Computers and Chemical Engineering 87 (2016) 111–124

Contents lists available at ScienceDirect

Computers and Chemical Engineering

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

Solution of bivariate population balance equations with high-order moment-conserving method of classes

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ARTICLE INFO

Article history:
Received 4 July 2015
Received in revised form 6 December 2015
Accepted 18 December 2015
Available online 16 January 2016

Keywords:
Population balance
High-order moment-conserving method of classes (HMMC)
Bivariate
Two-component aggregation
Particulate processes
Numerical methods

ABSTRACT

In this work the high-order moment-conserving method of classes (HMMC) (Alopaeus et al., 2006) is extended to solve the bivariate Population Balance Equation (PBE). The method is capable of guaranteeing the internal consistency of the discretized equations for a generic moment set, including mixed-order moments of the distribution. The construction of the product tables in the case of aggregation, breakage and convection in internal coordinate space are discussed. Eventually, several test cases are considered to assess the accuracy of the method. The application to a realistic mass transfer problems in a liquid–liquid system is preliminarily discussed. The comparison with analytical solutions of pure aggregation problems shows that the proposed method is accurate with only a limited number of categories.

1. Introduction

Population balance modeling is nowadays a widely used tool in many areas of chemical engineering and process industry, useful for describing the evolution of those systems characterized by dispersed elements with a distribution of properties in a continuous phase, such as particles, droplets and bubbles with different size, composition, velocity and temperature. This modeling approach involves the solution of the so-called Population Balance Equation (PBE), which requires efficient numerical techniques due to its complex integro-differential form.

First applications of the population balance methodology were limited to the one-dimensional case, i.e., only one property of the distribution is considered. For this reason, the development of solution methodologies was firstly focused on mono-dimensional problems (Hulburt and Katz, 1964; Valentas and Amundson, 1966; Hounslow et al., 1988; Ramkrishna, 2000). Most of the known approaches belong to one of the following groups: Monte Carlo, moment-based and classes (or sectional) methods. For further details on this subdivision, the reader may refer to specialized literature (Marchisio and Fox, 2013). Monte Carlo methods can be thought as direct numerical simulations and are based on the solution of stochastic differential equations that are able to reproduce a finite number of artificial realizations of the system under investigation (Hsu and Tsao, 1992; Laurenzi et al., 2002; Zhao et al., 2007; Zhao and Zheng, 2009; Terrazas-Velarde et al., 2009; Braumann et al., 2010). The main drawback of this group of methods is represented by the unsustainable computational costs in order to have a physically meaningful solution, since the error is inversely proportional to the square of the number of notional elements considered. On the other hand, moment-based methods became very popular due to their low computational demand and the easy integration in CFD codes (Hulburt and Katz, 1964; McGraw, 1997; Frenklach, 2002; Marchisio et al., 2003; Kostoglou and Karabelas, 2004; Strumendo and Arastoopour, 2008, 2009; Lage, 2011; Marchisio and Fox, 2013); with these methods the internal coordinate dependency is integrated out, solving only few equations for the moment of the distribution. Due to this integration procedure, the information related to the shape of the distribution is lost and this might be critical for certain type of applications.

Classes methods are in between the former two approaches in terms of computational time (Vanni, 2000; Marchisio and Fox, 2013): this wide group of methods is characterized by the fact that the internal coordinate space is discretized in a finite number of bins, transforming the PBE into a coupled set of differential equations for the expected number of elements within each bin, giving the possibility to the modeler to track the actual shape of the distribution. Many methods belong to this group, such as discretization methods by Hounslow et al. (1988), Litster et al. (1995), Kumar and Ramkrishna (1996a, 1996, 1997), Wynn (2004),

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http://dx.doi.org/10.1016/j.compchemeng.2015.12.013
0098-1354/

Chakraborty and Kumar (2007), Nandanwar and Kumar (2008), Chauhan et al. (2010), Singh et al. (2013); the method of characteristics by Rhee et al. (1986), Lim et al. (2002), Qamar et al. (2009), John and Suciu (2014); the cell-average technique Kumar et al. (2006, 2008); the method of weighted residuals by Rawlings et al. (1992), Wulkow et al. (2001), Mahoney and Ramkrishna (2002), Immanuel et al. (2002), Immanuel and Doyle (2003, 2005); Lattice Boltzmann methods by Majumder et al. (2012a,b) and the finite volume methods by Gunawan et al. (2004), Qamar et al. (2006, 2007), Qamar and Rehman (2013). Due to it is easy implementation and accuracy (Vanni, 2000), one of the most popular numerical schemes of the method of classes is the fixed-pivot technique of Kumar and Ramkrishna (1996a), where the internal consistency is restored by conserving two moments of the distribution.

Recently, Alopaeus et al. (2006) extended the approach of Kumar and Ramkrishna (1996a) by proposing an efficient method, based on the idea of solving the internal consistency issue of the discretized equations by accommodating a defined number of moments of the distribution. This method, known as the high-order moment-conserving method of classes (HMMC), has been proven to be very accurate in the prediction of both moments and shape of the population distribution in a variety of problems (Alopaeus et al., 2006, 2007), by significantly reducing the numerical error inherent to the sectional methods even with a reasonable number of discretization classes.

However, there are a number of industrially relevant problems whose description requires the formulation of a multi-dimensional Population Balance Equation (PBE), where two or more properties of the population are taken into account to properly describe the investigated system. Practical examples are powders granulation, where size, porosity, binder content, and compositions of the granule should be considered as independent coordinates of the population balance to properly evaluate the evolution of the granule morphology (Iveson, 2002; Cameron et al., 2005; Matsoukas et al., 2006; Braumann et al., 2010), synthesis of nanoparticles, where at least the knowledge of another property together with particle size or mass is required (e.g. the fractal dimension, the actual surface area or the radius of gyration) (Haseltine et al., 2005; Celnik et al., 2007; Zucca et al., 2007; John and Suciu, 2014), mass transfer and chemical reactions in multiphase systems, where both particle size and particle composition affects the mass transfer rates, especially if the mass transfer is faster than other process involved compared to coalescence and breakage, possibly enhanced by chemical reactions (Buffo et al., 2013; Buffo and Marchisio, 2014; Alopaeus, 2014), just to cite a few examples. For this reason, in the latest years, many methods were extended to treat bivariate/multivariate problems (Buffo et al., 2013b). Vale and McKenna (2005) performed an extension of the fixed-pivot technique of Kumar and Ramkrishna (1996a) to solve a two-component aggregation problem by preserving four specified moments of the distribution. Kumar et al. (2008) proposed a multivariate version of the cell average technique (Kumar et al., 2006) and then Chauhan et al. (2010) and Singh et al. (2013) explored the possibility to use different discretization grids for the internal coordinate space than Cartesian grids. However the main limitation of these bivariate methods lays on their capability of predicting the moments of the distribution: all other methods are based on preserving a very limited number of moments (four mixed-order moment moments), which leads to a poor predictions for all the other moments not preserved by the method. This aspect can be problematic, since the moments of the distribution are usually the quantities of interest from the engineering point of view and they often are the only properties that can be measured rather than the actual distribution. For this reason, it is crucial that the solution method is consistent with the mixed-order moments of interest for a specific bivariate problem.

In this work, we first propose an extension of the HMMC of Alopaeus et al. (2006) for the solution of bivariate problems, making the solution procedure consistent with arbitrary moments of the distribution. The implementation is verified on a number of relevant test cases, considering coalescence and breakage problems, growth and mass transfer. The remainder of the paper is the following. In Section 2, the proposed numerical method is presented, with particular focus on the procedure to preserve a defined moment set for aggregation, breakage and convection (or drift) in the internal coordinate space. Then the investigated test cases, namely pure two-component aggregation and mass-transfer in a liquid–liquid system, are introduced and eventually simulation results and comparisons with available analytical solutions are discussed.

2. Moment-conserving numerical method

The population balance equation for a homogeneous volume element and for a generic internal-coordinates vector of M components $\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots, \xi_M)$ can be written as follows:

$$\frac{\mathrm{d}n(\boldsymbol{\xi}, t)}{\mathrm{d}t} = \frac{1}{T}\int_{\Omega_{\boldsymbol{\xi}'}} f(\tilde{\boldsymbol{\xi}}, \boldsymbol{\xi}', t) n(\tilde{\boldsymbol{\xi}}, t) n(\boldsymbol{\xi}', t) J(\tilde{\boldsymbol{\xi}}, \boldsymbol{\xi}) \mathrm{d}\boldsymbol{\xi}' - \int_{\Omega_{\boldsymbol{\xi}'}} f(\boldsymbol{\xi}, \boldsymbol{\xi}', t) n(\boldsymbol{\xi}', t) n(\boldsymbol{\xi}, t) \mathrm{d}\boldsymbol{\xi}' + \int_{\Omega_{\boldsymbol{\xi}'}} P(\boldsymbol{\xi}'|\boldsymbol{\xi}) g(\boldsymbol{\xi}', t) n(\boldsymbol{\xi}', t) \mathrm{d}\boldsymbol{\xi}' - g(\boldsymbol{\xi}, t) n(\boldsymbol{\xi}, t) + \dot{n}(\boldsymbol{\xi})_{\mathrm{in}} - \dot{n}(\boldsymbol{\xi})_{\mathrm{out}} - \frac{\partial}{\partial \boldsymbol{\xi}} \cdot (n(\boldsymbol{\xi}, t)\dot{\boldsymbol{\xi}}). \quad (1)$$

The left-hand side term of Eq. (1) represents the time rate of change of the number density function $n(\boldsymbol{\xi}, t)$ (NDF). The first right-hand side term describes the rate of birth of new particles due to aggregation, where $\Omega_{\boldsymbol{\xi}'}$ is the phase space, namely the space generated by the choice of the internal-coordinates $\boldsymbol{\xi}'$, $f(\tilde{\boldsymbol{\xi}}, \boldsymbol{\xi}', t)$ is the coalescence frequency, $J(\tilde{\boldsymbol{\xi}}, \boldsymbol{\xi})$ is the Jacobian of the variable transformation relating to the internal-coordinate space before aggregation $\tilde{\boldsymbol{\xi}}$ and after aggregation $\boldsymbol{\xi}$ and the integer number T is the symmetry factor used to avoid multiple pairs counting, and is equal to two for identical particles and one for different particles. The second right-hand side term represents the rate of death due to aggregation, while the third and the fourth are respectively the birth and the death terms due to particle breakage, where $P(\boldsymbol{\xi}'|\boldsymbol{\xi})$ represents the daughter distribution function, $g(\boldsymbol{\xi}', t)$ is the breakage frequency. The fifth right-hand side term is the flow of particles into the control volume, while the sixth term is the flow out of the domain. The last term represents the continuous rate of change in the internal-coordinate space, with $\dot{\boldsymbol{\xi}}$ expressing the phase space drift vector, composed in each component by the rate of change of the ith internal-coordinate due to continuous processes.

Although there is no limitation in the number of internal-coordinates that the proposed method can tackle, we limit the discussion to two generic internal-coordinates, ξ_1 and ξ_2, therefore simplifying the notation for a better comprehension of the text. When the method of classes is used to solve Eq. (1), the internal-coordinate space is discretized into a finite number of classes N, by denoting with $Y_i(t)$ the number density of particles belonging to each class, where the index $i = 1, 2, \ldots, N$ and $[\xi^-_{1,i}, \xi^+_{1,i}; \xi^-_{2,i}\ \xi^+_{2,i}]$ is the interval of the internal-coordinate space belonging to the ith class. In other words, $Y_i(t)$ represents the particle number concentration belonging to each category associated with a pair of internal