Elementary-Volume-Scale Simulations of Inertial Flow in Sphere Pack: Improvement of Di Felice Drag Model in High Porosity

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In this study, we studied the elementary volume (EV) size in pore scale simulations of flow in sphere packs and evaluated existing drag models in wide porosity range. The EV size in different porosities were modeled with the discrete-element method. Through a parametric study, we confirmed that as the EV size grows large, the simulated values of porosity, permeability and hydraulic tortuosity nearly converge to their respective constants. This trend agrees well with previously reported experimental and numerical results. Using the EV size determined by the parametric study, we simulated the inertial flow in sphere packs of porosity range between 0.3 and 0.95. We found that the simulated drag force disagreed drastically with the existing drag models for high porosity range. Accordingly, we improved the Di Felice equation suitable in high porosity range. [doi:10.2320/matertrans.M-M20208099]

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1. Introduction

Fluid-solid multiphase flow plays an important role in the powder processing in various industries. As an example in material sorting in mineral processing, density separator, such as jig separator and fluidized bed separator, separate particles depending on density by the differences in particles’ translation velocity caused by fluid drag forces. The motion of particles in fluid flows is complex and is difficult to evaluate quantitatively with conventional laboratory tests alone.

To analyze fluid-solid multiphase flows, simulations coupled with computational fluid dynamics (CFD) and the discrete-element method (DEM) have been employed in past studies. Coarse-grid and fine-grid approaches are available for grid-based CFD-DEM coupling. In this study, we focus on the coarse-grid approach. In CFD-DEM coupling, the motion of fluids is calculated by CFD and the motion of particles is calculated by DEM. Fluid-particle interaction forces are calculated using the fluid drag model, meaning that the motion of fluids and particles depends strongly on the drag model used.

The Ergun equations and Di Felice equations are often used to model drag forces in conventional CFD-DEM coupling simulations. The Ergun equation cannot be used in the high porosity range; hence, a combination of the Ergun and Wen-Yu equations, the latter being a drag model for high porosity flows, has been used in the past studies. This combination is referred to as the Ergun-Wen-Yu equation. This equation calculates the drag force using the Ergun equation for porosities lower than 0.8. When the porosity becomes higher than 0.8, the Wen-Yu equation is used instead of the Ergun equation. The Di Felice equation is not limited by porosity, and it has been used successfully in CFD-DEM coupling simulations. However, Di Felice determined the parameter values in his model from laboratory tests with a porosity of around 0.4. Particle packs with a porosity of around 0.4 behave like a solid, but packed particles can be fluidized in the high porosity range. Makkawi and Wright conducted fluidized bed experiment and reported that the measured parameter value in Di Felice equation disagreed with that predicted by the Di Felice equation. The parameters for the Di Felice equation to describe high porosity flows are difficult to determine in laboratory tests because the porosity of fluidized particles varies constantly during an experiment.

Pore-scale flow simulation (PFS) technology makes it possible to directly simulate flows in particle packs. The PFS using particle packs generated by DEM have been proposed in past studies and enables us to simulate the flow in sphere packs in the high porosity range. Many of the past studies used a small-scale volume element, i.e., elementary volume (EV) of the particles pack, and its size quantifies by the ratio of a side of cubic 3D-structure to the particle diameter \( L/D \). The smallest EV size that can simulate the response of laboratory experiment can be referred to as representative elementary volume (REV). The past studies reported that the EV size considerably influences the results of PFSs; however, they targeted at granular “solid”, i.e., the porosity of around 0.4. The porosity can increase during the density separation process, e.g., the past studies have reported that the porosity in jig separation can vary between 0.4 to 0.627 and that in fluidized bed separation can reach up to 0.9 near the head of fluidized particles. This fact implies that the conventional Di Felice equation should not be applicable in high porosity range.

Beestra et al. has conducted a pioneering work to evaluate an applicability of Di Felice equation in high porosity range by the PFSs using sphere packs generated by Monte-Carlo method. They found that the Di Felice equation disagreed with their simulations of porosity higher than 0.4 and proposed a novel empirical equation. The \( L/D \) has ranged between 3.6 and 6.5 in the PFSs by Beestra et al. The \( L/D \) values used have not been justified in the study of Beestra et al. Moreover, studies that determine the REV for the high porosity range are lacking in the literature.

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In this study, we evaluate the EV size for simulations of flow in sphere packs with a porosity higher than 0.4. Particle packs with porosities of 0.3, 0.4, 0.5, 0.6, and 0.7 were generated by DEM. Then, the EV size was varied systematically, conducting a series of PFSs to evaluate the influence of EV size on porosity, permeability, and hydraulic tortuosity. Using the EV size determined, we conducted simulations in the inertial flow regime. Fluid drag forces were calculated from the simulations, and then they were compared quantitatively with those estimated by the Di Felice equation and also the existing drag models.

2. Overview of the Simulation Procedure

To simulate flows in sphere packs, we conducted a series of CFD simulations using sphere pack models generated by DEM. The workflow of the simulation procedure is illustrated in Fig. 1. Since the simulation methodology is detailed in the previous study,22) we give only a brief overview in this section.

2.1 Discrete-element modeling of sphere packing

DEM is a simulation method for frictional rigid-particle systems. In this study, we employed a conventional contact model that is comprised of a set of linear springs, local damping, and frictional slider. Following the previous study of Katagiri et al. (2017), the spring constant, damping, and static friction coefficient were set to 1.0 \( \times 10^5 \) N/m, 0.02, and 0.0, respectively.

We modeled monodisperse spheres with a diameter of 0.24 mm. These spheres were generated randomly in cubic domains 8 mm on a side. The porosity (\( \eta \)) of the sphere pack varies with the number of spheres in the model. In the present study, we generated sphere packs of target porosity: \( \eta_T = 0.3, 0.4, 0.5, 0.6, \) and 0.7; the number of spheres was 49,514, 42,441, 35,367, 28,294, and 21,220, respectively.

2.2 Generation of a three-dimensional surface model

The open-source software OpenFOAM was used for CFD analysis. The meshing algorithm in OpenFOAM enabled us to generate calculation meshes for external regions of the 3D surface model with stereolithography (STL). To generate calculation meshes for the void spaces of the sphere packs, we decided to generate STL models of REVs of the sphere packs.

Nakano31) developed software for manipulating image assemblies obtained from X-ray computed tomography (CT) imaging. This software enabled us to convert the image assembly into an STL model. The image assembly is referred to as a 3D image. We first generated a 3D image of a cubic REV of sphere pack, and then the 3D image was converted into an STL model using Nakano’s software.

The 3D image is expressed as an assembly of binary images, in which white and black pixels represent the spheres and void spaces, respectively (see Fig. 1). A cubic region in the DEM domain was partitioned into a lattice with unit length \( 5 \times 10^{-3} \) mm. The value of unit length used was determined on the basis of an evaluation of influence of the unit length on the simulated hydraulic properties in the previous study of Katagiri et al. (2015).22) The partitioned lattices represent pixels in the binary images. If the lattice cell is covered by a sphere, the pixel value is set to 1 (i.e., white). The pixel’s value is zero if the lattice cell is covered by a void. This procedure was repeated for all lattices; as a result, we obtained 3D images of the EV for each sphere packing. The length of a side of the cubic regions is referred to as the model length. We generated nine sets of STL models from the 3D images of model lengths between 0.25 mm and 2 mm.

2.3 Flow simulation

Sphere packs that were generated by the procedure described above have no permeability anisotropy;23) thus, in this study, we simulated the flow along the z-direction only.

We generated calculation meshes for the void space in the STL models. An additional five meshes were included in the STL models at the bottom and top along the z-direction to control the boundary conditions. Constant velocity \( U \) and zero pressure were applied to the bottom and top planes, respectively. A no-slip condition was applied to the other four sides and particle surfaces. The value of \( U \) was set to 0.4 mm/s to yield a Reynolds number (Re) of approximately 0.1. The determination of Re in this study is follows:
where, $D$, $\rho$, and $\mu$ are the sphere’s diameter (0.24 mm), density, and viscosity of water, respectively. The governing equations are steady state Navier-Stokes equations and are as follows:

\[
\nabla : U = 0
\]

(2)

\[
\rho U (\nabla : U) = -\nabla p + \mu \nabla^2 U
\]

(3)

Permeability ($K$) is calculated by Darcy’s law as follows:

\[
\frac{\Delta p}{L} = -\frac{\mu}{K} U
\]

(4)

where, $\Delta p$ and $L$ are the pressure drop due to porous flow and the model length (from 0.25 mm to 2 mm), respectively.

Hydraulic tortuosity ($\tau_h$) quantifies the degree to which streamlines twist and is conventionally determined as the ratio of streamline length to model length. Following the past study, $\tau_h$ was calculated using the following equation:

\[
\tau_h = \frac{\langle u \rangle}{\langle u_w \rangle}
\]

(5)

where $\langle u \rangle$ and $\langle u_w \rangle$ are the volume averages of the magnitude of flow velocity and the velocity component along the flow direction, respectively. Note that $\tau_h$, as calculated using eq. (5), is almost identical to the conventional streamline-based $\tau_e$.33

3. Preliminary Analysis: EV Size Evaluation

3.1 Porosity

The $n$ value is calculated by counting the black and white pixels in the 3D image. The relation between the normalized model length ($L/D$) and $n$ is plotted in Fig. 2. The $n_f$ is the porosity of cubic domains 8 mm on a side. For $L/D$ greater than 2, the values of $n$ tend to converge with their respective constants. When the $L/D$ is greater than about 4.2, the calculated porosities are nearly constant. The relation between the $L/D$ and the measured porosity of glass beads34 is plotted in Fig. 2. The measured value of $n$ will be almost constant if the $L/D$ is greater than about 2.9; this value is in agreement with the value obtained in this study.

3.2 Permeability

The relation between the $L/D$ and $K$ is plotted in Fig. 3. The Kozeny-Carman (KC) equation is a semi-empirical equation to estimate the porosity-permeability relation.35-37

\[
K = \frac{D^2}{180} \frac{n^3}{(1-n)^2}
\]

(6)

Note that eq. (6) assumes (a) cubic sphere packing ($n = 0.486$) and (b) that geometric tortuosity is used instead of $\tau_h$ in the original KC equation developed by Carman.35,36 The lines in Fig. 3 are the estimated $K$ values for $n = 0.4$, 0.5, 0.6 and 0.7. The simulated $K$ values become almost constant when the $L/D$ is greater than 4. The simulated $K$ values for $n = 0.4$ and 0.5 agree well with the KC equation. It is reasonable that the simulated $K$ values for $n = 0.6$ and 0.7 disagree with the KC equation because of assumption (a) which is described in the beginning of this paragraph. Hence, the flow simulation for $L/D > 4$ quantitatively characterizes macroscopic flow in sphere packs.

3.3 Hydraulic tortuosity

The relation between the $L/D$ and $\tau_h$ is plotted in Fig. 4(a). The value of $\tau_h$ becomes nearly constant when the $L/D$ is greater than about 6. The relation between porosity and the simulated $\tau_h$ for $L/D > 6$ is shown in Fig. 4(b). The figure also includes a plot of $\tau_h$ for monodisperse spheres as obtained with Lattice Boltzmann Method simulations39 and the electric tortuosity ($\tau_e$) of glass beads as obtained by the finite-element simulation of electrical resistivity.34 The simulated values of $\tau_h$ agree well with those reported by Matyka and Koza,38 but they are slightly larger than the $\tau_e$ values reported by Saomoto et al.34 This disagreement is explained by differences in $\tau_h$ and $\tau_e$. According to the past study,39 $\tau_h$ and $\tau_e$ are slightly different; $\tau_h < \tau_e$.

The simulated values of $K$ and $\tau_h$ when the $L/D$ is greater than 6 are almost constant and agree well with past studies. $K$ and $\tau_h$ represent the macroscopic and the microscopic characteristics of the flow in the sphere pack; hence, we conclude that PFSs using $L/D > 6$ can quantitatively characterize flows in sphere packs.
4. Inertial Flow Analysis

4.1 Overview of the Di Felice fluid drag model

The fluid-drag force acting on a fixed sphere \( F_D \) in this study is calculated using the following equation:

\[
F_D = C_{D0} \frac{\pi \rho D^2 U^2}{8}
\]

where, \( C_{D0} \) is the drag coefficient. The following equation is commonly used to calculate \( C_{D0} \):

\[
C_{D0} = \left( 0.63 + \frac{4.8}{\sqrt{Re}} \right)^2
\]

According to Di Felice,\(^{11} \) the drag force acting on a sphere from surrounding spheres \( F_D \) is calculated by the following equation:

\[
F_D = F_{D0} \cdot g(n)
\]

where, \( g(n) \) is the voidage function. Di Felice used the following form of the voidage function based on the work of Richardson and Zaki:\(^{40} \)

\[
g(n) = n^{-\chi}
\]

where, \( \chi \) is an empirically determined coefficient. On the basis of past experimental studies, Di Felice proposed the following equation.

\[\chi = 3.7 - 0.65 \exp \left( -\frac{(1.5 - \log Re)^2}{2} \right)\]  

The voidage function using eq. (11) agrees well with the Ergun equation when the porosity is around 0.4.\(^{11} \)

4.2 Validation of simulation

We conducted a series of flow simulations with low to high \( Re \). The \( U \) values were varied between \( 4 \times 10^{-3} \) m/s and 4 m/s, equivalent to \( Re \) values between 0.001 and 1,000. The \( L/D \) of the STL models are 6.25.

Note that the initial sphere configuration can influence the flow characteristics; hence we generated spheres several times to obtain different initial sphere configurations. The values of \( n \) in each sphere configuration are listed in Table 1.

The relation between \( Re \) and the velocity-dependent \( K \) for Run-1 in Table 1 is shown in Fig. 5(a). This velocity-dependent \( K \) is normalized in the figure with respect to the square of the sphere radius \( R = 0.12 \) mm. The \( K \), determined by eq. (6), has been proposed to characterize low \( Re \) flows; however, eq. (6) has also been applied to characterize inertial flows in past study.\(^{41} \) The velocity-dependent \( K \) is almost constant when \( Re \) is lower than 1; for higher \( Re \), it tends to decrease. This trend has also been observed in two-dimensional simulations for \( n = 0.36 \).\(^{41} \)

The simulated \( \Delta p \) for high porosity differs slightly from the prediction of eq. (12) because the Ergun equation is based on experimental results for \( n \) lower than 0.5.\(^{10} \) The simulated \( \Delta p \) for \( n < 0.4 \) agrees well with the Ergun equation, meaning that PFSs using \( L/D = 6.25 \) can effectively model inertial flow in sphere packs.

Table 1 The \( n \) values of STL models with \( L/D = 6.25 \) for the different initial sphere configurations.

<table>
<thead>
<tr>
<th>Target porosity ((n^+))</th>
<th>Run 1</th>
<th>Run 2</th>
<th>Run 3</th>
<th>Run 4</th>
<th>Run 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>0.297</td>
<td>-</td>
<td>0.295</td>
<td>0.301</td>
<td>0.325</td>
</tr>
<tr>
<td>0.4</td>
<td>0.390</td>
<td>0.391</td>
<td>0.389</td>
<td>0.390</td>
<td>0.393</td>
</tr>
<tr>
<td>0.5</td>
<td>0.542</td>
<td>0.484</td>
<td>0.486</td>
<td>0.480</td>
<td>0.442</td>
</tr>
<tr>
<td>0.6</td>
<td>0.569</td>
<td>0.594</td>
<td>0.594</td>
<td>0.594</td>
<td>0.569</td>
</tr>
<tr>
<td>0.7</td>
<td>0.683</td>
<td>0.684</td>
<td>0.684</td>
<td>0.684</td>
<td>0.571</td>
</tr>
<tr>
<td>0.8</td>
<td>0.787</td>
<td>0.830</td>
<td>0.830</td>
<td>0.788</td>
<td>0.700</td>
</tr>
<tr>
<td>0.9</td>
<td>0.888</td>
<td>-</td>
<td>-</td>
<td>0.888</td>
<td>-</td>
</tr>
<tr>
<td>0.95</td>
<td>0.945</td>
<td>0.945</td>
<td>0</td>
<td>0</td>
<td>0.942</td>
</tr>
</tbody>
</table>

The voidage function using eq. (11) agrees well with the Ergun equation when the porosity is around 0.4.\(^{11} \)
4.3 Discussion

The voidage function is calculated using the following equation.11)

$$g(n) = \frac{4}{3C_{D0}} \frac{n}{1 - n} D \Delta p L$$

(13)

Following Di Felice,11) we calculated the value of $\chi$ using eqs. (9) and (13). The relation between Re and $\chi$ is shown in Fig. 6(a). The porosity-dependency of $\chi$ can be predicted by eq. (14) which is detailed as follows. The simulated $\chi$ values for $n \leq 0.4$ in this study and for $n = 0.4$ in the study of Beetstra et al.29) is similar to the values predicted by eq. (11). Contrastingly, we found that the simulated $\chi$ value is drastically different from the eq. (11) for high $n$. This is because eq. (11) is based on laboratory experiments using porous media with $n < 0.5$.

Previous studies have reported that the CFD-DEM coupling simulations agree well with laboratory results even when using the Di Felice equation.15,18) These studies have mainly focused on the time evolution of $n$ due to flow-induced particle removal from the host matrix for $n < 0.4$, and hence they do not require great precision in modeling the motion of the removed particles. However, the motion of the removed particles plays an essential role in material sorting in the fluidized bed separator and the jig separator. Di Felice equation’s underestimation of drag forces has a considerable influence on the particle motion in CFD-DEM coupling simulations. This finding implies that the Di Felice equation needs to be improved if it is to be used to simulate flows in high porosity sphere packs.

On the basis of the discussion above, we propose an improved phenomenological $\chi$ model as follows:

$$\chi = \frac{1}{\phi^2} \left[ 3.7 - 0.65 \exp \left( - \frac{(1.5 - \log Re)^2}{2} \right) \right]$$

(14)

where, $\phi$ is volume fraction: $\phi = 1 - n$. Equation (14) is shown in Fig. 6(a). The porosity-dependency of $\chi$ can be predicted by eq. (14).

The values of $g(n)$ simulated are shown in Fig. 6(b). The original Di Felice equation, the Di Felice equation using eq. (14), Ergun equation, and equation proposed by Beetstra et al. (2007)29) are also plotted in Fig. 6(b). As described above, eq. (11) is based on the laboratory test of $n$ around 0.4; hence the Di Felice equation can accurately predict the simulation results in low to medium porosity. The equations of Di Felice, Ergun and Beetstra et al. underestimate the drag force in high porosity. The proposed model agrees well with the simulated $g(n)$ in high porosity range; this is an advantage of the proposed model.

The past studies have conventionally used the CFD-DEM coupling to understand qualitative behavior of solid-fluid multiphase flow. The conventional CFD-DEM coupling has not focused on faithful reproducibility of real multiphase flow. Several factors can cause the low reproducibility of the
simulation. Among them, one of the most critical issues is that the past CFD-DEM coupling simulations had to use the drag models based on laboratory experiments for low porosity. An advantage of the proposed model is to calculate accurately the drag force for wide porosity range and have a positive impact on simulation accuracy of CFD-DEM coupling analysis. The existing drag models are based on the laboratory experiment in low porosity. Contrastingly, the proposed model is based on the CFD simulations from low to high porosity, and hence is expected to improve the accuracy of CFD-DEM coupling simulation in wide porosity range. This advantage against the existing drag models will lead to computer “virtual” experiment which deepens our understanding of complex powder behavior. The CFD-DEM coupling simulation has been extensively used in powder engineering industry to model fluidized bed, pneumatic conveying and so on. Moreover, powder is frequently used in various industries not only as a raw material but also an end product. The computer virtual experiment enables us to conduct design evaluation test on the computer, which should significantly speed up design and production processes of powder equipment.

5. Conclusion

A series of simulations of flow in sphere packs for $n = 0.4, 0.5, 0.6,$ and 0.7 were conducted to evaluate the influence of EV size on the response of PFSs. When the normalized model length is greater than 6, the simulated values of $n, K,$ and $r_b$ converge to their respective constants. Moreover, the simulated values are almost identical to those reported previously in experimental and numerical studies. Therefore, we conclude that PFSs using a normalized model length greater than 6 can quantitatively characterize the flow in a sphere pack.

We simulated inertial flow in sphere packs for $0.295 \leq n \leq 0.945$ to evaluate the Di Felice fluid drag model. The trend of simulated velocity-dependant $K$ against varying Re is similar to that obtained in a previous study. Moreover, the pressure drop due to flow was almost identical to that predicted by the Ergun equation in the low porosity range. When low $n$, the simulated value of the parameter $\alpha$ agrees well with that estimated by the Di Felice and Beestra et al.\(^{29}\) equations. However, the simulated value of $\chi$ was drastically different from that predicted by such existing equations for middle to high porosity range. We improved $\chi$ model in the Di Felice equation; as a result, we confirmed that the proposed model agreed well with the simulations for wide porosity range, especially for high porosity.

The particles behavior in high porosity is important to understand the powder processing including fluidized bed. In future work, we plan to simulate fluidized bed CFD-DEM coupling simulations using the proposed model and the existing models, and to evaluate the performance of the proposed model.

REFERENCES