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An improved and efficient finite volume scheme for bivariate aggregation population balance equation

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ABSTRACT

In this work, a finite volume scheme for the numerical solution of bivariate pure aggregation population balance equations on non-uniform meshes is derived. The new method has a simple mathematical structure and it provides high accuracy with respect to the number density distribution as well as different moments. The method relies on weights to conserve the total mass of the system. The new method is compared to a recently developed finite volume scheme by Forestier-Coste and Mancini (2012) for some selected benchmark problems. It is shown that the proposed method is not only computationally more efficient but also more accurate than the method by Forestier-Coste and Mancini (2012).

1. Introduction

Aggregation is a formation process in which at least two individual (primary) objects form a new object, called the aggregate. In this formation process, which can be due to various physical effects, some properties of the individual objects are conserved in the aggregate, e.g., mass, whereas other properties may change, for instance the size or shape of the aggregate. Aggregation is a size enlargement process that takes place in many technical applications or natural phenomena, e.g., rain formation from tiny cloud drops, formation of polymers from monomers, production of instant food materials, as well as in biological processes or in astronomy [1–5].

In applications, aggregation may be a desired effect as in the examples stated above, however, it can also be an undesired effect, e.g., the instant and flow behavior of food granules will initially improve with increasing agglomerate size but beyond a composition-dependent limit size it will decrease again. Due to its importance in many industries, there is a need for understanding and predicting aggregate formation—not only on single particle level, but also on apparatus and plant level. On apparatus and plant level, the population balance framework [6] is usually used to study the dynamics of aggregate formation.

In solids processing, e.g., in foods and pharmaceuticals, product quality is characterized by multiple particle properties, for example the volume and composition of aggregating particles. In the following, the bivariate case is considered, i.e., particles (or individual objects) are characterized by two properties, named x and y.

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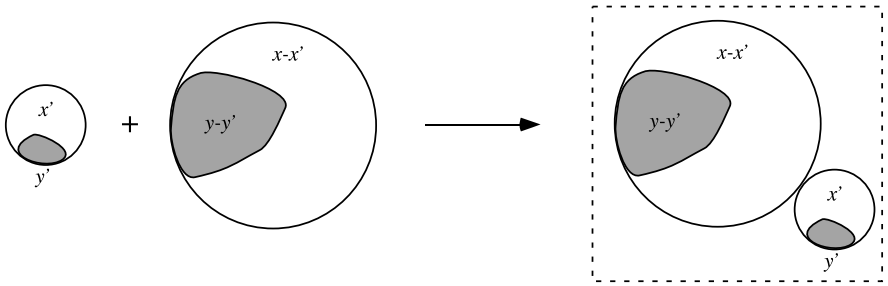

Fig. 1. Schematic depiction of bivariate aggregation by binary collision.

Aggregation is taking place in a well-mixed apparatus, i.e., neglecting spatial dependencies, the bivariate population balance equation (PBE) is written as

$$\frac{\partial f(t,x,y)}{\partial t} = \frac{1}{2}\int_0^x \int_0^y \beta(t,x-x',y-y',x',y')f(t,x-x',y-y')f(t,x',y')dx'dy' - \int_0^\infty \int_0^\infty \beta(t,x,y,x',y')f(t,x,y)f(t,x',y')\,dx'dy', \tag{1}$$

with initial data

$$f(0,x,y) = f_0(x,y), \quad x,y \in]0,\infty[.$$

Here, $f(t,x,y)$ is the number density distribution of particles having properties $x > 0$ and $y > 0$ at time $t \geq 0$, i.e., the number of particles in the infinitesimal range $[x, x+dx] \times [y, y+dy]$ at any time t is given by $f(t,x,y)\,dx\,dy$. The bivariate aggregation process is depicted schematically in Fig. 1.

The first term on the right hand side of Eq. (1) corresponds to the birth of particles with properties (x,y) due to the aggregation of particles with properties $(x-x', y-y')$ and (x',y'). Similarly, the second term describes the loss of particles having properties (x,y) due to the collision with particles having properties (x',y'). The aggregation kernel $\beta(t,x,x',y,y')$ describes the kinetics of successful collision of two particles with properties (x,y) and (x',y'). It is a non-negative function and is symmetric in its arguments. The structure of the kernel can be arbitrarily complex; often used simple expressions are of the form $\beta = \beta_0(t)\beta^*(x,x',y,y')$. In case of $\beta^*(x',x,y,y') = 1$, the kernel is named as the constant kernel; in case of $\beta^*(x,x',y,y') = (x+x') + (y+y')$, it is called the sum kernel; and the structure $\beta^*(x,x',y,y') = (x\,x')(y\,y')$ is called multiplicative kernel. The pre-factor $\beta_0(t)$ is interpreted as a collision efficiency, accounting for all other process conditions.

In applications, integral properties of the number density function f are also of importance, for instance total number and total volume of particles. These can be obtained from moments of a given number density function. The ijth moment of the distribution f is defined by

$$\mu_{ij}(t) = \int_0^\infty \int_0^\infty x^i y^j f(t,x,y)\,dxdy. \tag{2}$$

In most applications i and j are integers, i.e., $i,j = 0, 1, 2, \ldots$, however, depending on the interpretation of the properties x and y, fractional order moments are also of interest. The order of a moment is given by the sum of the indices i and j: $i+j$. The zeroth order moment μ_{00} represents the total number of particles in the system. If, e.g., x and y are interpreted as masses of two components in a particle, then the first order moments μ_{10} and μ_{01} can be interpreted as the total mass of the individual components. Note, that there are two first-order moments (μ_{10} & μ_{01}); there are three second-order moments (μ_{20}, μ_{11} & μ_{02}), and so on.

The bivariate aggregation PBE (1) is a non-linear integro-differential equation, for which explicit solutions are known only for some simple kernels. Therefore, in order to study bivariate aggregation processes in real life applications, numerical methods have to be used to get the dynamics of these processes. So far, several numerical methods have been proposed, including finite difference methods [7], finite element methods [8,9], finite volume schemes [10–12], direct quadrature method of moments [13–16] or sectional methods like the fixed pivot technique (FPT) [17,18] and cell average technique (CAT) [19,20].

It is established in the literature that the sectional methods do not only produce highly accurate results for different moments but also provide accurate approximations to the number density distributions. Initially, FPT and CAT were formulated for rectangular grids (Fig. 2). Later, Chakraborty and Kumar [21] extended FPT to triangular grids (see Fig. 3) and found that the results obtained were in better agreement with the analytical results. Following, Kumar et al. [22] extended CAT to triangular grids and concluded the similar observation. Other applications of sectional methods can be found in [23–27]. Although sectional methods provide accurate results for number density as well as different order moments, their formulations are quite complex; rendering these techniques computationally expensive.