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Direct calculation of voidage in the fine-grid CFD–DEM simulation of fluidized beds with large particles

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ABSTRACT

Voidage is important in determining the hydrodynamic behavior of a fluidized bed and estimating the drag force. Exact calculation methods are limited, especially in terms of determining the intersection of a particle and cell. This paper presents a method of directly calculating voidage. First, a judgment criterion of particle–cell overlap, which relies on the relationship of the distance from the particle to a cell face, edge, or vertex, is proposed. Eight cases of the overlap volume of a particle and cell are then ascribed to a unified formula in the framework of the cuboid cell. This formula relies on the volume of two kinds of segments named the hemispherical segment and quarter-spherical segment. The presented method is validated by calculating the voidage of simple cubic packing. Moreover, a three-dimensional fluidized bed with large particles is simulated and the results of numerical simulation are compared against experimental and simulation results reported in the literature. All numerical results are in good agreement with corresponding experimental data, and demonstrate the accuracy and reliability of the presented method in the three-dimensional simulation of fluidized beds.

Introduction

The combination of computational fluid dynamics and the discrete element method (CFD–DEM) has been shown to well predict gas–solid flows in recent years (Ebrahimi & Crapper, 2017; Link, Cuypers, Deen, & Kuipers, 2005; Tsuji, Yabumoto, & Tanaka, 2008; Tsuji, Kawaguchi, & Tanaka, 1993; Xu & Yu, 1997; Xu, Zhong, Yuan, & Yu, 2017; Xu, Ge, & Li, 2007; Zhu, Zhou, Yang, & Yu, 2008). The two phases are coupled by the fluid–particle force (i.e., drag force), which is computed using a correlation. In CFD–DEM simulations, one critical parameter is the voidage, which not only is incorporated in the governing equations of the gas phase but also affects the accuracy of the drag force. The accurate calculation of voidage is thus essential.

The voidage ε_g defined as the ratio of the gas volume within one grid cell is often calculated according to the volume occupied by the solid phase (i.e., $\varepsilon_g = (V_{cell} - V_{solid})/V_{cell} = 1.0 - \varepsilon_s$, where V_{cell} is the volume of the computational cell, V_{solid} is the sum of all particle volumes in the cell, and ε_s is the solid volume fraction). Different methods have been applied to compute the voidage: e.g., the particle centroid method (PCM) (Alobaid & Epple, 2013; Alobaid, Ströhle, & Epple, 2013; Wu, Ouyang, Yang, & Li, 2013; Zhao & Shan, 2013), non-analytical method (Freireich, Kodam, & Wassgren, 2010; Hilton, Mason, & Cleary, 2010; Khawaja, Scott, Virk, & Moatamedi, 2012; Link et al., 2005; Natsui et al., 2011; Okaya, Sadaki, & Fujita, 2008), and analytical method.

Each method has its own advantages and disadvantages. The PCM has a lower computational cost as it only requires searching of the particle centroid host cell. However, the PCM may introduce errors as high as 50% (Peng, Doroodchi, Luo, & Moghtaderi, 2014) when the particle centroid is near the cell boundary and the cell is not large enough. Such large errors eventually result in an incorrect voidage and impractical behavior in simulation. Nonanalytical methods can handle complex domains and/or nonspherical particles with the sacrifice of accuracy.

Analytical methods have been proposed to accurately calculate voidage, where the actual volume of particles in each cell is exactly calculated by means of the geometrical relationships between the particles and cell. Hoomans, Kuipers, Briels, and Van Swaaij (1996) accounted for partial areas using square cells with circular particles and used a formula for translation from two-dimensional (2D) porosity to three-dimensional (3D) porosity in their 2D simulations of a fluidized bed. Wu and Ouyang (2015) proposed a 3D porosity model in fine-grid DEM simulation. 3D analytical expressions for

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Nomenclature

C_d	drag coefficient
d_p	particle diameter (m)
$\mathbf{F}_c$	collision force (N)
$\mathbf{F}_p$	momentum exchange term (N/m^3)
$\mathbf{g}$	gravity vector (m/s^2)
l_{fij}	distance from the center of the ith particle to the jth face (m)
l_{eik}	distance from the center of the ith particle to the kth edge (m)
l_{vik}	distance from the center of the ith particle to the lth vertex (m)
l_{fx}, l_{fy}, l_{fz}	distances from the particle centroid to the cell faces that correspond to the x, y, and z axes (m)
l_{ex}, l_{ey}, l_{ez}	distances from the particle centroid to the cell edges that correspond to the x, y, and z axes (m)
l_v	distance from the particle centroid to the cell vertex (m)
m_p	mass of particle (kg)
$\mathbf{n}=(A, B, C)$	normal vector of the jth face
p	pressure (Pa)
Re	particle Reynolds number
R	particle radius (m)
X_i, Y_i, Z_i	center coordinates of the ith particle
x_{il}, y_{il}, z_{il}	vertex coordinates of the main cell containing the ith particle
$\mathbf{u}$	gas velocity (m/s)
V_{cell}	volume of the gas cell (m^3)
V_{fx}, V_{fy}, V_{fz}	volumes of the spherical segment along the x, y, and z axes (m^3)
V_{ex}, V_{ey}, V_{ez}	volumes of the hemispherical segments that correspond to the x, y, and z axes (m^3)
V_f	sum of the volume of spherical segments belonging to one sphere (m^3)
V_e	sum of the volume of hemispherical segments belonging to one sphere (m^3)
$\mathbf{v}_p$	particle velocity (m/s)
V_p	exact partial volume inside the main cell (m^3)
V_{sphere}	volume of particle (m^3)
V_{solid}	sum of all particle volumes in the gas cell (m^3)
V_v	volume of the quarter-spherical segment (m^3)

Greek symbols

ρ_g	gas density (kg/m^3)
τ_g	viscosity stress tensor (Pa)
μ_g	gas viscosity (kg/(m s))
β	interphase momentum exchange coefficient (N/m^3)
ε_g	ratio of the gas volume within one grid cell
ε_s	solid volume fraction
ε_{sphere}	ratio of the spherical volume within one grid cell
ε_f	ratio of the spherical segment volume within one grid cell
ε_e	ratio of the hemispherical segment volume within one grid cell
ε_v	ratio of the quarter-spherical segment volume within one grid cell

Superscripts and subscripts

x, y, z	x, y, z axes
i	ith particle
s	solid
p	particle
n	number of particles in a cell
j, k, l	indices of cell faces, edges, and vertices
ij, ik, il	center of the ith particle to the jth cell face, kth cell edge, lth cell vertex

Abbreviations

SCP	simple cubic packing
PCM	particle centroid method

each scenario of the particle–cell geometrical relation in structured rectangular cells were detailed by Peng, Doroodchi et al. (2014). However, they mainly discussed the effect of the cell size selection and the corresponding method for voidage calculation. An analytical method for the cell void fraction on 2D and 3D unstructured meshes was developed by (Wu, Berrouk, & Nandakumar, 2009; Wu, Zhan, Li, Lam, & Berrouk, 2009) for the discrete particle model. However, the implementation of their approach was difficult and time consuming.

To capture the mesoscale structure of gas–solid fluidized beds, the grid size used in the numerical simulation should be sufficiently small (Wang, Van der Hoef, & Kuipers, 2009). There is thus a need to develop a method of accurately calculating the voidage in fine-grid CFD–DEM simulations. The present paper proposes an easily implemented direct method of calculating voidage. The case of particle–cell overlap is important to the accurate calculation of voidage. To the best of our knowledge, there has been no study on how to judge the particle–cell overlap. The present work therefore gives a judgment criterion of spherical particle cell overlap derived from the distance relationship of nodes, lines, and planes. Eight cases of particle cuboid cell overlap are then demonstrated. The solutions of all cases of the overlap volume of the particle and cell are ascribed to a unified formula by the combination relations of a partial sphere, which requires the volumes of two kinds of special segments. To test the validity of the presented method, the voidage of the unit cell of simple cubic packing (SCP) is solved and compared with the analytical and PCM results. Moreover, a 3D fluidized bed with large particles is used to illustrate the extended application and accuracy of the presented method.

Direct calculation of voidage

The following analysis assumes the particle to be a sphere with radius R. When the particle centroid is near a cell boundary, the particle volume is divided into two sub-volumes: the volume inside the cell and the volume outside it. The judgment criterion of particle–cell overlap is therefore vital for determining the actual particle volume inside the cell. Subsequently, this paper focuses on all cases of particle cuboid cell overlap and solves the overlap volume of all cases using a unified formula.

Judgment criterion of particle–cell overlap

We give a judgment criterion of particle–cell overlap based on Cartesian geometry. The judgment criterion relies on the relationship between particle radius R and l_{fij}, R and l_{eik}, and R and l_{vil}, where l_{fij}, l_{eik} and l_{vil} are respectively the shortest lengths from the center of the ith particle to the jth cell face, to kth cell edge and lth cell vertex.

The centroid coordinates of particles are denoted (X_i, Y_i, Z_i) $(i = 1, 2, \ldots, N)$. Generally, the particle centroid should be included in one cell that is named the main cell once the mesh is generated; if (X_i, Y_i, Z_i) lies on a cell vertex, edge, or plane, we randomly choose a cell as the main cell from the corresponding cells. We then suppose the vertex coordinates of the main cell are (X_{il}, Y_{il}, Z_{il}), where l denotes the number of vertices of the main cell; e.g., the cuboid cell $l = 1$,

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