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Accurate void fraction calculation for three-dimensional discrete particle model on unstructured mesh

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ABSTRACT

An accurate and efficient analytical method for computing the three-dimensional local void fraction is proposed in the context of discrete particle modeling. It is developed for the general case of unstructured meshes whose use is unavoidable to efficiently simulate modern gas–solid fluidized bed reactors characterized by complex geometries. The method relates the three-dimensional void fraction to several geometrical parameters. This allows the exact voidage evaluation for the frequently occurring case of having particles not wholly contained within one grid cell regardless its shape. Failing to accurately account for these common particle configurations in dense gas–particle systems has proven detrimental to the accuracy of their simulations.

1. Introduction

Discrete particle models (DPMs) coupled to a finite volume description of the gas-phase dynamics have been used in a panoply of chemical and petrochemical applications since they were first introduced by Tsuji et al. (1993) for the soft-sphere version and Hoomans et al. (1996) for the hard-sphere approach. Using DPMs, the particle motion is resolved at such a particle scale that many important features related to the particle motion in gas–solid systems could be reasonably captured. Many parameters contribute to the level of accuracy of the DPMs, such as the restitution and friction coefficients for the hard-sphere version and stiffness and damping coefficients for the soft-sphere version. In addition, the void fraction should be accurately determined since the empirical or theoretical relations that describe gas–solid interactions are found to be strongly dependent on it. Also, in discrete particle modeling the solid particles occupy part of the gas-phase volume and this is incorporated in the conservation equations of the fluid phase through multiplying all the gas properties by the void fraction. Therefore inaccurate computation of the void fraction would adversely affect the general performance of the model.

Early DPM studies were based on the two-dimensional (2D) model using structured regular grids. The voidage ε_{2D} in 2D DPMs is calculated according to the space or area occupied by the particles in the 2D grid cells. This is not consistent with the empirical drag formula in which the correlated porosity ε_{3D} is derived for real three-dimensional (3D) systems. To correct this inconsistency, two strategies have been used to transform the 2D porosity. The first one was suggested by Hoomans et al. (1996) and it is described by the following equation:

$$\varepsilon_{3D} = 1 - \frac{2}{\sqrt{\pi\sqrt{3}}}(1-\varepsilon_{2D})^{3/2} \tag{1}$$

This equation was derived on the basis of a comparison between a 2D hexagonal lattice and a 3D cubic lattice assuming equal interparticle distances. Ouyang and Li (1999) gave a formula similar to the above. The second strategy was presented by Xu and Yu (1997), and it gives

$$\varepsilon_{3D} = 1 - \frac{\sum V_i}{\Delta V} \tag{2}$$

where V_i is the volume of particle i, and the summation is taken over all the particles in the cell volume $\Delta V = \Delta x \Delta y d_p$, which means the 2D domain is regarded as a pseudo-3D one with a thickness of one particle diameter, d_p. Van Wachem et al. (2001) introduced an empirical parameter containing the maximum experimental solids packing in practice. They gave a slightly different equation from the one given by Hoomans et al. (1996). Their numerical results indicated that the 2D discrete particle simulations are sensitive to the porosity estimation strategies.

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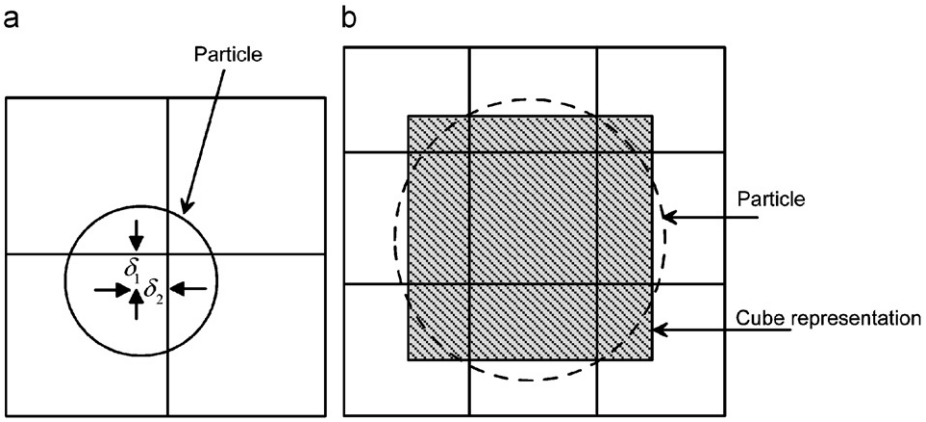

Fig. 1. Approximate method to calculate the 2D and 3D porosity (2DAM and 3DAM).

With the massive increase in the computing capacities, 3D DPMs have become tractable for the simulation of gas–solid flows in complex domains such as cylindrical beds, tapered beds, or flat beds with immersed tubes or baffles. For such complex system geometries, the use of unstructured grids is more appropriate. It is in many cases the only possibility to avoid unnecessary high resolution and to locally accommodate the mesh to the complicated geometry boundaries. The use of unstructured grids constitutes a challenge when it comes to the estimation of the void fraction for both 2D and 3D DPMs, in particular when particles are not fully contained in one cell that can have any shape (wedged, tetrahedral, or hexahedral) and/or can intersect particles through any of its boundaries (node, edge, or face). Indeed, when the center of a particle locates on an edge shared by two 2D cells or on a face shared by two 3D cells, there will be considerable errors in the calculated porosity if the volume of this particle is not accurately shared between these two cells. If the cell volume is 20 times that of the particle, for example, neglecting the share of the particle volume between two cells results in particle volume fractions of 0.05 and 0. This represents a 50% relative error or 2.5% absolute error in the volume fraction. Since the porosity plays a very important role in the local mass and momentum balance of the gas phase, the said errors should be avoided as far as possible.

In case of 2D square cells, the particle area shared by the four neighboring cells can be calculated approximately as follows (see Fig. 1a):

$$A_i = \frac{\pi}{4}(r_p \pm \delta_1)(r_p \pm \delta_2) \quad (i = 1, 2, 3, 4) \tag{3}$$

where r_p is the particle radius. We refer to this approach as the 2D approximate method (2DAM). In case of 3D cubic cells, Darmana et al. (2005) give the following formula for the particle volume (see Fig. 1b):

$$V_i = \zeta_i V_p \tag{4}$$

where V_p is the particle volume. The particle is treated as a cube and ζ_i is the cube volume fraction in the cell under consideration (hereafter referred to as the 3D approximate method, 3DAM).

The use of the above two methods is limited to regular structured grids. They are relatively simple to apply yet inaccurate. For solution domain discretized by unstructured grids, an approach named point approximate method (PAM) is often used. In this approach, the particle shape is omitted and the particle is considered as a point. Thus, the split of particles between cells is neglected and particles are considered to belong only to one cell.

In the following two sections, an analytical method to calculate the void fraction for general unstructured meshes is proposed. It is developed for cells of different shapes (wedged, tetrahedral, or hexahedral) and for different particle–cell intersections (node, edge, or face). It is validated in the context of discrete particle simulations of 3D dense gas–particle systems and its numerical efficiency is improved using the look-up table strategy. The method is detailed for the 2D and 3D configurations separately.

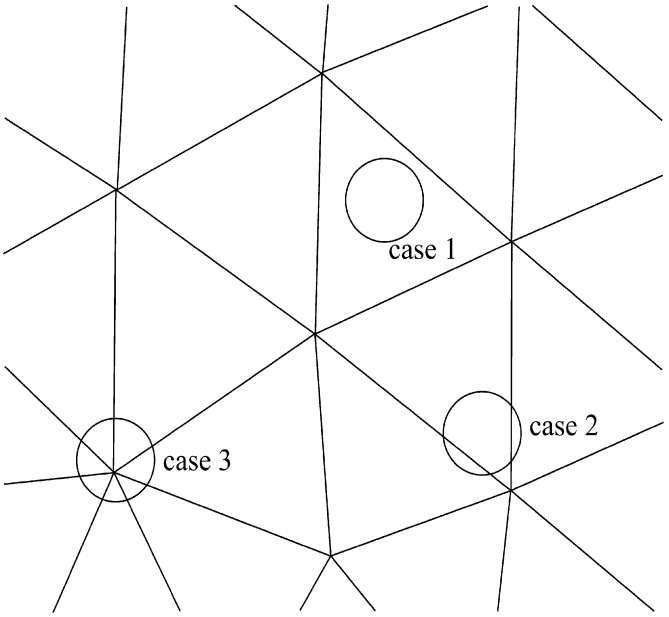

Fig. 2. Different particle positions in an unstructured 2D grid.

2. The 2D case

The 2D unstructured mesh is often composed of triangular, quadrilateral cells, or combinations of these two geometrical entities. All possible particle–cell intersections can be studied using three generic cases as it is depicted in Fig. 2. The covered area is the full particle area for case (1). It is calculated for case (2) once the intersection points between the edges of the cell and the particle circumference are located. Case (3) is more complex. Hereafter we call C_0 the cell that hosts the center (O) of the particle while the other cells that share the said particle are denoted by C_n ($n = 1, 2, \ldots$) as depicted in Fig. 3. The corresponding areas that the said particle occupies in these cells are denoted by A_0 and A_n ($n = 1, 2, \ldots$),