feasible, even with large-scale parallel computers. Hence researchers studying this problem have used Reynolds-averaged Navier-Stokes (RANS) models (e.g. k-ε models) for simulating the turbulent fluid dynamics, or compartmental models for otherwise representing the macromixing within the crystallizer. For the reactive and antisolvent crystallization processes in which non-ideal mixing can be especially important, micromixing models must be incorporated into the overall system of equations, to account for the mixing of multiple streams on a molecular scale.

An approach for computing average and aggregate properties of the crystalline phase involves coupling a computational fluid dynamics (CFD) code with moment equations for describing the effects of nucleation and growth on the crystals, and subgrid-scale models for describing micromixing effects (Baldyga and Orciuch, 1997; Marchisio et al., 2001). One drawback of this approach is that realistic models of the localized crystal growth kinetics have a nonlinear dependence on crystal size, in which case a closed set of moment equations do not exist. A second drawback of the approach of using moments to represent the crystal size distribution is the inability of a low number of moments to resolve complexities in the shape of crystal size distribution, such as having multiple modes. An alternative is to integrate the Lagrangian multi-zonal approach (Baldyga et al., 1995; Schwarzer and Peukert, 2004; Kresta et al., 2005), which models mixing at a coarse spatial resolution, with solution of a spatially-varying population balance equation (SPBE), to simulate the crystal size distribution. A drawback of this, and other compartmental approaches, is the inability to resolve mixing effects at the smaller length scales of importance throughout the entire crystallizer domain.

This poster considers a crystallizer model that integrates computational fluid dynamics (CFD) with the spatially-varying population balance equation (Hulburt and Katz, 1964) and micromixing models (Fox, 2003) to model the effects on hydrodynamics on industrial-scale crystallizers. A high spatial resolution of the turbulent flow field is needed to determine the impact of hydrodynamics on the local nucleation and growth rates of the crystals, and the population balance equation has to be solved to resolve distributions that are non-unimodal, and to simulate the nonlinear dependence of local growth and dissolution rates on crystal size, which cannot be achieved with the method of moments.

We adapt and integrate state-of-the-art numerical algorithms for hyperbolic equations with computational methods for turbulent fluid dynamics to simulate antisolvent crystallization processes. Here, the full crystal size distribution is solved numerically using the high-resolution, finite-volume, semidiscrete central scheme proposed by Kurganov and Tadmor (2000) for nonlinear hyperbolic equations. The numerical advantages of using a high-resolution method have been discussed in some detail by Gunawan et al. (2004). The micromixing is modeled by a multi-environment probability

density function (PDF) model (Fox, 2003), which provides a statistical description of the fluctuating scalars at the subgrid scale. An advantage of these methods is their relative ease of implementation with commercially available CFD codes, in which the additional models can be directly simulated within the CFD solver. The authors believe that this is the first time a high-resolution method for solving population balance equations is coupled with a CFD code to simulate micro- and macro-mixing effects in industrial-scale crystallizers.

The integrated algorithm is used to simulate an antisolvent crystallization process with different crystallizer configurations to quantitatively predict the effects of hydrodynamics on crystal nucleation, growth, and dissolution and on the size distribution of the product crystals. The effects of operating variables and geometry of crystallizer internals on the hydrodynamics, crystallization rates, and the resulting crystal size distribution are investigated, which result in specific recommendations on the design of the crystallizer to obtain crystals of desired characteristics. This case study illustrates how the integrated CFD-PDF-SPBE can be used in a systematic engineering approach to the design and scale-up of crystallizers.

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