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A Laplace transformation based technique for reconstructing crystal size distributions regarding size independent growth

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Abstract

This article introduces a technique for reconstructing crystal size distributions (CSDs) described by well-established batch crystallization models. The method requires the knowledge of the initial CSD which can also be used to calculate the initial moments and initial liquid mass. The solution of the reduced four-moment system of ordinary differential equations (ODEs) coupled with an algebraic equation for the mass gives us moments and mass at the discrete points of the given computational time domain. This information can be used to get the discrete values of size independent growth and nucleation rates. The discrete values of growth and nucleation rates along with the initial distribution are sufficient to reconstruct the final CSD. In the derivation of current technique the Laplace transformation of the population balance equation (PBE) plays an important role. The proposed technique has dual purposes. Firstly, it can be used as a numerical technique to solve the given population balance model (PBM) for batch crystallization. Secondly, it can be used to reconstruct the final CSD from the initial one and also vice versa. The method is very efficient, accurate and easy to implement. Several numerical test problems of batch crystallization processes are considered here. For validation, the results of the proposed technique are compared with those from the high resolution finite volume scheme which solves the given PBM directly.

Keywords: Population balance models; Crystallization processes; Laplace transformation; Model reduction; Mathematical modeling; Reconstruction technique

1. Introduction

The problem of obtaining a reliable reconstruction of a crystal size distribution (CSD) from a finite number of its low-order moments has been investigated since the last century (Akhiezer, 1975; 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 arise 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 (Barrett and Jheeta, 1996; Madras and McCoy, 2004; Marchisio et al., 2003; Vollmer, 2005), mainly due to their low computational costs. 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 is 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 crystal size, a chord length distribution or even directly the complete CSD. Once the CSD is known the corresponding moments can be readily computed, see Marchisio et al. (2002).

After having these moments, the problem which remains open is to reconstruct the corresponding CSD in a best possible manner. The CSD generally constitutes the key information for the judgement of the quality of a process.

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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 et al., 2007; Taglian, 1999, 2001, and references therein). However, no satisfactory unified numerical method is available in literature for the reconstruction of a function from a finite number of its 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 CSD. 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.

An approach similar to the technique proposed in this article was introduced by Hounslow and Reynolds (2006) for the one-dimensional (1D) batch crystalization 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 this paper, we propose an efficient technique for the reconstruction of CSD of 1D batch crystallization models. In this derivation the Laplace transformation (Doetsch, 1974; Jaeger and Newstead, 1949; Wylie, 1995) has been used as a basic tool. The Laplace transformation transforms the given population balance equation (PBE) to a linear ordinary differential equation (ODE). 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 required four initial moments. These initial moments along with the given initial mass can be used as initial data for the four-moment system of ODEs coupled with an algebraic equation for the mass. The solution of this coupled system gives us moments and mass at the discrete points of the computational time domain. This discrete data can be used to get the discrete values of growth and nucleation rates in the same 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 PBM directly. For validation, the numerical results of the current technique are compared with the high resolution finite volume scheme of Koren (1993). This and other types of high resolution finite volume schemes have already been used for solving batch crystallization models (see Ma et al., 2002; Qamar et al., 2006, 2007).

The current work is inspired by our recent work (Qamar and Warnecke, 2007) on the analytical and numerical investigations of the 1D batch crystallization model. In that article we have proved the local existence and uniqueness of the solution of a batch crystallization model for the size independent growth rate. Moreover, the issues of positivity (monotonicity), consistency, stability and convergence of the proposed high resolution scheme of Koren (1993) were analyzed and proved.

This article is organized as follows. In Section 2, we give the proposed 1D batch crystallization model. In Section 3, we present the reduced four-moment system of the given PBE coupled with a mass balance equation. The Laplace transformation is used to transform the given PBE to a linear ODE which is then solved analytically, 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 1D particle size distribution. In Section 4, we present some numerical test problems for the 1D batch crystallization processes. Lastly, Section 5 gives conclusions and remarks.

2. One-dimensional batch crystallization model

We consider a relatively simple population balance model (PBM) for a batch crystallization process. Attrition is not explicitly included in this batch crystallization model. Instead, the production of small fragments by attrition is incorporated implicitly in the nucleation rate. Moreover, breakage and agglomeration of crystals are also neglected. Consequently, the resulting batch models are not expected to be able to predict the effects of, e.g., scale-up or changes in the operating conditions. Nevertheless, they are capable of describing the behavior of a given process in the relevant operating range fairly well.

In the 1D batch crystallization model, the size of crystals is defined by a characteristic length x. The CSD is described by the number density function $n(t,x)\geqslant 0$, which represents the number of crystals per crystal length. Balancing the number of crystals in an infinitesimal interval of crystal length, a partial differential equation is obtained which, together with appropriate initial and boundary conditions, describes the temporal evolution of the CSD (Miller and Rawlings, 1994)

$$\frac{\partial n(t,x)}{\partial t} = -G(t,m)\frac{\partial n(t,x)}{\partial x} + B_0(t,m)\,\delta(x-x_0), \quad (t,x)\in\mathbb{R}^2_+, \tag{2.1}$$

$$n(t_0,x) = n_0(x), \quad x\in\mathbb{R}_+, \tag{2.2}$$

where $t_0\geqslant 0$ and $\mathbb{R}_+ := (0,\infty)$. Here, $m := m(t) > 0$ represents the solute mass in the liquid phase, $n_0(x)\in\mathbb{R}_{\geqslant 0}$ denotes the CSD of seed crystals added at the beginning of the batch, $G(t,m)\geqslant 0$ is assumed to be size independent growth rate, $B_0(t,m)\geqslant 0$ is the nucleation rate at minimum crystal size $x_0 > 0$ and δ is the Dirac delta distribution.

The jth moment $\mu_j(t)$ of the number density $n(t,x)$ is defined as

$$\mu_j(t) := \int_0^\infty x^j n(t,x)\,\mathrm{d}x. \tag{2.3}$$