Chemical Engineering Science 63 (2008) 3988 – 3997

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

A new discretization of space for the solution of multi-dimensional population balance equations: Simultaneous breakup and aggregation of particles

Mahendra N. Nandanwar, Sanjeev Kumar*

Department of Chemical Engineering, Indian Institute of Science, Bangalore 560012, India

ARTICLE INFO

Article history:
Received 27 December 2007
Received in revised form 5 April 2008
Accepted 28 April 2008
Available online 6 May 2008

Keywords:
Population balance modelling
Discretization methods
Multi-dimensional population balance equations
Modelling and simulation

ABSTRACT

In this work, we show that straight forward extensions of the existing techniques to solve 2-d population balance equations (PBEs) for particle breakup result in very high numerical dispersion, particularly in directions perpendicular to the direction of evolution of population. These extensions also fail to predict formation of particles of uniform composition at steady state for simultaneous breakup and aggregation of particles, starting with particles of both uniform and non-uniform compositions. The straight forward extensions of 1-d techniques preserve 2^n properties of non-pivot particles, which are taken to be number, two masses, and product of masses for the solution of 2-d PBEs. Chakraborty and Kumar [2007. A new framework for solution of multidimensional population balance equations. Chemical Engineering Science 62, 4112–4125] have recently proposed a new framework of minimal internal consistency of discretization which requires preservation of only $(n+1)$ properties. In this work, we combine a new radial grid [proposed in 2008. part I, Chemical Engineering Science 63, 2198] with the above framework to solve 2-d PBEs consisting of terms representing breakup of particles. Numerical dispersion with the use of straight forward extensions arises on account of formation of daughter particles of compositions different from that of the parent particles. The proposed technique eliminates numerical dispersion completely with a radial distribution of grid points and preservation of only three properties: number and two masses. The same features also enable it to correctly capture mixing brought about by aggregation of particles. The proposed technique thus emerges as a powerful and flexible technique, naturally suited to simulate PBE based models incorporating simultaneous breakup and aggregation of particles.

1. Introduction

Population balance equations (PBEs), first proposed by Hulburt and Katz (1964), Randolph (1964), and Fredrickson et al. (1967), find applications in both physical and biological processes. Particulate systems in which particles continuously change their identity can be described by PBEs with internal state of particle as continuous variable. Crystallizers, liquid–liquid and gas–liquid contactors, fermenters, fluidized beds, polymer reactors, etc. (Ramkrishna, 2000) are few of the process equipment which have been simulated using PBEs. In a number of industrial processes (granulation for example), particles need to be identified with more then one independent (internal) variable. In general, if n internal variables are required to identify a particle uniquely, the population balance equations required to characterize such processes become n-dimensional in nature. In many such processes, breakup and aggregation of particles occur simultaneously. A general PBE in n-d space for simultaneously and independently occurring processes of breakup and aggregation of particles is given by

$$\frac{\partial n(\mathbf{v},t)}{\partial t} = \frac{1}{2}\int\int Q(\mathbf{v}',\mathbf{v}'')n(\mathbf{v}',t)n(\mathbf{v}'',t) \times P(\mathbf{v}'+\mathbf{v}''|\mathbf{v})\,\mathrm{d}\mathbf{v}'\,\mathrm{d}\mathbf{v}'' - \int_0^{\infty} Q(\mathbf{v}',\mathbf{v})n(\mathbf{v},t)n(\mathbf{v}',t)\,\mathrm{d}\mathbf{v}' + \int \beta(\mathbf{v},\mathbf{v}')\Gamma(\mathbf{v}')n(\mathbf{v}',t)\,\mathrm{d}\mathbf{v}' - \Gamma(\mathbf{v})n(\mathbf{v},t) \quad (1)$$

where $\mathbf{v}$ is a vector of n internal attributes of particles, $n(\mathbf{v},t)\,\mathrm{d}\mathbf{v}$ is number of particles in range $\mathbf{v}$ to $\mathbf{v}+\mathrm{d}\mathbf{v}$, $Q(\mathbf{v},\mathbf{v}')$ is aggregation frequency, $\Gamma(\mathbf{v})$ is breakage frequency, $\beta(\mathbf{v},\mathbf{v}')\,\mathrm{d}\mathbf{v}$ is average number of particles formed in range $\mathbf{v}$ to $\mathbf{v}+\mathrm{d}\mathbf{v}$ when a particle of state $\mathbf{v}'$ breaks, and $P(\mathbf{v}',\mathbf{v}''|\mathbf{v})$ is the probability of formation of a particle with attribute $\mathbf{v}$ when two particles with attributes $\mathbf{v}'$ and $\mathbf{v}''$ aggregate. When a particle can be adequately identified for its role in a process system by just one internal variable, for example its size, the above general equation leads to 1-d PBE, and vector $\mathbf{v}$ reduces to

* Corresponding author. Tel.: +91 80 2293 3110; fax: +91 80 2360 8121.
E-mail address: sanjeev@chemeng.iisc.ernet.in (S. Kumar).

0009-2509/$ - see front matter
doi:10.1016/j.ces.2008.04.054

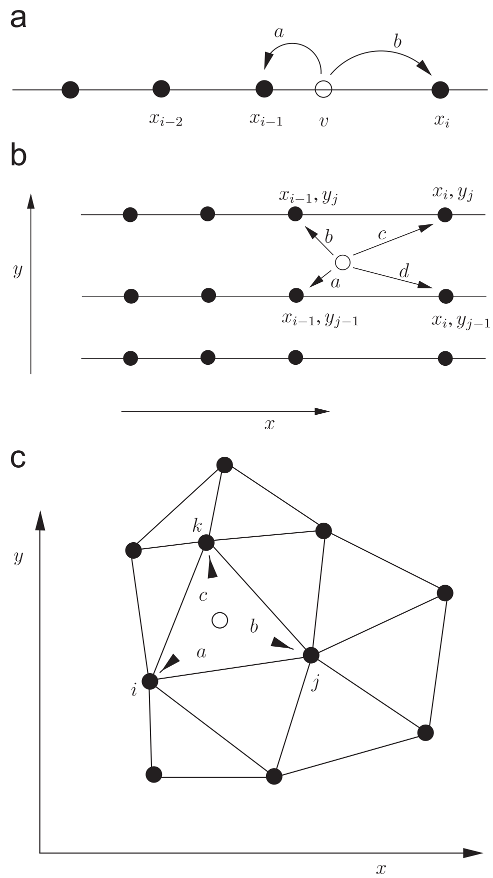

Fig. 1. Representation of a non-pivot particle of size v through neighbouring fixed pivots: (a) in 1-d (Kumar and Ramkrishna, 1996a), (b) extension of Kumar and Ramkrishna (1996a) to 2-d (preservation of 2^n properties), (c) framework of minimal internal consistency (Chakraborty and Kumar, 2007) applied to 2-d (preservation of $n+1$ properties).

a scalar. Vector **v** for 2-d PBEs can simply consist of masses of two constituents of particles.

Analytical solutions of the above equation for number density are available for simple cases: pure aggregation (Scott, 1968) and pure breakup (Ziff and McGrady, 1986, 1987; Ziff, 1991) of particles identified by one internal coordinate. Analytical solution for simultaneous breakup and aggregation is limited to a special combination of breakup and aggregation kernels (Blatz and Tobolsky, 1945). Analytical solutions for multi-variate number density are available for a few cases (Gelbard and Seinfeld, 1978). Most often, numerical solutions are required. Several numerical approaches to solve PBEs are available, e.g., method of weighted residuals (Subramanian and Ramkrishna, 1971), finite difference method (Mantzaris et al., 2001), method of moments (McGraw, 1997). These techniques are reviewed by Ramkrishna (2000). Among the discretization techniques, the fixed pivot technique (FPT) of Kumar and Ramkrishna (1996a) is quite useful for the solution of 1-d PBEs due to its simplicity and robustness (Vanni, 2000; Attarakih et al., 2004; Roussosa et al., 2006). In this technique, continuous particle population is discretized into bins, and represented through representative volumes called *pivots*, one for each bin. The non-pivot particles formed through breakup and/or aggregation of particles located on pivots are represented through pivots adjoining non-pivot particles as shown in Fig. 1(a). Discretized version of Eq. (1) is obtained in terms of particle populations at discrete pivots.

Direct extensions of 1-d discretization techniques to 2-d PBEs, using rectangular grids (Fig. 1(b)), are reported by Kumar and Ramkrishna (1995) and Alexopoulos and Kiparissides (2007) for simultaneous breakup and aggregation, and Vale and McKenna (2005) and Kumar et al. (2007) for pure aggregation. In its generalized form, this approach uses line segments as bins for 1-d, rectangles for 2-d, cuboids for 3-d, hyper-cuboids with 16 vertices (pivots) for 4-d PBEs, and so on. A non-pivot particle is represented through 2^n neighbouring pivots, and requires preservation of 2^n of its properties to determine fractions assigned to the neighbouring pivots. These properties are: x^0 and x^1 for 1-d; x^0y^0, x^1y^0, x^0y^1, and x^1y^1 for 2-d; $x^0y^0z^0$, $x^1y^0z^0$, $x^0y^1z^0$, $x^0y^0z^1$, $x^1y^1z^0$, $x^0y^1z^1$, $x^1y^0z^1$, and $x^1y^1z^1$ for 3-d; sixteen properties for 4-d PBEs; and so on.

A new framework of *minimal internal consistency*, proposed by Chakraborty and Kumar (2007), preserves only $n+1$ properties of a non-pivot particle and represents it through $n+1$ adjoining pivots. This has proved to be an effective extension of the original fixed pivot technique. The bins required for discretization in this framework are line segments, triangles, tetrahedrons, an object with five vertices in 4-d space, and so on to solve 1, 2, 3, and 4-d PBEs respectively. Incidently, these objects are also known as *natural objects* which enclose a region of n-d space with minimum number of vertices. The authors have demonstrated the usefulness of their framework by solving 2 and 3-d PBEs for pure aggregation using *randomly* oriented triangles (Fig. 1(c)) and tetrahedrons, with preservation of number and n constituent masses of particles (their internal attributes).

Nandanwar and Kumar (2008) proposed a new type of structured radial grid to harness the advantages of the framework of Chakraborty and Kumar easily and effectively. In comparison to a random grid, a regular structured grid can be generated easily and searched easily to locate a non-pivot particle in space. It also offers numerous other advantages. Nandanwar and Kumar demonstrated the effectiveness of their radial grid for the solution of 2-d PBEs for pure aggregation processes. The present paper is an extension of our previous work (Nandanwar and Kumar, 2008). Here, we demonstrate the usefulness of radial grid for discretization of 2-d PBEs for pure breakup and simultaneous breakup and aggregation of particles. The results obtained suggest that the framework of minimal internal consistency combined with radial grid offers a natural solution methodology to predict evolution of particle population correctly when particles undergo breakup with or without simultaneous aggregation.

2. Previously developed discretization methods for PBEs

An equation for time variation of particle population in a bin represented by a pivot can be obtained by integrating Eq. (1) over the domain of the bin. As most of the non-pivot particles born into a bin are of sizes different from that of the pivot that represents it, one can choose to either preserve their numbers or mass. Batterham et al. (1981) conserved mass for pure aggregation problems. As the resulting discretized equations did not preserve numbers, the variation of total number of particles with time could not be predicted correctly. Hounslow et al. (1988), who recognized the above problem, were the first to propose a discretization technique which preserved number of particles formed and also conserved mass of particles. Instead of choosing particles in a bin to be represented by a pivot, they assumed uniform number density of particles in a bin. They preserved numbers in their derivation of discretized equations, multiplied the terms accounting for birth of particles with an unknown parameter, and estimated its value to enforce mass conservation. Their final equations were derived for a fixed geometric grid—the ratio of the largest to the smallest particle in a bin being two. Litster et al. (1995) expanded the scope of the technique of Hounslow et al. by deriving discretized equations for geometricc grids with the ratio of the largest to the smallest particle being $2^{1/q}$, where q is an integer. These approaches appear to be closely tied to the grids they use. Extension of these approaches to include breakup processes is not possible (Vanni, 2000).