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Comparison and pitfalls of different discretised solution methods for population balance models: a simulation study

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Abstract

One way of solving population balance equations in a time efficient way, necessary for using the model in non-linear parameter estimation, process control or for combination with computational fluid dynamics (CFD), is by means of discretisation of the population property of interest. Several methods are available in literature, but which one should be used in which case? Do they all perform equally well or do some of them have unexpected pitfalls? In this study, three discretisation methods (the Hounslow method, the fixed pivot and the moving pivot) were compared for three different processes (pure aggregation, pure binary breakage into equally sized daughters and combined aggregation/breakage) and six different initial conditions (two monodispersions, one uniform polydispersion and three partially uniform polydispersions). Their performances were compared in terms of accuracy and calculation speed and their pitfalls addressed and explained where possible. Overall, it was concluded that the moving pivot with a geometric factor of 2 performs good in all studied cases (not for finer or coarser grids). The eventual choice of discretisation scheme is highly dependent on the particular goal of the study and is a compromise between accuracy and calculation speed.

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Keywords: Population balances; Discretisation; Aggregation; Breakage; Numerical solution

1. Introduction

Population balance models (PBM) have been widely applied to describe processes involving dynamical behaviour of population properties. Applications can be found in a variety of scientific areas such as crystallisation, flocculation of inorganic dispersed systems, polymerisation, precipitation, flotation, granulation, cell culture dynamics, bioflocculation and aerosol dynamics, to name but a few. Depending on the number of properties being described by the model, a PBM can be categorized as either one- or multidimensional. The general format of a one-dimensional number-based PBM looks like (Hulburt & Katz, 1964; Ramkrishna, 2000):

$$\frac{\partial n(x,t)}{\partial t} + \frac{\partial}{\partial x}(\dot{X}(x,t)n(x,t)) = h(x,t) \quad (1)$$

where x is a property of the individuals, in our case particle size (expressed as volume), $n(x, t)$ is the number-based property distribution function (L^{-3}), $\dot{X}(x, t)$ is the time derivative of the property x (T^{-1}) and $h(x, t)$ the net generation rate of particles ($L^{-3} \cdot T^{-1}$). The right-hand-side of Eq. (1) often contains integral functions of $n(x, t)$ describing aggregation and/or breakage processes, turning it into an integro-differential equation which is hard to solve analytically. Alternative, numerical, techniques to solve this type of equations are summarised in Ramkrishna (2000). One of these techniques resulting in an acceptable calculation time and accuracy is the discretisation of the particle size x. Acceptable

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calculation speeds are important when using the model for parameter estimation, process control or in combination with CFD. This was the authors' main drive to solely investigate discretisation techniques to solve the PBE in this work, along with the ease of implementation and compatibility with our existing modelling and simulation software platform WEST (Hemmis NV, Belgium).

Discretisation techniques divide the property range of interest into a finite number of classes (M), transforming the integro-differential equation into a set of M ordinary differential equations that can be solved simultaneously. Several discretisation schemes exist, mainly differing in terms of (1) freedom of discretisation grid choice and (2) conserved properties (at least two) during the discretisation (Hounslow, Ryall, & Marshall, 1988; Kumar & Ramkrishna, 1996a, 1996b; Litster, Smit, & Hounslow; 1995; Nopens & Vanrolleghem, 2003; Vanni, 2000). In this study three discretisation algorithms were compared in terms of accuracy to describe different processes (pure aggregation, pure breakage and combined aggregation/breakage) using different initial conditions and grid densities. Pitfalls were addressed and explained where possible.

2. The population balance model

Since this work fits in the authors' study of activated sludge flocculation, a PBM without growth, but with aggregation and breakage included was selected. The growth term can be omitted because biological growth dynamics are significantly slower than aggregation/breakage dynamics.

A Smoluchowski type aggregation model was used (Ramkrishna, 2000; Thomas, Judd, & Fawcett, 1999):

$$h(x,t)_{\text{agg}} = \frac{1}{2}\int_0^x \alpha\beta(x-x',x')n(x-x',t)n(x',t)\,\mathrm{d}x' - n(x,t)\int_0^\infty \alpha\beta(x,x')n(x',t)\,\mathrm{d}x' \quad (2)$$

where $\beta(x,x')(L^3\cdot T^{-1})$ is the collision frequency for particles of volume x and x' and α $(-)$ is the collision efficiency. The former describes the transport of particles towards one another, whereas the latter describes the probability that these collisions lead to aggregation taking into account short-range forces like van der Waals attraction, charge repulsion and hydrodynamic interaction. In this study an orthokinetic kernel $\beta(x-x',x)$ was borrowed from Spicer and Pratsinis (1996a):

$$\beta(x-x',x) = 0.31\bar{G}[(x-x')^{1/3}+x^{1/3}]^3 \quad (3)$$

α was chosen to be a constant between 0 and 1. In the latter case, all collisions are considered to be successful. Other aggregation efficiency expressions are available in literature (Adler, 1981; Ducoste, 2002; Kusters, Wijers, & Thoenes, 1997) but not considered here since this was not the goal of this work.

Breakage models typically look like (Ramkrishna, 2000):

$$h(x,t)_{\text{break}} = \int_x^\infty n(x',t)S(x')v(x')\Gamma(x,x')\,\mathrm{d}x' - n(x,t)S(x) \quad (4)$$

where $S(x)$ is the breakage rate of particles of size $x\,(s^{-1})$, $v(x')$ the average number of particles resulting from a breakage event and $\Gamma(x,x')$ the breakage distribution function. $S(x)$ was assumed to be a power law (Spicer & Pratsinis, 1996b):

$$S(x) = Ax^a \quad (5)$$

where a is a constant (=1/3) and A is the breakage rate coefficient $(L^{-1}\cdot T^{-1})$. Binary breakage into equally sized daughters is assumed

$$v(x')\Gamma(x,x') = 2\delta(x-\tfrac{1}{2}x') \quad (6)$$

Other more complex breakage functions can be found in literature (Ducoste, 2002; Konno, Aoki, & Saito, 1983; Kramer & Clark, 1999; Vanni, 2000) but were not considered in this particular study focusing on solution methods.

3. Discretisation techniques

In this study, three different discretisation techniques were compared: (1) the method of Hounslow et al. (1988), (2) the fixed pivot technique (Kumar & Ramkrishna, 1996a) and the moving pivot technique (Kumar & Ramkrishna, 1996b). In this section the different methods are briefly presented.

3.1. The method of Hounslow

Hounslow et al. (1988) used a geometric grid with factor 2 based on volume ($v_{i+1}=2v_i$, with v the particle volume) and were the first to develop a set of equations conserving both numbers and mass for purely aggregating systems:

$$\frac{\mathrm{d}N_i}{\mathrm{d}t} = N_{i-1}\sum_{j=1}^{i-2}2^{j-i+1}\beta_{i-1,j}N_j + \frac{1}{2}\beta_{i-1,i-1}N_{i-1}^2 - N_i\sum_{j=1}^{i-1}2^{j-i}\beta_{i,j}N_j - N_i\sum_{j=i}^{\infty}\beta_{i,j}N_j \quad (7)$$

Litster et al. (1995) expanded the method for finer geometric grids, whereas Hill and Ng (1995) developed similar equations for breakup and finer grids. The main disadvantage of these methods is their inflexibility in terms of grid and conservation of distribution properties, which is restricted to numbers and mass. When the properties of interest are different, new equations need to be derived from scratch which is quite straightforward but time consuming.