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A comparative study of different discretizations for solving bivariate aggregation population balance equation

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ABSTRACT

In this work, a comparative study on how the solution of a pure bivariate aggregation population balance equation depends on different structured grids is presented. Numerical results obtained using the most commonly used cell average and fixed pivot techniques on four different types of structured grids are compared with the exact solutions. As expected, the cell average technique predicts more accurate solution than the fixed pivot technique for all different grids. Moreover, the results predicted using the cell average technique using X-type grid with logarithmic scale in the radial direction provide solutions of high quality among all other grids.

1. Introduction

Population balance equations (PBE) describe changes of number density in a particulate system. Very often in applications, two or more properties are required to characterize a particle and thus multidimensional population balance equations are needed to model such systems. Many applications of multidimensional population balance equations like crystallization, liquid–liquid contraction, fluidized bed, etc. can be found in the literature, see [21] and references therein. Moreover, engineers most extensively use population balances to model and optimize several processes like liquid–liquid extraction, leaching, polymerization etc. Population balance equations are integro-partial differential equations and the solution of such equations depends solely on how the property domain is discretized.

In this work, we consider two dimensional pure aggregation population balance equation in a well mixed system given by Hulburt and Katz [9] as:

$$\frac{\partial f(\mathbf{x},t)}{\partial t} = \frac{1}{2}\int_0^{\mathbf{x}} \beta(\mathbf{x}-\mathbf{x}',\mathbf{x}',t)f(\mathbf{x}-\mathbf{x}',t)f(\mathbf{x}',t)d\mathbf{x}' - \int_0^{\infty} \beta(\mathbf{x},\mathbf{x}',t)f(\mathbf{x},t)f(\mathbf{x}',t)d\mathbf{x}'; \quad t \in [0,\infty). \tag{1}$$

Whereas $f(\mathbf{x},t)$ is the transient number density distribution and $\mathbf{x}$ is the particle state vector given in terms of some additive properties like mass or volume. Each component of the vector $\mathbf{x}$ lies in the interval $[0,\infty)$. The bold notations are used to denote vector quantities. Here the aggregation kernel β describes the rate at which two particles of state vectors $\mathbf{x}$ and $\mathbf{x}'$ aggregate. The first term on the right hand side of Eq. (1) corresponds to the birth of particles of properties $\mathbf{x}$ due to the aggregation of smaller particles of properties $\mathbf{x}-\mathbf{x}'$ and $\mathbf{x}'$. Similarly, the second term describes the death of particles having properties $\mathbf{x}$ due to the collision of particles having properties $\mathbf{x}'$. Not only the property distribution f, we are also interested in some integral properties like moments. The ijth moment of the particle size distribution is defined as

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

where the zeroth moment μ_{00} denotes the total number of particles and μ_{10} or μ_{01} usually denotes the total mass of particles in the system.

Numerical solution of the PBE (1) is difficult due to the presence of complex double integral and the non-linearity of the equation. Earlier, the analytical solution of PBE were found by Gelbard and Seinfeld [8] and Fernández-Díaz and Gómez-García [7] for simple kernels like constant and sum, respectively. Therefore, numerical techniques have been proved to be very essential in solving these equations. Many authors proposed different techniques in the literature to solve 2-D PBE including finite difference method [22], finite element method [10,1], Monte Carlo method [18], finite volume schemes [20], Galerkin's method [2], sectional methods [16,12] and method of moments [24,3]. Among various techniques, sectional methods are very popular for their speed and accuracy [17,13,11]. However, the solution obtained using sectional methods depend on how the property domain is discretized, [23]. In particular, accuracy of solution of a PBE highly depends on the shape and orientation of triangular elements.

In sectional methods, the continuous number density is represented by fixed discrete 'pivots' obtained after discretization of the given domain. One of the most popular methods in this category known as the fixed pivot technique [16]. This method was further extended to solve two dimensional PBE by Vale and McKenna [25] using rectangular grids. Later, Kumar et al. [12] presented a new technique based on averaging of particle properties over the discretized rectangular bin (see Fig. 1) around a pivot. This method is well known as the cell average technique. It was also reported by Kumar et al. [12] that the results obtained by the cell average technique (CAT) were better than the fixed pivot technique (FPT) on rectangular grid.

Chakraborty and Kumar [4] proposed a new framework to discretize two dimensional PBEs using triangular grids known as *minimum internal consistency*. It was proved that for solving a n-D PBE, $n+1$ surrounding neighbors were required to represent a non-pivot particle instead of 2^n pivots reported earlier in the literature by Vale and McKenna [25] as well as Kumar et al. [12]. Several research articles like Nandanwar and Kumar [19] and Chauhan et al. [5] have identified this as a smarter space discretization. Nandanwar and Kumar [19] also established FPT for the 2-D PBE using radial grids formed by section of radial lines starting from origin and arcs of increasing radii. Later, Kumar et al. [15] applied the CAT on triangular grids obtained by slicing the rectangular grids across and along diagonal (Fig. 2) and found very accurate results. Furthermore, Chauhan et al. [6] have also used FPT on X-Type grids for solving 2-D aggregation PBE. Recently, Singh et al. [23] developed CAT for the unstructured grids and realized that a suitable grid refinement leads to provide a very accurate and efficient solution of bivariate PBE.

As mentioned before, Singh et al. [23] concluded that the cell averaging with improved irregular triangular grid is one of the smartest numerical techniques. Moreover, working with irregular grid are advantageous over regular triangular grid because it serves to refine the grid to any desired location. However, the irregular grid is not easy to produce and handle as reported in [23]. Chakraborty and Kumar [4] as well as in Singh et al. [23], irregular grids were generated by Fluent and stretched the grid to cover several orders of magnitude.

Recent development of various different structured grids by Nandanwar and Kumar [19] and Chauhan et al. [6] has led to renewed interest in performing a comparative study of numerical solutions on different structured grids. Few attempts have been made to check performance of the cell average as well as fixed pivot techniques on different structured grids. Comparative study of [12] was limited to only two different types of triangular grids. Therefore, the aim of this work is to provide a

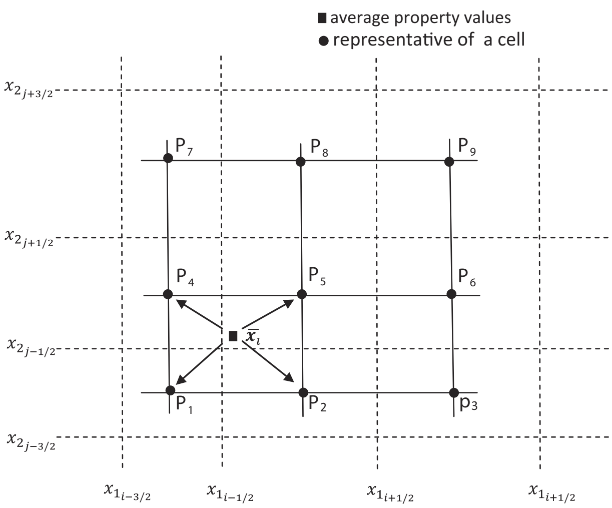

Fig. 1. Particles assignment to four neighboring notes in a rectangular partitioning of the domain.