

# A framework for the simulation of mass crystallization considering the effect of fluid dynamics

Viatcheslav Kulikov, Heiko Briesen\*, Wolfgang Marquardt

*Lehrstuhl für Prozesstechnik, RWTH Aachen University, Turmstr. 46, D-52064 Aachen, Germany*

Received 11 May 2005; received in revised form 28 July 2005; accepted 20 September 2005

Available online 31 March 2006

## Abstract

The behavior of large-scale crystallizers is strongly affected by the fluid dynamic characteristics of the apparatus like e.g. local supersaturation and velocity profiles. The simulation of this effect is a complex multi-scale and multi-phenomena problem. This contribution presents an approach to solve the coupled problem of crystallization and fluid dynamics by means of software integration. Existing specialized software tools (Fluent and Parsival) are employed for the solution of specific subproblems, namely the solution of population balance models and fluid dynamics. To reflect the phenomena on their characteristic scales different grids are used during the simulation of the respective subproblems. The population balance and crystallization kinetics are formulated in the coarse scale compartments while the fluid dynamics are solved on the fine CFD grid. The problem decomposition needed for the formulation of the subproblems and the proper selection of the compartments are discussed. The approach is validated with a simple model of a crystallization in a tubular reactor which can be solved using reduced methods without introducing a systematic error.

© 2006 Elsevier B.V. All rights reserved.

*Keywords:* Crystallization; Population balance; Software integration; Problem decomposition; Compartment model

## 1. Introduction

Over the past decades, the rapid development of computer technology and the need for improved process modeling resulted in many specialized software tools. Particularly for fluid phase processes, many established models, formulated as algebraic equation (AE) systems or differential-algebraic equation (DAE) systems, and corresponding solution algorithms have been implemented in commercial software tools. Simulation tools like Aspen Plus, Hysys<sup>1</sup> or gPROMS<sup>2</sup> have become standard tools supporting the solution of many fluid phase chemical engineering problems in process design, scale-up or optimization. Also problems in fluid dynamics can be solved using specialized commercial computational fluid dynamics (CFD) tools (e.g. FLUENT<sup>3</sup>).

While model-based techniques have become a standard for many fluid phase processes, their use for particulate processes

has not yet reached the same level of spreading. This can be attributed to the higher physical complexity of the processes and the associated higher mathematical complexity of the corresponding models. Though most of the concepts presented in this work may carry over to other particulate applications, we will focus on crystallization processes. In case of crystallization processes the physical behavior is determined by the interaction of multiple phenomena. Various kinetic phenomena (growth, nucleation, aggregation, breakage) all directly affect the particulate phase (total mass, size and shape of the crystals). To reflect this complex interaction, the mathematical model structure also becomes complex. Usually, a population balance approach [31] is employed, which results in a partial (integro) differential algebraic equation (PIDAE) system. In the literature a number of methods have been presented to discretize and solve this type of PIDAE models [13,17,18,30,42], and commercial tools (e.g. Parsival<sup>4</sup>, SediFloc project on sedimentation and flocculation<sup>5</sup>) have become available. The main problem, how-

\* Corresponding author. Tel.: +49 241 8094861.

E-mail address: [briesen@ipt.rwth-aachen.de](mailto:briesen@ipt.rwth-aachen.de) (H. Briesen).

<sup>1</sup> Aspen Technology Inc., <http://www.aspentech.com> (accessed 18.04.2005).

<sup>2</sup> Process Systems Enterprise Ltd., <http://www.psenterprise.com> (accessed 18.04.2005).

<sup>3</sup> FLUENT Inc., <http://www.fluent.com> (accessed 18.04.2005).

<sup>4</sup> Computing in Technology GmbH (CiT), <http://www.cit-wulkow.de> (accessed 18.04.2005).

<sup>5</sup> University of Ghent, <http://biomath.ugent.be/~sedifloc/> (accessed 21.04.2005).

ever, is the correct choice of the constitutive equations for the kinetic phenomena. As it will be discussed in more detail in Section 2, many of the kinetic phenomena directly depend on the fluid dynamic behavior in the crystallizer. Additionally, the typically made assumption of ideal mixing in the crystallizers is highly questionable.

Besides the difficult experimental analysis of the interaction of fluid dynamics and crystallization, the rigorous consideration of fluid dynamic effects is hindered by software restrictions. Generally, current simulation tools often use process knowledge and tailored numerics to improve efficiency. On the other hand this gain in efficiency is paid by restrictions with respect to the problem formulation. The population balance equation and crystallization kinetics can efficiently be solved in population balance solvers like Parsival, but fluid dynamics are not taken into account due to the assumption of an ideally mixed crystallizer. On the other hand CFD tools like FLUENT are capable of solving complicated fluid dynamics problems involving reactions and turbulence models, but meet difficulties to rigorously represent particulate rate processes. Though there has been a considerable progress in extending CFD tools in this direction [23,24,38], restrictions regarding the reconstruction of the particle size distributions and the systematic errors introduced by moment discretization still have to be taken into account (see Section 4).

Instead of developing completely new software tools and algorithms for the coupled problem of fluid dynamics and crystallization, it is more desirable to exploit the modeling capabilities of existing simulation tools to the maximum possible extent. By integration of various tools, the variety of problems is extended over the standard range that can be addressed by single, stand-alone tools. To realize such integration, a high-level software framework for the software-technological integration of different specialized simulation tools is proposed [33]. In our previous work [19], this framework has been used to solve flow-sheet simulation problems, where the models of individual units have been simulated in appropriately selected, specialized tools. In this contribution, we discuss the extension of this approach to the simulation of crystallization processes considering the effect of fluid dynamics.

## 2. Effect of fluid dynamics

The effect of fluid dynamics on crystallization is a topic, which has been addressed in many studies. However, there is still a shortcoming of reliable quantitative models for the physics of these processes. Many effects are only described qualitatively based on the results of the experiments.

Generally, the flow field in a crystallizer is anisotropic. This leads to local differences in the crystallization behavior. The effects of local fluid dynamics on crystallization can be classified into direct and indirect influences. For direct influences the crystallization rate processes directly depend on the flow characteristics (e.g. shear rate). Thus, the anisotropic flow field directly leads to locally distributed crystallization behavior. The main influence on crystallization is given by the actual driving force, the supersaturation. Supersaturation itself, determined by

the local distribution of temperature and concentration, is often affected by fluid dynamics. Thus, the local profile of the supersaturation, induced by fluid dynamics, strongly but indirectly affects the crystallization behavior.

Direct influences appear for collision-dominated phenomena. Particle–particle, particle–wall and particle–impeller collisions can frequently occur in industrial crystallizers and can lead to different phenomena. In case of particle–particle collisions the most important phenomenon is aggregation. The kinetics of aggregation are primarily determined by the collision frequency and the collision efficiency [14]. The shear rate affects both the frequency (increases with increasing shear rate) and efficiency (decreases with increasing shear rate) of particle–particle collisions. This results in a complex dependence of aggregation kinetics on the shear rate as shown by the analysis of calcium oxalate aggregation [28]. In case of highly turbulent flows, shear- and drag-induced disaggregation of particles can become an important factor [34,36]. Disaggregation of particles also often occurs during particle–impeller or particle–wall collisions. This affects in particular particle attrition and breakage. In the literature [12], the attrition kinetics are defined as a function of impact energy and target efficiency of particle–impeller collisions, which in turn depend on the relative velocity of particle and streamlines along the impeller blade. Although to a less extent, the same is true for particle–wall collisions which contribute to the overall disaggregation kinetics observed in a crystallizer [21].

Fluid dynamics also directly affect diffusion-limited growth. In turbulent flows the thickness of the boundary layer decreases, which enhances the mass transport to the crystal surface [27].

Note that all phenomena discussed above generally have to be considered as spatially distributed due to significant local variations of velocities, turbulence and fixed impeller and boundary regions.

Indirect influences of fluid dynamics on crystallization stem from local variations of the supersaturation and the particle size distribution. There are several ways how supersaturation and particle size distribution can be affected by fluid dynamics. In reactive crystallization (precipitation), this influence is especially important on the micro-scale (Kolmogorov turbulence scale) where the effect of micro-mixing plays an essential role in the generation of the supersaturation profiles [2]. In evaporation or cooling crystallizers micro-mixing is not the primary concern. However, non-ideal mixing characteristics on the meso- and macro-scale already lead to a local distribution of solids in the crystallizer as well as to local temperature and concentration variation [35].

Since the rates of crystallization kinetics (primary nucleation, growth, aggregation) almost always depend on the supersaturation and/or the particle size distribution, their local variation obviously lead to an indirect influence of the fluid dynamics.

In return, locally varying crystallization rates produce local variations of concentration and particle size distribution. This introduces a back-coupling of crystallization on fluid dynamics. This influence increases with increasing solids fraction in the slurry. Thus, fluid dynamics and crystallization in real pro-

Download English Version:

<https://daneshyari.com/en/article/688568>

Download Persian Version:

<https://daneshyari.com/article/688568>

[Daneshyari.com](https://daneshyari.com)