Computing drag and interactions between fluid and polydisperse particles in saturated granular materials

Chris Knight, Catherine O’Sullivan, Berend van Wachem, and Daniele Dini

Abstract

Fundamental numerical studies of seepage induced geotechnical instabilities and filtration processes depends on accurate prediction of the forces imparted on the soil grains by the permeating fluid. Hitherto coupled Discrete Element Method (DEM) simulations documented in geomechanics have most often simulated the fluid flow using computational fluid dynamics (CFD) models employing fluid cells that contain a number of particles. Empirical drag models are used to predict the fluid-particle interaction forces using the flow Reynolds number and fluid cell porosity. Experimental verification of the forces predicted by these models at the particle-scale is non-trivial. This contribution uses a high resolution immersed boundary method to model the fluid flow within individual voids in polydisperse samples of spheres to accurately determine the fluid-particle interaction forces. The existing drag models are shown to poorly capture the forces on individual particles in the samples for flow with low Reynolds number values. An alternative approach is proposed in which a radical Voronoi tesselation is applied to estimate a local solids volume fraction for each particle; this local solids fraction can be adopted in combination with existing expressions to estimate the drag force. This tesselation-based approach gives a more accurate prediction of the fluid particle interaction forces.
Notation

\( b \) radius retraction coefficient

BCC body centred cubic packing configuration

\( C_H \) empirical coefficient in the Hazen equation

\( C_u \) coefficient of uniformity

\( D \) particle diameter

\( \langle D \rangle \) Sauter mean diameter

\( D_{10} \) 10% of particles are smaller than \( D_{10} \)

\( D_i \) diameter of particle \( i \)

\( D_{\text{min}} \) minimum particle diameter

\( dA_{i}^{BC} \) area of the surface element on the boundary surface of particle \( i \)

\( D_C \) coarse particle diameter in bimodal simulations

\( D_F \) fine particle diameter in bimodal simulations

\( ds_c \) target element edge length used in the mesh generation process

FCC Face centered cubic packing configuration

\( F_{d}^{\text{corr}} \) drag force calculated using correlation expression

\( F_b \) buoyancy force due to a hydrostatic pressure gradient acting on each particle

\( \overline{F_b} \) \( F_b \) normalized by drag force calculated using Stokes drag expression (magnitude)

\( F_i^b \) buoyancy force due to a hydrostatic pressure gradient acting on particle \( i \)

\( F_d \) drag force acting on each particle

\( \overline{F_d} \) magnitude of drag force normalized by Stokes drag

\( F_{d}^{s} \) drag force calculated using Stokes drag expression

\( F_i^d \) drag force on an individual particle in size class \( i \)

\( \langle F_{d}^{F} \rangle \) mean drag force from the monodisperse expression proposed by Tenneti et al. (2011) for the finer fraction

\( \langle F_{d}^{C} \rangle \) mean drag force from the monodisperse expression proposed by Tenneti et al. (2011) for the coarse fraction

\( F_f \rightarrow s \) total flow induced force acting on each particle

\( \overline{F_f \rightarrow s} \) \( F_f \rightarrow s \) normalized by drag force calculated using Stokes drag expression (magnitude)

\( \langle F_{f \rightarrow s}^{C} \rangle \) average magnitude of the flow induced force acting on the coarse particles
average magnitude of the flow induced force acting on the finer particles

\( \langle F^c_{f-s} \rangle \)

\( F^i_{f-s} \) total flow induced force acting on particle \( i \)

\( F^i_p \) pressure component of flow induced force acting on particle \( i \)

\( F^i_v \) viscous component of flow induced force acting on particle \( i \)

\( F^i_{v,norm} \) viscous component of flow induced force acting on particle \( i \) in direction normal to the particle surface

\( f^i_{f-s} \) fluid-particle interaction force per unit volume

\( f_{f-s} \) fluid-particle interaction force per unit mass

\( g \) gravity

\( I \) identity matrix (tensor)

IBM immersed boundary method

\( k \) permeability of sample

\( k_h \) hydraulic conductivity

\( K \) fluid particle interaction coefficient

\( L^D_{x,DEM} \) length of periodic cell in the \( x \)-direction

\( n \) porosity

\( N^i_c \) number of fluid cells adjacent to particle \( i \)

\( N_p \) number of particles in the sample

\( N^C_p \) number of coarse particles in bimodal samples

\( N^F_p \) number of fine particles in bimodal samples

\( \hat{n}^i_{f-c=1} \) vector normal to surface element on the boundary surface corresponding to particle

\( p \) fluid pressure

PBC periodic boundary condition

PSD particle size distribution

\( R \) Particle radius

\( Re \) Reynold’s number

SC simple cubic packing configuration

\( S_v \) ratio of internal surface area to volume of solids

\( t \) time

\( u \) fluid velocity vector
\( u_x \) component of fluid velocity vector in the \( x \)-direction

\( u_y \) component of fluid velocity vector in the \( y \)-direction

\( u_z \) component of fluid velocity vector in the \( z \)-direction

\( U \) component of fluid velocity vector in the \( x \)-direction at \( x = x_{\text{min}} \) for IBM simulations

\( v \) particle velocity vector

\( V \) Total volume

\( V_p \) particle volume

\( V^i_p \) volume of particle \( i \)

\( V^i_{VC} \) Volume of Voronoi cell associated with particle \( i \)

\( \Delta x \) Fluid cell size

\( x_i \) volume fraction

\( x_{\text{min}} \) minimum \( x \) coordinate

\( x_{\text{max}} \) maximum \( x \) coordinate

\( y_i \) diameter fraction

\( \phi \) solids fraction

\( \phi^i_{VC} \) solids fraction for each particle \( i \) calculated using Voronoi tessellation

\( \mu \) dynamic viscosity

\( \rho_f \) fluid density

\( \sigma \) hydrodynamic stress tensor

\( \psi \) volumetric fines content

\( \tau \) viscous stress tensor

\( \chi \) Size ratio for bimodal simulations
Introduction

Use of the discrete element method (DEM) is now well established in fundamental geomechanics research. Many problems associated with sand involve seepage flow. Coupling DEM with computational fluid dynamics (CFD) enables particle-scale analyses of these problems. Within the geotechnical research community most published examples documenting the coupling of a discrete element method (DEM) code with computational fluid dynamics (CFD) have used a coarse grid approach for the fluid phase; this is sometimes termed unresolved DEM-CFD. This means that the discretization used to solve the Navier Stokes equations describing the fluid phase is coarser than the particles making up the solid phase considered in the DEM analyses. Semi-empirical drag expressions are used to model the fluid-particle interactions. Unresolved DEM-CFD implementations are outlined in Tsuji et al. (1993); Kafui et al. (2002); Xu & Yu (1997). This approach has been applied to consider liquefaction-induced lateral spreading (El Shamy et al. 2010), submarine landslides (Jiang et al. 2015) (2D study), backward erosion piping (Tao & Tao 2017), particle migration in filters (Huang et al. 2014), suffusion (Kawano et al. 2018) and sand production (Climent et al. 2014). This contribution shows that despite the growing use of DEM-CFD in geomechanics, the approaches used have limited accuracy. A new, more accurate approach to calculate the fluid-particle interaction forces is proposed.

In this contribution the fluid flow between the grains is fully resolved using an immersed boundary method (IBM) to enable a detailed analysis of the fluid-particle interaction forces. Consideration is restricted to spherical particles, saturated flow with a low Reynolds number and the fluid is assumed to be incompressible and Newtonian. The data generated are used to investigate the limitations of the drag expressions currently used in coupled DEM-CFD simulations in geomechanics. The paper shows that the application of a previously proposed polydispersity correction can improve the predictability of these expressions only in some cases; significant errors remain for many of the samples considered here. Therefore, a new approach that uses local void ratios calculated from a radical Voronoi tessellation is proposed and it is shown to better capture both the total fluid-particle interaction force as well as the forces on individual particles.

Fluid-particle interaction forces

In unresolved DEM-CFD the discretization used to solve the Navier-Stokes equations describing the fluid phase is coarser than the particles making up the solid phase considered in the DEM analyses. Assuming incompressible and Newtonian flow, and adopting the local averaging technique proposed by Anderson & Jackson (1967) the Navier-Stokes equations are then given by (e.g. Xu & Yu 1997)

\[
\frac{\partial n}{\partial t} + \nabla \cdot (nu) = 0 \tag{1}
\]

\[
\frac{\partial (nu)}{\partial t} + \nabla \cdot (n\nu u) = -\frac{n\nabla p}{\rho_f} + \frac{1}{\rho_f} \nabla n \tau + n g - f_{f\rightarrow s} \tag{2}
\]

where \(t\) is time, \(n\) is porosity, \(u\) is the fluid velocity vector, \(\tau\) is the viscous stress tensor, \(\rho_f\) is the fluid density, \(p\) is the fluid pressure, \(g\) is gravity, and \(f_{f\rightarrow s}\) the fluid-particle interaction force per unit volume. Note that in this contribution vector quantities are indicated in bold font, i.e. \(f\), and the corresponding magnitude of the vector in the direction of the applied flow is given in regular weight, i.e. \(f\).

In unresolved CFD-DEM the total flow induced force, \(F_{f\rightarrow s}\) acting on each particle is added to the resultant force acting on that particle in the DEM equations of motion. \(F_{f\rightarrow s}\) can be separated into a buoyancy force due to a hydrostatic pressure gradient, \(F_b = -\nabla_p (\nabla_p (V_p)\) is the particle volume) and a
drag force ($F_d$) which arises from viscous friction as the fluid moves relative to the surface of the particle. At Reynolds numbers $Re \to 0$ the drag imposed on a single particle is given by Stokes drag:

$$F_d = 3 \pi \mu D |u - v|$$

where $D$ is the particle diameter, $\mu$ is the dynamic viscosity of the fluid, and $v$ is the particle velocity vector. Table 1 lists some of the available expressions used to estimate the drag force on a particle within a particle assembly with solids fraction $\phi$, where $\phi = \frac{\sum V_i}{V}$, and $V$ is the total volume considered ($\phi = 1 - \eta$ where $\eta$ is the sample porosity). Referring to Table 2, the empirically-derived expressions proposed by Ergun (1952) and Di Felice (1994) are the most commonly used drag expressions in published geomechanics studies. In experiments the drag force is not directly measured, rather it is derived from the pressure drop. $F_{F-e}$ for individual grains can be obtained in simulations where the fluid flow is resolved using a grid discretization that is smaller than the particles. The expressions proposed by Tang et al. (2015) and Tenneti et al. (2011) were obtained using immersed boundary method (IBM) simulations, while the formula proposed by Beetstra et al. (2007) was derived using lattice Boltzmann method (LBM) simulations. The Ergun, Tang and Tenneti correlations have a similar form; all include a $\phi (1 - \phi)^2$ term and a $\frac{Re}{(1 - \phi)^2}$ term, and are based on the Kozeny-Carmen model. Di Felice followed the analytical form used by Richardson & Zaki (1954); this is well suited to describe sedimentation at low values of $\phi$.

The expressions listed in Table 1 were mainly developed for mono-disperse assemblies. Corrections to enable application of the expressions to polydisperse assemblies have been proposed. The correction of van der Hoef et al. (2005), which was derived using LBM simulation data, is expressed in terms of the volume fraction, $x_i$, diameter fraction, $y_i$, and Sauter mean diameter $\langle D \rangle$ of size component $i$:

$$x_i = \frac{\phi_i y_i}{\phi}, y_i = \frac{D_i}{\langle D \rangle}, \langle D \rangle = \left( \sum_i x_i y_i \right)^{-1}$$

Then the drag on an individual particle in size class $i$ is given by applying a multiplicative factor to the preferred expression in Table 1:

$$F^{i}_{d} = [(1 - \phi) y_i + \phi y_i^2 + 0.064(1 - \phi) y_i^3] F_d(\phi, Re)$$

Further research by van der Hoef and co-workers (also using LBM) (Beetstra et al. (2007) and Sarkar et al. (2009)) supports the use of this expression.

While polydisperse assemblies have been considered in most of the studies noted in Table 2 no polydispersity correction such as is given in Equation 5 was applied. Consequently it is important to establish the need to use such a correction for the dense packings of interest in geomechanics applications.

**Simulation Approach**

**Numerical Method**

IBMs are a class of CFD methods in which the fluid equation system is modified by the introduction of additional boundary conditions inside the internal region of the fluid domain (Mittal & Iaccarino 2005). In this case the Navier-Stokes equations are given by:

$$\nabla \cdot \mathbf{u} = 0$$

(6)
\[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = \frac{1}{\rho_f} \nabla \cdot \mathbf{\sigma} + f_{f \rightarrow s}, \tag{7} \]

where in this case \( f_{f \rightarrow s} \) is a volume source term representing the fluid-particle interaction force per unit mass and (for an incompressible fluid) \( \nabla \cdot \mathbf{\sigma} = -\nabla p + \mu \nabla^2 \mathbf{u} \) is the divergence of the hydrodynamic stress tensor.

Referring to Figure 1, the Navier-Stokes equations are solved on a fixed Eulerian mesh with a grid spacing that is smaller than the particles. Points representing the surfaces of the solid objects are inserted in the fluid domain at which no-slip and no-penetration boundary conditions are imposed by the application of source terms representing the fluid-particle interaction force into the fluid equation system. These points are called Lagrangian or IB points and they track the motion of the solid surfaces as they move across the Eulerian fluid mesh. They do not necessarily coincide with the fluid cell points. The locations of the IB points are taken as the centroids of the triangles comprising the convex hull of a point set generated following the generalised spiral point method of Rakhmanov et al. (1994). A volume is associated with each surface triangle corresponding to a subvolume of a spherical shell centred about the IB points, which are located a distance of the particle radius from the sphere centre.

The spiral point generator implemented in the current study can achieve a close match between the triangle volume and the fluid cell size, while achieving a narrow distribution of triangle areas; these features are both requirements of the direct forcing type IBM.

A multi-direct forcing type IBM implemented in Multiflow (Denner & van Wachem 2014; Azis et al. 2019) was used in the current study. As outlined by Uhlmann (2005) in a direct forcing scheme the force required to impose the no-slip condition at each IB point is sought. This force depends upon the velocities and the derivative fields for the pressure, viscous and convective terms in the Navier-Stokes equations, which are interpolated from the fluid grid to the IB point. The interpolation process for each IB point considers a support region comprising a number of fluid cells. The support regions of neighbouring IB points will overlap, so that the forcing from one IB point will affect the neighbours; consequently the no-slip condition will not be well-satisfied at the end of each time-step. Luo et al. (2007) proposed a multi-direct forcing scheme in which the forces are calculated iteratively until the no-slip error is within a specified tolerance. For each particle, the sum of the forces on all of the IB points on its surface gives a fluid particle interaction force \( \mathbf{F}_{f \rightarrow s} \). In the IB scheme fluid is present throughout the domain analyzed and so \( \mathbf{F}_{f \rightarrow s} \) includes a contribution from the fluid inertia within the particle domain. The correction proposed by Uhlmann (2005) was implemented, however in the current study the particles remain stationary and \( \mathbf{F}_{f \rightarrow s} \) does not require correction.

Following Uhlmann (2005) the Dirac-delta function of Roma et al. (1999) is used to interpolate the velocities and spread the forces out in the fluid and particle domains. Uhlmann noted that the smoothing of the particle interface caused by the interpolation and spreading procedures leads to an enhancement of the particle size from the perspective of the fluid which increases \( \mathbf{F}_d \) and reduces the method to first order accuracy in space. Following Yu & Shao (2007), Breugem (2012), and Tang et al. (2014) the radius of each particle is retracted so that the IB points are located a distance of \( R - b \Delta x \) from the particle centroid, where \( R \) is the particle radius and \( b \) is a radius retraction coefficient. Breugem (2012) suggested \( b = 0.3 \), however Tang et al. (2014) showed that the optimal \( b \) depends on \( \phi \) and the Reynolds number, Re.
The approximations associated with the IBM (most notably radius retraction) are avoided if the regular fluid grid is replaced by an unstructured mesh conforming to the pore space geometry as detailed in Hu et al. (2001). The overlapping of the fluid and particle domains is avoided. However significant computational cost is associated with mesh generation. In the case of dense packings associated with geomechanics applications the mesh topology is complex and generating a high quality mesh is not easy. In the case of CFD, having very small, i.e., thin, elements neighbouring very large elements or in regions of high flow velocity can result in high Courant numbers in the badly shaped cells, which in turn can prevent the solver from converging. As detailed in Knight (2018b; 2018a), in the current study a mesh generator was developed to enable selected IBM simulations to be repeated using an unstructured tetrahedral mesh.

In the unstructured mesh simulations the force on particle \(i\), \(F_{f \rightarrow s}^i\), is then calculated from the hydrodynamic stress tensor, \(\sigma\), integrated over the particle surface; in discrete form this is given by a summation over the \(N_c^i\) cells adjacent to the hole representing particle \(i\):

\[
F_{f \rightarrow s}^i = \sum_{j}^{N_c^i} \left[ -I p_j + \mu(\nabla u_j + \nabla u_j^T) \right] \cdot \hat{n}_{j}^{BC=i} dA_{j}^{BC=i}
\]  
(8)

where \(I\) is the identity matrix (tensor) and the normal vector, \(\hat{n}_{j}^{BC=i}\), and the area of the surface element, \(dA_{j}^{BC=i}\), are those corresponding to the triangular face of cell \(j\) which lies on the boundary surface corresponding to particle \(i\).

\(F_{f \rightarrow s}^i\) can be separated into a viscous component, \(F_{v}^i\), and a pressure component \(F_{p}^i\) given by

\[
F_{v}^i = \sum_{j}^{N_c^i} \mu(\nabla u_j + \nabla u_j^T) \cdot \hat{n}_{j}^{BC=i} dA_{j}^{BC=i}
\]  
(9)

\[
F_{p}^i = \sum_{j}^{N_c^i} -I p_j \cdot \hat{n}_{j}^{BC=i} dA_{j}^{BC=i}
\]  
(10)

The pressure in Eqn. 6 includes a contribution from the fluid velocity equal to the normal component of \(F_{v,norm}\). Therefore, to avoid double counting for the unstructured mesh data

\[
F_{f \rightarrow s}^i = F_{p}^i + F_{v}^i - F_{v,norm}^i
\]  
(11)

Both the IBM and unstructured mesh implementations were developed to enable fully resolved DEM-CFD simulations. The current study aimed to improve understanding of the fluid-particle interaction force and the data required could be obtained keeping the particle phase static.

**IBM Verification and Selection of \(b\)**

Zick & Homsy (1982) considered particles with regular simple cubic (SC), body centred cubic (BCC), and face centred cubic (FCC) configurations over a range of \(\phi\) values. They developed two-dimensional integral equations of the stress at the sphere surfaces and evaluated these equations numerically to obtain \(F_{f \rightarrow s}\) (although they use the term drag in their discussion). The results are presented in terms of a fluid particle interaction coefficient: \(K = \frac{F_{f \rightarrow s}}{F_d}\), where \(F_d\) is calculated using Equation 3. In the current study, \(K\) values determined for IBM simulations of flow through ordered arrays of spheres were compared with values obtained by Zick & Homsy (1982). SC, BCC and FCC configurations were considered, each sample was considered at the maximum packing density and the sphere radii were systematically reduced to vary \(\phi\) so that both disperse non-contacting configurations as well as dense configurations more representative of soil were considered; this enabled definition of the \(K - \phi\) relationship. Figure 2 illustrates the FCC simulation set up. The comparison focussed on the sensitivity of the IBM \(K\) values to the value of \(b\) used. The results informed
the choice of $b$ for simulations on polydisperse systems. The sensitivity to grid resolution was explored by systematically varying the number of fluid cells per particle diameter, i.e. $\frac{D}{\Delta x}$, where $D$ is the sphere diameter. Referring to Figure 3(a) it is clear that $K$ increases non-linearly with increasing $\phi$; and that $K$ becomes very sensitive to $\phi$ at the close-packed limit which is representative of stress-transmitting sand samples. Figure 3(a) illustrates that for $\frac{D}{\Delta x} = 16$ the value of $b = 0.3$ recommended by Breugem (2012) does not effectively capture $K$. As $\phi$ increases the value of $b$ giving the most accurate $K$ estimate reduces, however at the close-packed limit even the minimum value of $b = 0.0$ gives a substantial error. There is a fabric sensitivity, slightly different trends were observed for the SC and BCC configurations (data for these cases is presented in Knight (2018a)). As might reasonably be expected, the $K - \phi$ relationship is dependent on $\frac{D}{\Delta x}$; Figure 3(b) illustrates that the variation in $K$ with $b$ is less marked for $\frac{D}{\Delta x} = 64$, however at the highest solid fractions considered the smallest error is given with $b = 0.3\Delta x$. Considering the FCC data presented in Figure 3, as well as the SCC and BCC data given in Knight (2018a), it was concluded that a resolution of $\frac{D}{\Delta x} = 24$ would give sufficiently accurate results for dense grain packings, with the resolution calculated based on the smallest particle diameter for polydisperse systems. The value of the radius retraction parameter should be chosen based on the global solid fraction with the optimal values selected as follows: $b = 0.30$ for $\phi < 0.60$ (maximum relative error: $\left| \frac{\Delta K}{K} \right|_{max} \approx 0$), $b = 0.15$ for $0.60 < \phi < 0.70$ ($\left| \frac{\Delta K}{K} \right|_{max} \approx 0$), and $b = 0.00$ for $\phi > 0.70$ ($\left| \frac{\Delta K}{K} \right|_{max} \approx 0$).

Considering the unstructured mesh simulations, Zick & Homsy (1982) data were also used to assess the influence of the element size on the accuracy by considering the ratio $\frac{D_{esc}}{D}$ where $D_{esc}$ is the target element edge length used in the mesh generation process. As illustrated in Figure 4(a) (for the FCC case) the unstructured mesh simulations more accurately reproduce the Zick & Homsy data than the IBM simulations with $\frac{D}{\Delta x} = 64$. The sensitivity of the results to the spatial discretization for the FCC case is illustrated in Figure 4(b); the error is highest for the densest packings, and to achieve $\left| \frac{\Delta K}{K} \right| < 0.05$ across all packing densities a $\frac{D}{D_{esc}}$ of at least 40 is required. As before, consideration of the SC and BCC data along with the FCC data indicates that the results depend on $\phi$. For $\phi$ values of 0.65 a $\frac{D}{D_{esc}}$ of 30 gives $\left| \frac{\Delta K}{K} \right|_{max} \approx 5\%$ for all samples considered.

**IBM simulations**

A total of 74 IBM simulations of flow through assemblies of randomly packed spheres were completed as detailed in Knight (2018a). In all cases the virtual numerical samples were generated as an initial cloud of randomly placed non-contacting spheres confined within cubic periodic boundaries. They were subject to isotropic compression up to a mean isotropic effective stress of 100 kPa using the DEM capabilities of Multiflow. Snapshots were taken of the system during compression so that IBM simulations were carried out over a broad range of $\phi$ values, including $\phi$ values at which the samples were not stress transmitting (i.e. where a percolating contact force network was not formed). This provided the range of $\phi$ values needed to critically analyze the equations to predict the drag, as documented in Table 2. 26 of the samples considered had linear particle size distributions (PSDs) as illustrated in Figure 5. Computational considerations restricted the maximum coefficient of uniformity, $C_u$, to be 2.5. 48 bimodal samples were considered, 24 with a size ratio, $\chi = \frac{D_{sc}}{D_F} = 2$ and 24
with \( \chi = \frac{D_C}{D_F} = 4 \), where \( D_C \) and \( D_F \) are the coarse and fine particle diameters respectively. For these bimodal samples the volumetric fines content \( \psi = N_F^C D_F^3 / (N_F^C D_F^3 + N_F^C D_C^3) \) was varied \((N_F^C \text{ is the number of fine particles and } N_F^C \text{ is the number of coarse particles})\). The computational cost of the IBM simulations limited the number of particles between 491 and 629 for the samples with linear PSDs and between 317 and 1363 for the bimodal samples.

The particle radii and positions, along with the boundary positions were taken as the input for the IBM simulations. Figure 6 illustrates the IBM simulation set up. The periodic boundary conditions (PBCs) applied in the compression stage remained in the \( y \) and \( z \) directions. In the \( x \) direction an inlet boundary condition was applied at \( x = x_{\min} \) with \( \mathbf{u} = (u_x, u_y, u_z) = (U, 0, 0) \) and \( \frac{dp}{dx} = 0 \); for the outlet at the opposite end of the domain, at \( x = x_{\max} \), \( (\partial u_x / \partial x, \partial u_y / \partial x, \partial u_z / \partial x) = 0 \) and \( p = 0 \).

A constraint of the IBM is that all the Lagrangian control points must lie inside the fluid domain. Placing IBM points too close to the inlet results in an unphysical solution as the no-slip condition imposed by these points conflicts with the constant velocity enforced at the inlet. Analysis of the simulations with regular packings discussed above indicated that \( F_{f_{\rightarrow s}} \) is over-predicted for particles close to the inlet and under-predicted for particles close to the outlet. In the inlet region, all the fluid cells have the same velocity; this is not representative of flow through a bed of particles. Similarly close to the outlet the flow does not encounter the resistance it would experience if there were additional layers of particles and \( F_{f_{\rightarrow s}} \) is under-predicted. To overcome this challenge in a computationally effective way, particles that intersect the DEM simulation boundaries are duplicated and translated by \( L_x \) to the opposite end of the domain as illustrated in Figure 6. Therefore, the particle locations are periodic in the \( x \) direction. The domain is then extended in the \( x \) direction so that all IBM points are at a distance of at least \( 2\Delta x \) from the inlet and outlet boundaries.

Computational considerations restricted the cases considered to small numbers of particles. Balancing considerations of accuracy and cost, a resolution of \( \Delta x = 24 \) was used, where \( \Delta x \) was the minimum particle diameter for that simulation. A typical IBM case comprising about 600 particles embedded in a fluid mesh with 60 million cells took 16 hours to run on 400 processing cores (using compute nodes each having two 12-core Intel Ivy Bridge series processors, EPCC (2013–2018)). For the samples with linear gradings three values of \( b \) were considered to establish the sensitivity of \( F_{f_{\rightarrow s}} \) to \( b \) for different values of \( \phi \) and \( C_u \). Informed by the simulations on lattice packings discussed above, the data presented here are restricted to consider only simulations with \( b = 0.30 \) when \( \phi < 0.60 \) and \( b = 0.15 \) when \( \phi > 0.60 \). The computational cost restricted the study to use only one value of \( b \) for each bimodal sample; with \( b = 0.30 \) when \( \phi < 0.60 \), \( b = 0.15 \) when \( 0.60 < \phi < 0.70 \) and \( b = 0.0 \) when \( \phi > 0.70 \). For each sample with a linear PSD considered, the flow was simulated along each of the 3 Cartesian directions to obtain three distinct flow fields for each combination of \( \phi \) and PSD. For the simulations with a bi-model PSD, the computational cost restricted consideration to one flow field in the x-direction for each \( \phi \) considered.

**Results**

**Overall Flow Response**

The overall permeabilities \( k \) of the samples were determined as \( k = \mu U L_{DEM}^D / \Delta p \) where \( \mu \) is the viscosity and \( \Delta p \) is the difference in pressure over a length \( L_{DEM}^D \), the length of the periodic cell as illustrated in Figure 6. These values of \( k \) were compared with analytical and empirical expressions for permeability to verify the flow data for the randomly packed assemblies. The comparison considered the empirical Hazen equation (Hazen 1892; 1911) which gives \( k_h = C_\mu D_{10}^2 \), where \( k_h = \frac{k p f \phi}{\mu} \) is the
hydraulic conductivity and $C_H$ is an empirical coefficient. Carrier (2003) noted that a wide range of $C_H$ values are reported in the literature but that a value of 100 is often used and so $C_H=100$ for the comparisons presented here. The Kozeny-Carmen equation, which is derived by assuming the porous medium can be approximated as a network of capillary tubes, gives:

$$k = \frac{(1-\phi)^3}{5S_\nu^2\phi^2}$$

(12)

Where $S_\nu$ is the ratio of internal surface area to volume of solids, and the factor 5 is the approximate value of the empirical tortuosity obtained by Carman (1937). $S_\nu$ was calculated using all $N_p$ particles in the assembly and is

$$S_\nu = \frac{6\sum_i N_p d_i^3}{\Sigma_{Ni} d_i^2}$$

(13)

Figures 7(a) and (b) show the permeabilities ($k$) against $\phi$ for random samples with the linear and bimodal PSDs respectively. The wide variation in $k$ reflects the broad range of $\phi$ values considered. The sensitivity of $k$ to both $\phi$ and $C_u$ is in line with the general understanding of sand permeability and the data are in good agreement with data obtained by application of the Kozeny-Carmen equation (these data are denoted KC on Figure 7). The Kozeny-Carmen and IBM values diverge at higher $\phi$ values; this may reflect the increase in error in the IBM simulations as indicated in the regular packing simulations discussed above, but we must also acknowledge that the way in which tortuosity is included in the Kozeny-Carmen equation lacks rigour (e.g. Taylor et al. (2017)). The comparison with data obtained by applying the Hazen equation (denoted Hazen on Figure 7) considers only the linear PSD samples and the maximum $\phi$ values, which are most representative of a stress transmitting sand sample, and the agreement is very good. Taylor (2016) reported experimental permeameter tests on glass ballotini samples with linear PSDs and $C_u$ values of 1.5 and 3 and the experimental data (denoted HT on Figure 7) show similar gradients to the IBM data. The experimental permeability values are lower, most likely reflecting the smaller $D_{10}$ values for Taylor’s samples (0.48 and 0.42 mm compared with the 0.56-0.72 for the IBM simulations). The $k$ - $\phi$ relationship was also obtained for $C_u = 1.01$ samples using the unstructured mesh approach (MSP data on Figure 7a), and was in very good agreement with the IBM data. Overall, the permeability data, combined with the simulations on regular packings discussed above, indicate that reasonable values for $F_{f\rightarrow s}$ can be extracted from the IBM simulations.

**Particle-fluid interaction forces**

For the IBM data two approaches can be used to decompose $F_{f\rightarrow s}$ into $F_d^i$ and $F_p^i$. The first approach, termed method A here, assumes that the pressure gradient acting across each particle is well approximated by the global pressure gradient. The buoyancy contribution acting on each particle can then be removed from the total fluid-particle interaction force acting on a given particle to obtain the drag contribution such that:

$$F_d^i = F_{f\rightarrow s}^i - V_p^i \nabla p.$$  

(14)

does not apply here. van der Hoef et al. (2005) and Tang et al. (2014) proposed that the total drag force $\sum_i N_p F_d^i$ should be calculated by considering the balance between $\nabla p$, and the total fluid-particle interaction force $\sum_i N_p F_{f\rightarrow s}^i$. The global force balance is then given by
\[ -\nabla V p = \sum_{i}^{Np} F_{i}^{d} = N_p \langle F_{d} \rangle = N_p \left( \langle F_{d} \rangle + \langle F_{p} \rangle \right) \]  

As \( \phi = \frac{N_{d}(V_{p})}{V} \) and assuming that \( \langle F_{p} \rangle = -\langle V_{p} \rangle \nabla p \), manipulation of the relevant terms leads to method B to extract the \( \langle F_{d} \rangle \) (Knight 2018a)

\[
\langle F_{d} \rangle = (1 - \phi) \langle F_{f-s} \rangle
\]

Method B cannot account for local fluctuations of \( F_{i}^{d} \) around \( \langle F_{d} \rangle \) and so it cannot be used to determine \( F_{i}^{d} \) (Municchi & Radl 2017).

The computationally expensive unstructured mesh simulations were employed to verify the use of the IBM to analyse the drag forces in the random samples. For the analyses presented here the individual particle drag force magnitudes were normalized by the Stokes drag, calculated using the mass weighted mean diameter \( \langle D \rangle \) and the superficial velocity (flow rate per unit area) and denoted \( \bar{F}_{d} \). Figure 8(a) shows good agreement in the variation in the total \( \bar{F}_{d} \) value per unit volume with \( \phi \) predicted using both the IBM and unstructured mesh approaches for the linear PSD with \( C_{u} = 1.01 \). The individual \( \bar{F}_{d} \) values for \( \phi = 0.651 \) are illustrated on Figure 8(b) and again a good agreement is observed, reflecting a Pearson correlation coefficient of 98.7\% when the \( F_{i}^{d} \) are compared.

**Meso-scale analysis**

The \( \sum_{i}^{Np} F_{i}^{d} \) data were averaged for flow in the \( x, y \) and \( z \) directions to obtain the \( \sum \bar{F}_{d} / V \) values presented in Figure 9. Figures 9(a) and (b) present the variation in \( \sum \bar{F}_{d} / V \) with \( \phi \) for the samples with linear PSDs and \( C_{u} = 1.01 \) and \( C_{u} = 2.0 \) respectively. Only a limited number of simulations were completed for the \( C_{u} = 2.5 \) samples and so there were insufficient data to enable consideration of this PSD. Considering the samples with bimodal PSDs, Figure 9(c) presents data for \( \chi = 2 \) and \( \psi = 0.1 \) and Figure 9(d) presents data for \( \chi = 4 \) and \( \psi = 0.11 \). Data obtained using both methods A and B are included and the results are compared with the \( \sum \bar{F}_{d} / V \) values calculated using the Ergun, DiFelice, Tang and Tenneti expressions to predict the drag listed on Table 1. For each PSD a cubic polynomial is fitted to the IBM data to describe the overall trend.

Each IBM sample is analogous to a single fluid cell in an unresolved DEM-CFD simulation, consequently this is a meso-scale analysis and the data give an indication of the applicability of the expressions listed in Table 1 in unresolved DEM-CFD. Table 3 summarizes the RMS errors in the \( \sum \bar{F}_{d} / V \) data comparing each of the drag expressions with the IBM data and also considering use of the polydispersity correction by van der Hoef et al. (2005) given in Equations 4 and 5. The RMS error is defined as:

\[
\overline{\Delta F_{d}} / V = \frac{1}{\sqrt{F_{d}^{\text{corr}}}} \left( \langle F_{d} \rangle - \langle F_{d}^{\text{corr}} \rangle \right)
\]

where \( F_{d}^{\text{corr}} \) is the drag force given by the expressions, to act on a single particle with \( D = \langle D \rangle \).

The IBM data obtained using methods A and B are in very close agreement. The small differences observed can likely be explained by the challenges in determining \( Vp \) exactly along the boundary cells that include regions that are inside the immersed boundaries (Knight 2018a). The unstructured mesh simulations for the \( C_{u} = 1.01 \) samples were in good agreement, having a Pearson correlation coefficient of 98.7\%.

Considering the linear PSD samples (Figures 9(a)-(b)), it is clear that the Tang, Ergun and Tenneti expressions give similar trends, reflecting their similar basis as discussed above. The Di Felice expression has the greatest error at low \( C_{u} \) values, most likely explained by its limited applicability at
low \(Re\) and high \(\phi\) values. Referring to Figure 9(a) and Table 3, for the linear PSDs and for the low \(C_u\) values of 1.01 and 1.2 only the expression proposed by Tenneti et al. (2011) gives a good agreement with the IBM data; however, even for this correlation the data diverge as \(C_u\) increases.

The errors evident from Figure 9(b) can partially be explained by the application of drag expressions developed for mono-disperse systems to a polydisperse assembly. In addition, the expressions for drag do not take into account the microstructure of the particles, and are derived for an average pressure drop (on a much larger scale). Figures 10(a) and (b) and the data on Table 3 illustrate that where the polydispersity correction (Equations 4 and 5) is applied using 8 size bins (size classes), there is a significant improvement in the comparison between the IBM and the data obtained using the expression proposed by Tenneti et al. (2011).

For the bimodal samples with \(\chi = 2\), Figure 9(c) indicates good agreement with the empirical expression of Tang et al. (2015); however the significant error associated with the empirical expression of Tang and co-workers for the \(\chi = 4\) samples show that this could be a coincidence. In any case the predictions obtained using the empirical expression of Tang et al. diverge from the IBM data as \(\psi\) increases. The data for the \(\chi = 4\) samples indicate that none of the monodisperse expressions listed in Table 1 can adequately predict the drag force for a bimodal sample. The data obtained using the expression of Tenneti et al. (2011), which gave such a good match for the linear PSDs, differ from the IBM data by at best a factor of 2 across the range of \(\psi\) and \(\phi\) considered.

As before, Figures 10(c) and (d) illustrate the \(\sum \overline{F_d}/V\) data for the expression of Tenneti et al. (2011) using the polydispersity correction in equations 4 and 5. Figure 10(c) shows that a good agreement is seen for \(\chi = 2\) and \(\psi = 0.1\) across all \(\phi\) values considered; similar good agreement was seen for the other \(\psi\) values considered (Knight 2018a). With \(\chi = 4\), excellent agreement is seen for all \(\psi\) and \(\phi\) values, except for the maximum \(\phi\) values considered; representative data are presented in Figure 10(d). However, it is expected that the IBM will underpredict \(\overline{F_{d-s}}\) for \(\phi > 0.7\) and so the divergence does not discount the use of the Tenneti expression with a polydispersity coefficient for stress-transmitting systems representative of soil, provided the particle scale data are reasonable.

**Particle-Scale Perspective**

In a polydisperse system, it is expected that larger particles will experience a higher local solids fraction than smaller particles, as the small particles can fit into the relatively large gaps between the large particles. As a consequence of this locally increased density, the fluid passes through narrower constrictions in the pore space in the vicinity of the large particles resulting in an increase in the flow velocity and larger fluid forces on particles in these regions. In this work, the radical Voronoi tessellation proposed by Gellatly & Finney (1982) was used to define a local volume associated with each particle; this approach gives a more reasonable partitioning of the void space than the classical Voronoi tessellation. The voro++ software (Rycroft 2009) was used. The solids fraction for each particle \(i\) is then given by \(\phi_{VC}^i = V_{VC}^i / V_{VC}\). Knight (2018a) showed that for the linear PSD samples considered here the range of \(\phi_{VC}\) values increased with increasing \(C_u\) with \(\phi_{VC}^{\text{min}}\) reducing and \(\phi_{VC}^{\text{max}}\) increasing.

Figure 11 considers the samples with linear PSDs and illustrates the normalized particle drag forces, \(\overline{F_d}\), where the particle drag force magnitudes, \(F_d^i\), were normalized by the Stokes drag calculated for the mass weighted mean diameter, \(\langle D \rangle\), and using a flow velocity equal to the flow per unit area; the data points are coloured by \(\phi_{VC}\). The trends predicted using both the expression proposed by Tenneti et al. (2011) listed in Table 1 and the expression proposed by Tenneti et al. along with the polydispersity correction (Equations 4 and 5) are also indicated. For the monodisperse case \((C_u=1.01,\)
Figure 11(a) and (b)), whether Method A or Method B is used to extract data from the IBM simulations, \( \bar{F}_d \) values are normally distributed about a mean value that is closely matched by the expression proposed by Tenneti et al. (2011). For this sample there is no clear link between \( \phi V_C \) and \( \bar{F}_d \) and the range of \( \phi V_C \) values is small. Even for a small amount of polydispersity \( (C_u = 1.20, \text{Figure 11(c) and (d))} \) the best fit to the data indicates a non-linear relationship between \( \bar{F}_d \) and \( D \), which can be linked to the increase in \( \phi V_C \) with \( D \) (illustrated by the colour of the data points). With further increases in \( C_u \) the curvature of the best fit line increases and the dependency of \( \bar{F}_d \) upon both \( D \) and \( \phi V_C \) becomes more apparent. Referring to Figure 11(e) and (f) which present the data for \( C_u = 2.50 \) and \( \phi = 0.701 \), the error associated with excluding the polydispersity correction (Equations 4 and 5) from the Tenneti drag prediction increases as \( C_u \) increases. This error is most evident for the larger particle diameters. The \( \bar{F}_d \) values calculated from the IBM data depend on whether method A or method B is used. The curve approximating the IBM \( \bar{F}_d - D \) relationship is clearly steeper when method B is used.

Figure 12 considers the total fluid particle interaction force \( \langle F_f \rangle \) as well as the components \( \bar{F}_b \) and \( \bar{F}_d \) (all normalized by the Stokes drag as described above) for \( C_u = 2.0 \) and \( \phi = 0.681 \) using method A to achieve the decomposition. Equation 16 indicates that as \( \phi \) increases the contribution of \( \Sigma_i \phi_i \bar{F}_d \) compared to \( \Sigma_i \phi_i \bar{F}_f \) decreases. Assuming \( \phi_i = -V_i \nabla p \) (Equation 14), all of the observed variation in \( \langle F_f \rangle \) for a given \( D \) value is due to variations in \( \bar{F}_d \). Consequently the variation in \( \langle F_f \rangle \) relative to \( \langle F_d \rangle \) increases with increasing \( \phi \). Where method B is used to decompose \( \langle F_f \rangle \) the variation in \( \langle F_f \rangle \) is split proportionally between \( \bar{F}_b \) and \( \bar{F}_d \). \( \bar{F}_b \) is proportional to \( D^3 \) and as \( \phi \) increases \( \bar{F}_f \) becomes dominated by the contribution from \( \bar{F}_b \). For the \( C_u \) and \( \phi \) values considered in Figure 11, \( \bar{F}_b \) is significantly larger than \( \bar{F}_d \) for the larger particles due to the different scalings of \( \bar{F}_d \) and \( \bar{F}_b \) with particle size. As a consequence, for large particles, the relative error on the overall fluid-particle interaction force is less than the error in \( \bar{F}_d \).

Figure 13 illustrates the polar distribution of the fluid-particle interaction forces for \( C_u = 2.0 \) and \( \phi = 0.681 \). It is clear that while the force is not always coincident with the overall flow field direction, all the force vectors are within \( \pm 45^\circ \) of the overall flow orientation and that the forces are the largest in the direction of the main flow field. This variation is to be expected as the tortuous nature of the flow path means there will be local variations in the flow velocity orientations.

Figures 14 (a) and (b) consider the distribution of the \( \langle F_f \rangle \) values for the two particle sizes in the bimodal samples for \( \chi = 2 \) and \( \psi = 0.10 \) and for \( \chi = 4 \) and \( \psi = 0.11 \) respectively. The distributions can be approximated by Gaussian kernel density estimates. The data for the \( \chi = 4 \) and \( \psi = 0.11 \) case are clearly affected by the small numbers of particles used. Figure 15 considers the variation of \( \langle F_f \rangle \) with \( \phi \) for all bimodal samples considered where, \( \langle F_f \rangle \) and \( \langle F_f \rangle \) are the \( \langle F_f \rangle \) values for the coarse and finer fractions. For \( \chi = 2 \) the ratio varies between 5.0 and 6.0 while for \( \chi = 4 \) the ratio varies between 22 and 36. In both cases, the minimum value of \( \langle F_f \rangle / \langle F_f \rangle \) occurs at the lowest \( \phi \) considered. The ratio initially increases with increasing \( \phi \), and then, depending on the \( \chi \) values, \( \langle F_f \rangle / \langle F_f \rangle \) attains maximum at a \( \phi \) of over 0.55, and subsequently decreases slightly. As illustrated in Figure 16, the polydispersity correction detailed in Equations 4 and 5 can neither give a good estimate of the value of \( \langle F_f \rangle / \langle F_f \rangle \) nor does it predict the pattern of variation in \( \langle F_f \rangle / \langle F_f \rangle \) with \( \phi \). The good agreement between the IBM data and the expression proposed by Tenneti et al. (2011) used along with a correction for polydispersity illustrated in Figure 10 (c) and (d) is therefore a coincidence.
Recognizing the poor prediction of the drag force obtained using the expression proposed by Tenneti et al. (2011) when it was applied to the bimodal samples, even where a polydispersity correction is applied, a new approach to correct for polydispersity was developed using the radical Voronoi tessellations illustrated in Figure 17. This approach recognises the link between $\langle F_d \rangle$, $D$ and $\phi_{VC}$ as is apparent in Figures 11 and 12 relates to the value of $\phi$ experienced by the fluid in the vicinity of cell $i$. As illustrated in Figure 17(a), for the case of a bimodal sample, there is a significant jump in the local solids fraction when the Voronoi cells for the large and small particles meet. It is possible, for each Voronoi cell, to define a volume weighted average solids fraction considering the volumes of the neighbouring Voronoi cells. However, for small particles the influence of the adjacent large cells on resultant weighted volume will be unrealistic when the aim is to understand the $\phi$ experienced by the fluid around that particle. Thus a weighted sum that considers the area of the common Voronoi faces has been used; it is given by:

$$\phi_{VC,W}^i = \frac{1}{3} \left[ 2\phi_{VC}^i + \sum_{j=1}^{N_n} \prod_{i=1}^{a_{ij}} \phi_{VC}^j \right]$$

(18)

where $a_{ij}$ is the area of the shared face of the Voronoi cells surrounding particles $i$ and $j$ and there are $N_n$ Voronoi cells abutting the Voronoi cell surrounding particle $i$.

The $\phi_{VC,W}$ values were used to calculate the mean $\phi_{VC,W}$ values for the coarse and finer fractions and these values were used to obtain a prediction of the mean drag force from the monodisperse expression proposed by Tenneti et al. (2011) for the fine and coarse fractions, $\langle F_d^F \rangle$ and $\langle F_d^C \rangle$ respectively. The total drag was calculated as:

$$\sum F_d = N_p^F \langle F_d^F \rangle + N_p^C \langle F_d^C \rangle$$

(19)

As illustrated in Figure 18, the ratios of the forces on the two size fractions capture the trends observed and are quantitatively in agreement with the IBM data on Figure 14. The total force values are also in agreement with the IBM data as illustrated in Figure 19.

The use of a weighted-sum, radical Voronoi tessellation method was also explored for samples with linear PSDs. Referring to Figure 11, the predictive ability of the expression proposed by Tenneti et al. (2011) used with the polydispersity correction was poorest for the dense samples with higher $C_u$ values. Figure 20 indicates that the predictive ability of the radical Voronoi-based method is significantly better considering the densest samples with $C_u = 2.0$ and $C_u = 2.5$; this is further supported by the good agreement with the overall force data as indicated in Figure 21.

While the dataset considered is relatively small, these results support the use of a weighted-sum radical Voronoi approach in conjunction with an accurate monodisperse correlation to estimate the total drag for bimodal samples. Calculating the Voronoi tessellation is comparable in computational cost to reconstructing the neighbour list and must occur with a similar frequency which should be chosen judiciously based on the particle dynamics of the specific problem at hand.

**Conclusions**

This contribution has described the application of the IBM to determine the fluid particle interactions acting on samples of spherical particles with both linear particle size distributions as well as bimodal particle size distributions. Laminar flow conditions with a low Reynolds number were considered. IBM
simulations considering flow through mono-sized spheres on lattice packings were used to validate the method's implementation and determine the appropriate radius retraction value to use. The validity of the IBM samples was further established by comparison with unstructured mesh simulation data and by considering the permeability values predicted from the simulation data. Finally, the predictions from these IBM simulations were compared to popular correlations presented in the literature, using a correction for polydispersity when appropriate. From this comparison the following points can be concluded for the laminar flow conditions considered:

1. While the expressions proposed by Ergun (1952) and Di Felice (1994) used in previous geomechanics studies can give reasonable predictions of total drag for monodisperse samples, their accuracy reduces with increasing polydispersity. The expression proposed by Tenneti et al. (2011) when used with the polydispersity correction proposed by van der Hoef et al. (2005) accurately predicts the overall drag over a range of packing densities for all of the linear PSDs considered here.

2. Even for a monodisperse sample, and for the laminar flow configurations considered here, there is significant scatter amongst the drag forces acting on individual particles about the mean. This variation is not captured by the Ergun / Di Felice expressions as applied in prior geomechanics studies. Use of the expression proposed by Tenneti et al. (2011) improves the predictive capacity of the drag expressions; however the forces on the largest particles are underpredicted.

3. Even when the polydispersity correction of van der Hoef et al. (2005) is applied, the expression proposed by Tenneti et al. (2011) does not predict the individual drag forces accurately for the bimodal samples.

4. For larger particles in particular, the pressure gradient force is significantly larger than the drag force.

5. Due to the tortuosity of the flow paths the orientation of the individual drag forces on the particles is not always co-linear with / parallel to the fluid flow direction. However all the force vectors are within ±45° of the main flow field.

6. There is correlation between the local solids fraction and the drag force. Motivated by this observation use of the drag expression proposed by Tenneti et al. (2011) with a local solids fraction, calculated using an area weighted mean of the radical Voronoi cells around each particle, was explored. Using of approach significantly improved predictions of the individual particle forces could be made.

This contribution has illustrated the ability of the IBM to enable highly accurate predictions of drag on particle assemblies. The IBM overcomes some of the computational challenges associated with unstructured mesh simulations, most notably achieving an effective unstructured mesh using periodic boundaries. The improved correlation obtained using the Voronoi tessellation shows promise as a computationally efficient means to significantly improve DEM-CFD models.

Acknowledgements

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<table>
<thead>
<tr>
<th>Reference</th>
<th>Drag expression</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ergun (1952)</td>
<td>[ F_d(\phi, Re) = \frac{150\phi}{18(1-\phi)^2} + \frac{1.75Re}{18(1-\phi)^2} ]</td>
<td>Developed from fluidization experiments; applicable for (0.53 &lt; \phi &lt; 0.68) and Re 1,000</td>
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<tr>
<td>Di Felice (1994)</td>
<td>[ F_d(\phi, Re) = \frac{C_dRe}{24}(1-\phi)^{-n} ] (n = 3.7 - 0.65e^{-0.5(1.5-\log(Re))}); (C_d) is the drag correlation for an isolated sedimenting particle from Dallavalle (1948)</td>
<td>Developed from sedimentation experiments; applicable for (0.10 &lt; \phi &lt; 0.65) and Re 10,000</td>
</tr>
<tr>
<td>Beetstra et al. (2007)</td>
<td>[ F_d(\phi, Re) = \frac{10\phi}{(1-\phi)^2} + (1-\phi)^2 \left( 1 + 1.5\phi^{\frac{1}{2}} \right) ] [ + \frac{0.413Re}{24(1-\phi)^2} \left[ (1-\phi)^{-1} + 3\phi(1-\phi) + 8.4Re^{-0.343} \right] \left[ 1 + 10^3Re^{\frac{1}{1+4\phi}} \right] ]</td>
<td>Developed from numerical Lattice Boltzmann Method simulations; applicable for (0.10 &lt; \phi &lt; 0.65) and Re 1,000; monodisperse and bidisperse assemblies.</td>
</tr>
<tr>
<td>Tenneti et al. (2011)</td>
<td>[ F_d(\phi, Re) = \frac{1 + 0.15Re^{0.687}}{(1-\phi)^2} + \frac{5.18\phi}{(1-\phi)^2} + \frac{0.48\phi^{\frac{1}{2}}}{(1-\phi)^{3/2}} + (1-\phi)\phi^3Re \left[ 0.95 + \frac{0.61\phi^3}{(1-\phi)^2} \right] ]</td>
<td>Developed from numerical Immersed Boundary Method simulations; applicable for (0.10 &lt; \phi &lt; 0.5) and Re 300. Monodisperse assembly.</td>
</tr>
<tr>
<td>Tang et al. (2015)</td>
<td>[ F_d(\phi, Re) = \frac{10\phi}{(1-\phi)^2} + (1-\phi)^2 \left( 1 + 1.5\phi^{\frac{1}{2}} \right) ] [ + Re \left[ 0.11\phi(1+\phi) - \frac{0.00456}{(1-\phi)^4} + Re^{-0.343} \left( 0.169(1-\phi) + \frac{0.644}{(1-\phi)^4} \right) \right] ]</td>
<td>Developed from numerical Immersed Boundary Method simulations; applicable for (0.10 &lt; \phi &lt; 0.6) and Re 1,000. Monodisperse assembly.</td>
</tr>
<tr>
<td>Reference</td>
<td>Drag expression cited</td>
<td>Application</td>
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<td>Climent et al. (2014)</td>
<td>Di Felice (1994)</td>
<td>Sand production in hydrocarbon reservoirs</td>
</tr>
<tr>
<td>Huang et al. (2014)</td>
<td>Ergun (1952), Wen &amp; Yu (1966)</td>
<td>Particle migration in filters</td>
</tr>
<tr>
<td>Kawano et al. (2018b)</td>
<td>Di Felice (1994)</td>
<td></td>
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<tr>
<td>Zou et al. (2013)</td>
<td>Highly simplified drag model</td>
<td>Particle transport in granular filters</td>
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</tbody>
</table>

Table 2: Drag force expressions reported in representative unresolved DEM-CFD simulations reported in the geomechanics literature
<table>
<thead>
<tr>
<th>Model</th>
<th>Linear PSDs</th>
<th>Bi-linear PSDs</th>
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<tbody>
<tr>
<td></td>
<td>$C_u=1.01$</td>
<td>$C_u=1.20$</td>
</tr>
<tr>
<td>Ergun (1952)</td>
<td>3.16</td>
<td>2.85</td>
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<tr>
<td>Di Felice (1994)</td>
<td>4.72</td>
<td>3.88</td>
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<td>Tang et al. (2015)</td>
<td>3.94</td>
<td>3.35</td>
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<tr>
<td>Tenneti et al. (2011)</td>
<td>1.61</td>
<td>1.01</td>
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<tr>
<td>Ergun (1952) with polydispersity correction</td>
<td>2.57</td>
<td>1.85</td>
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<tr>
<td>proposed by van der Hoef et al. (2005)</td>
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<td></td>
</tr>
<tr>
<td>Di Felice (1994) with polydispersity</td>
<td>4.52</td>
<td>3.47</td>
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<tr>
<td>correction proposed by van der Hoef et al. (2005)</td>
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<tr>
<td>Tang et al. (2015) with polydispersity correction</td>
<td>4.72</td>
<td>4.68</td>
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<tr>
<td>correction proposed by van der Hoef et al. (2005)</td>
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</table>

Table 3: Root Mean Square errors in $\sum F_d/V$ — comparing published empirical expressions with IBM data for the samples with linear PSDs and representative samples with bimodal PSDs
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