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A modified cell average technique for the solution of population balance equation

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ABSTRACT

A new generalized discretization technique, based on the cell average technique (CAT), for solving the population balance equation and predicting the zeroth and first moments has been developed. The proposed algorithm can be easily cast into computer programs, is conceptually straightforward and demonstrated to be computationally economic. Additionally, a new type of mesh, for breakage, aggregation and combined processes is introduced. A new solver, compatible with aforementioned processes, for improving the accuracy of technique has been also proposed. A number of solvable processes were simulated by this technique and compared with the analytical solution and the CAT method. The results were very close to the analytical solution and much more accurate than CAT results.

1. Introduction

Studies of the population balance equation (PBE) and its applications have been growing in the past decade. The PBE has a lot of application in polymer synthesis, powder technology, aerosol technology, and even in the fields like biotechnology and aerospace. The integro-differential nature of this equation alongside its hyperbolic behavior makes it analytically intractable for most cases. Most of the previous studies have neglected the dependency on the external variables (space) and have focused just on one internal variable. Even in this simplified form, the analytical solutions for the PBE are very scarce in the literature, so various numerical methods have been proposed to solve this equation. Solution methods such as the successive approximation (Liou et al., 1997; Ramkrishna, 2000), the finite element methods (Ahmeda et al., 2003; John et al., 2009; Mahoney & Ramkrishna, 2012), the finite volume methods (Kumar & Kumar, 2013; Vikas et al., 2013; Qamar et al., 2009), the Monte Carlo simulation (Lin et al., 2002; Xu et al., 2014; Zhao et al., 2007) and the method of moments (Attarakih et al., 2009; Bruns & Ezekoye, 2012; Marchisio & Fox, 2005; Santos et al., 2013; Yuan et al., 2012) are presented in the literature. The present work is based on the fixed-pivot technique (FPT) and cell average technique (CAT) that are usually classified as sectional methods. This type of methods discretize the whole particle size distribution (PSD) into a finite number of cells with a representative point for each cell. Subsequently by using the original equation, a set of ordinary differential equations (ODE) will be generated, which it should be solved with a proper ODE solver. Fixed-pivot technique

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(Kumar & Ramkrishna, 1996; Ramkrishna, 2000) besides estimating PSD tries to predict the two first moments of PSD too:

$$\mu_j(t) = \int_0^\infty x^j f(x,t)\,dx, \quad j = 0, 1 \tag{1}$$

This technique was successful in estimating these moments but failed to predict the PSD of the system and showed an over-predicting behavior towards the number density function (Attarakih et al., 2009). Instead, the cell average technique (Kumar et al., 2008) concentrated on the PSD more than the FPT and conforms with the nature of the processes, so it shows a better predicting behavior. However as it will be shown later, this method cannot predict the first two moments properly. In this paper, first of all, the CAT is rewritten in a new form which is handier and simpler for analysis and programming. Then, the predicted results of the moments of the PSD alongside the number density function are demonstrated. In addition, the modified CAT (mCAT) and CAT are compared to show the pros and cons of each one.

2. Mathematical description

The population balance equation (PBE) for a one-dimensional batch type process is expressed by Ramkrishna (2000):

$$\frac{\partial f(x,t)}{\partial t} + \frac{\partial (G(x,t) f(x,t))}{\partial x} = \mathbf{B_{agg}} + \mathbf{B_{break}} - \mathbf{D_{agg}} - \mathbf{D_{break}}. \tag{2a}$$

In which the birth and death terms are as follows:

$$\mathbf{B_{agg}} = \frac{1}{2}\int_0^x \beta(u, x-u, t) f(u,t) f(x-u,t)\,du, \tag{2b}$$

$$\mathbf{D_{agg}} = f(x,t)\int_0^\infty \beta(u,x,t) f(u,t)\,du, \tag{2c}$$

$$\mathbf{B_{break}} = 2\int_0^\infty S(u,t) f(u,t) P(x|u,t)\,du, \tag{2d}$$

$$\mathbf{D_{break}} = S(x,t) f(x,t), \tag{2e}$$

where f is the density function, G is the growth term, β donates the coagulation kernel, and functions S and P are the selection function and the breakage probability density function respectively.

By concentrating all particles of a cell into one point, the representative point, one can convert (2a) into a set of ordinary differential equation (ODE). The form of each ODE is like this

$$\frac{dN_i}{dt} = B_{i,in} - B_{i,out} + B_i - D_i, \quad i = 1, 2, \ldots \tag{3}$$

The variables B_i and D_i are the birth and the death rates respectively. The $B_{i,in}$ is the rate of forming new particles that leave other cells and enter the ith cell, the $B_{i,out}$ is also the birth rate of particles, which are not anymore in this cell. The last two variables are crucial because the precision of the presented method highly depends on determining them.

Suppose that all particles of each cell are concentrated at the representative point, then the density function would be

$$f(x,t) = \sum_{i=1}^{n_p} N_i(t)\delta(x - x_i). \tag{4}$$

The discretized equation, Eq. (3), can be arranged in a recursive way that preserves the zeroth moment:

$$\frac{dN_i}{dt} = -\frac{\lambda_i}{x_{i+1} - x_i} + B_i - D_i, \quad i = 1, \tag{5a}$$

$$\frac{dN_i}{dt} = \frac{\lambda_{i-1}}{x_i - x_{i-1}} - \frac{\lambda_i}{x_{i+1} - x_i} + B_i - D_i, \quad i = 2, \ldots, n_p - 1 \tag{5b}$$

$$\frac{dN_i}{dt} = \frac{\lambda_{i-1}}{x_i - x_{i-1}} + B_i - D_i, \quad i = n_p. \tag{5c}$$

The terms such as B_i and D_i can be achieved by the below formulas:

$$B_i = \int_{x_{b,i}}^{x_{b,i+1}} (\mathbf{B_{agg}} + B_{\mathbf{break}})\,dx, \tag{6a}$$

$$D_i = \int_{x_{b,i}}^{x_{b,i+1}} (\mathbf{D_{agg}} + \mathbf{D_{break}})\,dx. \tag{6b}$$

The variable λ_i (kernel of the discretized equation) also depends on the type of the process and must satisfy the following condition: