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An efficient numerical technique for solving multi-dimensional batch crystallization models with size independent growth rates

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ABSTRACT

This article introduces an efficient numerical technique for solving multi-dimensional batch models. The method requires initial crystal size distribution (CSD) and initial solute mass. The initial CSD is used to calculate the initial moments as an initial data for the reduced moments system. The solution of the moments system coupled with an algebraic equation for the mass gives moments and mass at the discrete points of the computational time domain. These values are then used to get the discrete values of growth and nucleation rates. The discrete values of growth and nucleation rates along with the initial CSD are sufficient to get the final CSD. In the derivation of current technique the Laplace transformation of the population balance equation (PBE) plays an important role. The method is efficient, accurate and easy to implement. For validation, the results of the proposed scheme are compared with those from the high resolution finite volume scheme.

1. Introduction

The problem of obtaining a reliable reconstruction of a crystal size distribution (CSD) from a finite number of its low-order moments remained the subject of interest since the last century, see Akhiezer (1975) as well as Shohat and Tamarkin (1943). In spite of its long history there are several issues which have still no unique answer. There are several scientific disciplines where such problems arises namely, chemical and process engineering, electronic engineering, nuclear physics, image analysis, biotechnology, and so on.

On the other hand, the standard method of moments (MOM) and related approaches like the quadrature method of moments (QMOM) and its direct alternative (DQMOM) have been applied in chemical engineering, see Barrett and Jheeta (1996), Madras and McCoy (2004), Marchisio, Vigil, and Fox (2003), and Vollmer (2005). The main reason of using these methods was their low computational cost. In particular, when external features like turbulent flow properties play an important role for the process under consideration, efficient numerical methods are needed for describing the population interacting with this flow. In the method of moments only a finite number of moments associated with the real distribution are finally determined by the numerical procedure. The other possibility is to find the values of different moments indirectly from experimental measurements, since the particle sizing devices provide general knowledge about e.g., the mean particle size or complete particle size distribution (PSD). Once the PSD is known the corresponding moments can be readily computed, see Marchisio, Barresi, and Garbero (2002).

After having these moments, the problem which remains open is to reconstruct the corresponding PSD in a best possible manner. The PSD generally constitutes the key information for the judgment of the quality of a process. Therefore, the reconstruction procedure is highly important and necessary.

Being an ill-posed inverse problem, theoretically and practically it is difficult to find an accurate and relatively fast method which can be generally applied in all fields. In the last decades, several authors have proposed different techniques, see Inglese (1994), John, Angelov, Öncül, and Thevenin (2007), Tagliani (1999, 2001), and references therein. However, no satisfactory unified numerical method is available in the literature for the reconstruction of a function from its finite moments. Most of the available methods were introduced for particular and simpler cases requiring specific assumptions.

Recently, John et al. (2007) have compared different possible methods namely, prescribed functions, discrete method and spline-based reconstruction allowing such a reconstruction of the PSD. They have compared these methods in terms of efficiency and accuracy. Their article also contains a nice review of the previous work in this direction.

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A close idea to the proposed technique in this article was introduced by Hounslow and Reynolds (2006) for the one-dimensional batch crystallization model. However, in their article instead of the Laplace transformation the method of characteristics was used as a basic tool for the scheme derivation.

In our recent article, see Qamar and Warnecke (2008), we have presented the analytical and numerical investigations of the one-dimensional batch crystallization model. In that article we have proved the local existence and uniqueness of the solution of batch crystallization model. Moreover, the issues of positivity (monotonicity), consistency, stability and convergence of the proposed high resolution scheme of Koren (1993, chap. 5) were analyzed and proved. In our second article, see Qamar, Warnecke, Elsner, and Seidel-Morgenstern (2008), we have presented an efficient numerical technique for the solution of one-dimensional batch crystallization model. The proposed numerical method can be used for dual purposes. Firstly, it can be used as an efficient and accurate numerical method for solving the given batch crystallization with size independent growth rate. Secondly, it can be used to reconstruct the final CSD from the initial one. The numerical experiments showed that the proposed numerical method is about thirteen times faster than the high resolution finite volume schemes. Furthermore, it was found that the proposed method preserves the mass balances up to the machine accuracy which was not the case for the high resolution finite volume schemes, see Qamar et al. (2008). Finally, the proposed numerical method can also be used for the control of batch crystallization processes, see for example the articles by Shi, Mhaskar, El-Farra, and Christofides (2005) and Shi, El-Farra, Li, Mhaskar, and Christofides (2006) and references therein. Similar to Shi et al. (2005, 2006), we are also using reduced moments model in our scheme. However, we get the CSD directly from an algebraic equation coupled with a nonlinear function of time variable. While, Shi et al. (2005, 2006) have used a second order finite difference scheme to solve the given PBE. Therefore, the proposed numerical scheme will be more efficient and accurate compared to their scheme.

In general, the particle size distribution (PSD) may depend on more than one internal coordinates. Therefore, a one-dimensional population balance equation (PBE) is not adequate to simulate such processes. There are several crystallization processes in the pharmaceuticals, photographic, and other industries where the product crystals are multi-dimensional. In such processes the crystals growth is associated with the change of multiple internal coordinates, see Braatz and Hasebe (2001) and Ma, Tafti, and Braatz (2002). Such internal coordinates can be volume, mass, length, width, composition, or the number of crystals in an agglomerate. This gives motivation for further investigation in this direction to understand multi-dimensional crystal growth and the development of optimal control strategies for such processes. A huge experimental literature is available on multi-dimensional crystal growth from the given supersaturatd solution, see Brown and Myerson (1989), Gabas and Lauerie (1991), Myerson and Saska (1984), Saska and Myerson (1987), Togkalidou and Braatz (1999), and Togkalidou, Johnson, Braatz, Davidson, and Andrews (2001). However, less work has been reported on the numerical simulation of multi-dimensional models. For modeling and simulation of two-dimensional batch crystallization processes see the articles by Gunawan, Fusman, and Braatz (2004, 2008), Ma et al. (2002), Qamar et al. (2007), and references therein.

This paper extends our work in Qamar et al. (2008) for solving two-dimensional batch crystallization models. In the derivation of the proposed method the Laplace transformation has been used as a basic tool. The Laplace transformation transforms the given population balance equation (PBE) to a linear ordinary differential equation. The transformed PBE can be solved analytically if the growth and nucleation rates are known. Afterwards, the inverse Laplace transformation has been used to get a relation for the actual number density which is coupled with an implicit function of time variable. The method works as follows. From the initial CSD one can calculate the initial moments. These initial moments can be used as an initial data for the reduced moments system coupled with an algebraic equation for the mass concentration. Note that, the initial mass concentration is also given. The solution of this coupled system gives us moments and mass concentration at the discrete points of the computational time domain. The resulting discrete data can be used to obtain the discrete values of growth and nucleation rates in the same computational time domain. The growth and nucleation rates along with the initial CSD are sufficient to reconstruct the final CSD. The current method is very efficient, accurate and easy to implement compared to the other methods solving the given population balance model (PBM) directly. For validation, the numerical results of the current technique are compared with the high resolution finite volume scheme of Koren (1993, chap. 5). This and other types of high resolution finite volume schemes have already been used for solving batch crystallization models, see Ma et al. (2002) and Qamar, Elsner, Angelov, Warnecke, and Seidel-Morgenstern (2006) and Qamar et al. (2007). Similar to the one-dimensional reconstruction technique, the two-dimensional method was found to be efficient and accurate compared to the existing finite difference and finite volume methods.

This article is organized as follows. In Section 2, we present a model for two-dimensional batch crystallization process. In Section 2.1, we present the reduced moments system of the given PBE coupled with a mass concentration balance equation reflecting the particular shape of crystals. The Laplace transformation is used to transform the given PBE to a linear ordinary differential equation which can be solved analytically by assuming that growth and nucleation rates are known. Afterwards, an inverse Laplace transformation is used to get back the actual number density. Finally, we present our numerical algorithm for the reconstruction of the two-dimensional particle size distribution. In Section 3, we present a numerical test problem for the two-dimensional batch crystallization process. Lastly, Section 4 gives conclusions and remarks.

2. Two-dimensional batch crystallization model

In the following we present a models for the two-dimensional batch process. The model uses the PBE as a balance law for the solid phase which is coupled with an integro-ordinary differential equation for the solute mass concentration in the liquid phase. The two-dimensional PBM for batch crystallization process with size independent growth rates is given as

$$\frac{\partial n(t,x,y)}{\partial t} = -G_1(t,c)\frac{\partial n(t,x,y)}{\partial x} - G_2(t,c)\frac{\partial n(t,x,y)}{\partial y} + B_0(t,c)\delta(x-x_0,y-y_0), \tag{1}$$

where $n{:=}n(t,x,y) \geq 0$ is the number density function, $t \geq 0$ denotes the time, $x, y \in \mathbb{R}_+$ are internal coordinates, $c{:=}c(t)$ represents the solute mass concentration in the liquid phase, $G_1(t,c)$ and $G_2(t,c)$ are the size independent growth rates along each characteristic length direction, and $B_0(t,c)$ is the nucleation rate which occurs at (x_0, y_0). Here, δ represents the Dirac delta distribution.

The moments of the PSD in two-dimensional case are defined as

$$\mu_{i,j}(t) = \int_0^\infty \int_0^\infty x^i y^j n(t,x,y)\,dx\,dy, \quad i,j = 0,1,2,\ldots. \tag{2}$$

The solute mass concentration reduces during the crystallization process. Hence, the above population balance equation for the solid phase must be coupled with a concentration balance equation for the liquid phase.