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Population balance discretization for growth, attrition, aggregation, breakage and nucleation

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ABSTRACT

This paper presents a new discretization method to solve one-dimensional population balance equations (PBE) for batch and unsteady/steady-state continuous perfectly mixed systems. The numerical technique is valid for any size change mechanism (i.e., growth, aggregation, attrition, breakage and nucleation occurring alone or in combination) and different discretization grids.

The developed strategy is based on the moving pivot technique of Kumar and Ramkrishna and the cell-average method of Kumar et al. A novel contribution is proposed to numerically handle the growth and attrition terms, for which a new representation of the number density function within each size class is developed. This method allows describing the number particle fluxes through the class interfaces accurately by preserving two sectional population moments.

By comparing the numerical particle size distributions with analytical solutions of one-dimensional PBEs (including different size change mechanisms and particle-size dependent kinetics), the accuracy of the proposed numerical method was proved.

1. Introduction

Particulate systems play an important role in a wide variety of industrial processes (among others: mining, food processing, pharmaceuticals and fertilizers manufacture). Changes in particle size distributions (PSDs) often take place in these industries due to different mechanisms, which can occur either alone or in combination, such as aggregation, growth, breakage, attrition and nucleation (Gerstlauer et al., 2006; Ramkrishna, 2000).

An appropriate modeling approach for quantify PSDs is the concept of population balance equation (PBE), which was developed several decades ago (Hulburtz and Katz, 1964). Ramkrishna (2000) defined the PBE as an equation to describe the density of a suitable extensive variable, usually the particle number (in terms of the number density function), so that the PBE represents a number balance on particles of a specific state. Significant efforts were those of Hulburtz and Katz (1964), Randolph and Larson (1971) and Ramkrishna (2000) to formalize a generic PBE capable of quantifying the different mechanisms by which particles of a specific state can either appear in or disappear from the system. Mathematically the PBE corresponds to a non-linear partial integro-differential equation, which presents only very few analytical solutions for some ideal cases. On the other hand, numerical solutions require substantial computational resources because, in practical engineering processes, PSDs may extend over several orders of magnitude and can be very sharp (Vanni, 2000; Qamar, 2008). Moreover, some methods exhibit lack of stability and accuracy of the solution. Since there is a great variety of processes that are studied by means of modeling and simulation (processes design, control and optimization), there is still need of numerical methods development to solve those mathematical models that include PBEs (Pinto et al., 2008; Utomo et al., 2009).

Several numerical methods have been proposed/used in the literature to solve PBEs, among others, the methods of: moments (Hulburtz and Katz, 1964; Motz et al., 2002; Madras and McCoy, 2004; Marchisio and Fox, 2005; Bajcinca et al., 2014), characteristics (Kumar and Ramkrishna, 1997; Pilon and Viskanta, 2003; Qamar and Warnecke, 2007), finite differences/discretization (Marchal et al., 1988; Hounslow et al., 1988; Kumar and Ramkrishna, 1996a,b; Ma et al., 2002) and Monte Carlo (Smith and Matsoukas, 1998; Kruis et al., 2000; Lee and Matsoukas, 2000; Lin et al., 2002). Frequent problems related to the numerical solution of PBEs include, among others, the inaccurate calculation of the PSD for strong aggregation processes, numerical instabilities for growth processes and stiffness of the equations system for rapid particle nucleation (Maurstad, 2002; Kiparissides, 2006).

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Nomenclature

A	attrition rate (m/s)
b	breakage rate (s^{-1})
b_0	constant in the breakage rate in Eq. (106) ($m^{-1}\ s^{-1}$)
b'_0	constant in the breakage rate in Eq. (129) ($m^{-3}\ s^{-1}$)
B_{nuc}	discrete nucleation rate (s^{-1})
C_{1i}	parameter for the linear approximation in Eq. (45) (m^{-2})
C_{2i}	parameter for the linear approximation in Eq. (45) (m^{-1})
d_p	particle diameter (m)
$d_{p_{crit}}$	critical diameter in Case 3 (m)
d_{p_i}	mean diameter in class i (m)
d_{nuc}	diameter of particles born by nucleation (m)
d_{nv}	number–volume mean diameter (m)
D_{p_i}	lower node in class i (m)
$\bar{D}_{p_i}$	arithmetic mean diameter in class i (m)
$\bar{D}^A_{p_i}$	average diameter of particles born by aggregation in class i (m)
$\bar{D}^B_{p_i}$	average diameter of particles born by breakage in class i (m)
$\bar{D}^B_{p_{j\to i}}$	average diameter of particles born by breakage in class i from class j (m)
$\bar{D}^{in}_p$	average diameter of particles of class i in the inlet flowrate (m)
G	growth rate (m/s)
G_0	constant in Eq. (82) (m^{1-q}/s)
G'_0	constant in Eq. (93) (m/s)
G''_0	constant in Eq. (119) (s^{-1})
h^{A+}	particle birth rate by aggregation ($m^{-1}\ s^{-1}$)
h^{A-}	particle death rate by aggregation ($m^{-1}\ s^{-1}$)
h^{B+}	particle birth rate by breakage ($m^{-1}\ s^{-1}$)
h^{B-}	particle death rate by breakage ($m^{-1}\ s^{-1}$)
H_i^{A+}	flow of particles born by aggregation in class i (s^{-1})
H_i^{A-}	flow of particles dead by aggregation in class i (s^{-1})
H_i^{B+}	flow of particles born by breakage in class i (s^{-1})
H_i^{B-}	flow of particles dead by breakage in class i (s^{-1})
I_0	modified Bessel function of the first kind of order zero
I_1	modified Bessel function of the first kind of order one
k	index of summation in Eqs. (76) and (77)
n	number density function (m^{-1})
n_0	number density function (m^{-1})
n_i	discrete number density function in class i (m^{-1})
$\dot{n}_{in}$	number density function of the particles entering the system ($m^{-1}\ s^{-1}$)
$\dot{n}_{nuc}$	rate of number density function of particles by nucleation ($m^{-1}\ s^{-1}$)
$\dot{n}_{out}$	number density function of the particles leaving the system ($m^{-1}\ s^{-1}$)
N_0	initial total particle number
N_i	particle number in class i
$\dot{N}_{i_{in}}$	inlet number flow rate of particles in class i
$\dot{N}_{i_{nuc}}$	flow of particles born by nucleation in class i (s^{-1})
$\dot{N}_{i_{out}}$	outlet number flow rate of particles in class i
p	exponent in Eq. (82)
P	breakage probability function (m^{-1})
q	index of the conserved population moment
$Q_{attrition}$	volume flow rate leaving the particles population by attrition (m^3/s)
Q_{growth}	volume flow rate fed to the system which contributes to the particle growth (m^3/s)
Q_{in}	inlet volumetric flow rate (m^3/s)
Q_{out}	outlet volumetric flow rate (m^3/s)
r	geometric grid ratio between classes
S	total particle surface area (m^2)
V	total particle volume (m^3)
V_0	initial total particle volume (m^3)
t	time (s)
T	dimensionless time
x	integration variable (m)
x'	integration variable (m)
x''	integration variable (m)

Greek letters

α_i	parameter defined in Eq. (52)
β	aggregation kernel (s^{-1})
γ_i	parameter defined in Eq. (57)
δ	Dirac delta function
λ	half width of the pulse defined in Eq. (96) (m)
Γ	Gamma function
μ_j	jth population moment (m^j)
μ_{j_i}	jth sectional population moment in class i (m^j)
$\bar{\mu}$	arithmetic mean diameter of the PSD (m)
μ_0	arithmetic mean diameter of the initial PSD (m)
ν	average number of particles formed by breakage
σ_0	standard deviation of the initial PSD (m)
τ	mean residence time (s)

Subscripts

i	class of the discrete PSD
j	class of the discrete PSD
k	class of the discrete PSD

In particular, discretization techniques have been one of the most popular numerical methods. They consist in dividing the continuous range of particle specific state (usually the particle size) into discrete classes and discretizing the density function in the domain of the internal coordinate by concentrating the particles within each class on a mean class size. Several discretization methods are available in the literature, which basically differ in the choice of the discretization grid and the global population properties that are conserved (Hounslow et al., 1988; Kumar and Ramkrishna, 1996a,b; Vanni, 2000; Nopens et al., 2005).

Hounslow et al. (1988) developed a discretization procedure for growth, nucleation and aggregation processes, limited to the use of a geometric grid. Vanni (2000) extended that method to breakage processes. Kumar and Ramkrishna (1996a) also developed a discretization method (called the fixed pivot technique) to solve PBEs for batch systems with aggregation and breakage, which is capable to predict desired global properties of the PSDs by using an arbitrary discretization grid. Although results of fixed pivot technique proved to be generally very accurate for estimating PSDs, the method failed to correctly predict the PSDs for aggregation processes in large size ranges represented on a coarse geometric grid. Then, Kumar and Ramkrishna (1996b) developed a new discretization technique to overcome this problem by defining moving pivots that concentrate the particle number of a given size range.

Kumar et al. (2006) developed a numerical procedure for solving PBEs for batch aggregation processes that guarantees the exact conservation of two population properties of interest. This technique (called the Cell Average Technique) involves the computation of the average size of newborn particles by aggregation and their