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On sectional techniques for the solution of the breakage equation

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ABSTRACT

The breakage equation is of great significance for modeling many physicochemical processes. The need for its extension to more than one internal coordinates in spatially distributed environment renders crucial the development of efficient numerical methods for its solution. In the present work two new sectional methods (Cell Average Technique and Extended Cell Average Technique) recently applied to the coagulation equation are implemented to breakage equation and tested extensively against the well-established Fixed Pivot Technique. The results of the analysis show that whereas the new methods cannot predict the complete particle size distribution better than the Fixed Pivot Technique (despite their superiority in the case of coagulation), they are very successful in predicting the moments of the distribution even for coarse grids. Thus, especially the Extended Cell Average Technique can be considered as a refinement of the moments method with increased number of degrees of freedom but also increased accuracy.

1. Introduction

Breakage (alternatively called fragmentation) is of paramount importance in several processes of technological and/or fundamental scientific interest. This phenomenon alone or in combination with other particle-level phenomena such as coagulation, growth-dissolution, particle size domain diffusion, etc., concerns several scientific disciplines. For example, regarding polymer technology, the mechanism of polymer degradation can be considered to be breakage (Staggs, 2004, 2006) whereas regarding catalytic processes it influences their efficiency through the catalyst attrition (Matsuda, Hatano, Muramoto, & Tsutsumi, 2004). In atmospheric sciences, it is related to rain formation (Shrivastava, 1982) and in astrophysics to the size distribution of asteroids (Piotrowsky, 1953). In biotechnology, the cell division process can be described as a spontaneous breakage process (Nielsen & Villadsen, 1994). Other processes where breakage is the essential mechanism are those related to size reduction of solids (e.g. crushing, milling, grinding) (Kelley & Spottiswood, 1982). Recently, it has been argued that the size distribution of the ice crystals in the Greenland ice sheet is the result of a breakage process (Olesen, Ferkinghoff-Borg, Jensen, & Mathiesen, 2005). The bubble size distribution in bubble columns is largely due to breakage, which in turn determines the characteristics of the flow field in the column (Jakobsen, Lindborg, & Dorao, 2005). Furthermore, breakage is very important in emulsion technology determining not only the droplet size distribution but in some cases even the phase inversion point (Hu, Matar, Hewit, & Angeli, 2006).

The dynamics of a particle population undergoing breakage is described by the breakage equation that belongs to the more general class of the population balance equations. The breakage equation is a linear partial integro-differential equation and its numerical solution requires special techniques. This is the primary reason for the development of several methods for its solution, obtained from various scientific disciplines. It is quite impressive that after 35 years of development of numerical techniques for the solution of population balance there is still room for the emergence of fresh ideas; e.g. the extension and application to cases of practical interest (Qamar & Warnecke, 2007a,b) of the completely new discretization approach introduced by Filbert and Laurencot (2004).

There are three general approaches to the numerical solution of the coagulation equation, in addition to the conventional finite differences-finite element-finite volume techniques. The so-called *higher order methods* are based on approximating the unknown particle size distribution (PSD) by sets of orthogonal functions (globally or locally) or spline polynomials. For example, cubic splines have been used for the solution of breakage equation by Eyre, Everson, and Campbell (1998). Liu and Tade (2004) proposed the expansion of the solution in terms of wavelets. Mantzaris (2005) employed local approximation with Legendre polynomials and Hamilton,

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Curtis, and Ramkrishna (2003) used global approximation by Hermitte polynomials. Canu (2005) attempted an expansion to a set of global non-orthogonal functions.

The second approach is the so-called *method of moments*. In this case the coagulation equation is transformed to a system of equations for some moments of the PSD. The closure problem is overcome by using relations between the moments of the PSD. The main advantage of the method is its computational efficiency as it has only a few degrees of freedom. On the other hand, the method has achieved some degree of success on the prediction of the moments of the PSD but its capability to predict the complete PSD is at best small. A rather extensive account of the application of the moments method to solve the breakage equation can be found in Kostoglou and Karabelas (2002, 2004).

The third approach is the so-called *sectional methods* (alternatively zero order methods or methods of classes). These methods offer a very attractive compromise between the very efficient but of limited accuracy moments methods and the very accurate but computationally demanding higher order methods. Of course the notion of computational efficiency is not crucial for the zero external and one internal coordinate problem examined here but it becomes important as the number of internal and external coordinates increases to simulate processes of practical interest (Livk & Illievski, 2007). Until today the state of the art sectional technique for the breakage equation is the so called Fixed Pivot Technique (Kumar & Ramkrishna, 1996a). Recently some new sectional techniques (Kostoglou, 2007; Kumar, Peglow, Warneke, Heinrich, & Morl, 2006) were developed to improve the Fixed Pivot Technique performance for the coagulation equation. The purpose of the present work is to examine whether similar principles can be employed for the development of improved sectional techniques for the breakage equation as well. It is noted that the breakage problem is in general easier than the coagulation problem due to its linearity.

The structure of the present work is as follows: in the next section the breakage problem is formulated and nondimensionalized. Then a rigorous mathematical derivation of sectional methods conserving just one integral property is presented. The implementation is described next of the Fixed Pivot (Kumar & Ramkrishna, 1996a,b), Cell Average (Kumar et al., 2006) and Extended Cell Average (Kostoglou, 2007) techniques to the breakage equation in order to overcome the restriction of the single conservation quantity. In the results section, the three sectional methods are assessed against the existing exact solutions of the breakage equation (moments or complete PSD). The outcome of the assessment is extensively discussed to reveal the advantages and disadvantages of the proposed techniques.

2. Problem formulation

2.1. The breakage equation

The linear breakage process (described as "continuous breakage" in physics literature, e.g. Astrom, 2006) can be described in general by the following linear partial integro-differential equation:

$$\frac{\partial f(x,t)}{\partial t} = \int_x^\infty p(x,y)b(y)f(y,t)\,dy - b(x)f(x,t) \tag{1}$$

where t time, x particle volume, $f(x, t)$ particle number density distribution, $b(x)$ breakage frequency and $p(x, y)$ the probability distribution of particles of volume x resulting from the breakup of a particle of volume y. The above equation must be solved for the evolution of the particle size distribution (PSD) having as initial condition a given PSD $f(x, 0) = f_0(x)$. For convenience, the following nondimensionalization is introduced, employing the initial total particle concentration, $N = \int_0^\infty f_0(x)\,dx$, and the mean particle volume of the initial PSD, $x_0 = \int_0^\infty x f_0(x)\,dx / \int_0^\infty f_0(x)\,dx$:

$$\bar{x} = \frac{x}{x_0}, \quad \bar{y} = \frac{y}{x_0}, \quad \bar{t} = b(x_0)t, \quad \bar{f}(x,t) = \frac{x_0 f(x,t)}{N}$$

$$\bar{b}(x) = b(x)/b(x_0), \quad \bar{p}(x,y) = p(x,y)/x_0$$

Thus, Eq. (1) can be written as

$$\frac{\partial \bar{f}(\bar{x},\bar{t})}{\partial \bar{t}} = \int_x^\infty \bar{p}(\bar{x},\bar{y})\bar{b}(\bar{y})\bar{f}(\bar{y},\bar{t})\,d\bar{y} - \bar{b}(\bar{x})\bar{f}(\bar{x},\bar{t}) \tag{2}$$

Since only dimensionless variables will be used in the rest of the present work the overbars are omitted for convenience. In that case the dimensionless coagulation equation looks exactly the same as the dimensional one. The dimensionless moments of the PSD are defined as

$$M_i = \int_0^\infty x^i f(x,t)\,dx \tag{3}$$

Multiplying the breakage Eq. (2) by x^i and integrating from $x = 0$ to ∞ the following system for the moments of the PSD results:

$$\frac{dM_i}{dt} = \int_0^\infty b(y)f(y,t)\left[\int_0^y x^i p(x,y)\,dx - y^i\right] dy \tag{4}$$

It is obvious that the parameters of the breakage equation are the breakage frequency $b(x)$ and the breakage kernel $p(x, y)$. The breakage frequency should go to a finite value as x goes to 0; instead, the so called "shattering" phenomenon appears (McGrady & Ziff, 1987). This phenomenon refers to the existence of a new phase with particles of zero size but finite mass. Under these conditions Eq. (2) does not conserve the total particle mass during breakage due to the mass loss towards the new particle phase. The breakage kernel should satisfy the mass conservation (total fragments mass equals to parent particle mass) condition $\int_0^y x p(x,y)\,dx = y$. The number of fragment resulting from the breakup of a particle of size y can be obtained as $\nu(y) = \int_0^y p(x,y)\,dx$.

A major classification of the breakage functions is made with respect to their homogeneity. The breakage frequency is homogeneous only if it has a power law form; i.e. $b(x) = x^b$. The breakage kernel is homogeneous if it has the form $p(x, y) = \theta(x/y)/y$. This means that the normalized (with respect to the parent particle size) fragment size distribution does not depend on the parent particle size. For the case of homogeneous breakage kernel, the no-shattering condition degenerates to the condition $b \geq 0$, the main properties of the breakage kernel given above are transformed to $\int_0^1 z\theta(z)\,dz = 1$ and $\nu = \int_0^1 \theta(z)\,dz$, respectively, and the moments equations are simplified as follows ($i = 0, 1, 2\ldots$):

$$\frac{dM_i}{dt} = (J_i - 1)M_{i+b} \tag{5}$$

where J_i are the moments of the homogeneous kernel, i.e. $J_i = \int_0^1 z^i\theta(z)\,dz$.

2.2. Sectional methods for the breakage equation

A typical discretization scheme transforms the breakage equation to a system of ordinary differential equations of the form:

$$\frac{dN_i}{dt} = \sum_{j=i}^{\infty} n_{ij} b_j N_j - b_i N_i \tag{6}$$