A velocity corrected unresolved CFD-DEM coupled method to reproduce wake effects at moderate Reynolds number

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Abstract

Purpose – The purpose of this paper is to develop a corrected unresolved CFD-DEM method that can reproduce the wake effects in modeling particulate flows at moderate Reynolds number.

Design/methodology/approach – First, the velocity field in the wake behind a settling particle is numerically investigated by a resolved method, in which the finite volume method (FVM) is applied to model the fluid flow, discrete element method (DEM) is applied to simulate the motion of particles and immersed boundary method (IBM) is used to tackle fluid solid interaction. Second, an analytical scaling law is given, which can effectively describe the velocity field in the wake behind the settling particle at low and middle Reynolds numbers. Third, this analytical expression is incorporated into unresolved modeling to correct the relative velocity between the particle and its surrounding fluid and enable the influence of the wake of the particle on its neighboring particles.

Findings – Two numerical examples, the sedimentation of dual particles, a list of particles and even more particles are provided to show the effectiveness of the presented velocity corrected unresolved method (VCUM). It is found that, in both examples simulated with VCUM, the relative positions of the particles changed, and drafting & kissing phenomenon and particle clustering phenomenon were clearly observed.

Practical implications – The developed VCUM can be highly beneficial for modeling industrial particulate flows with DKT and particle clustering phenomena.

Originality/value – VCUM innovatively incorporates the wake effects into unresolved CFD-DEM method. It improves the computational accuracy of conventional unresolved methods with comparable results from resolved modeling, while the computational cost is greatly reduced.

Keywords Flow similarity, Particulate flow, Unresolved CFD-DEM, Velocity field correction, Wake effect, Particle settling

Paper type Research paper

1. Introduction

Particle-laden flow widely exists in different natural phenomena and industrial applications. For example, in powder-based 3D printing (coaxial nozzle or selective laser melting), the

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distribution of the metal powders depends on the behavior of the particle flow and affects powder melting, porosity and the surface finish of the product (Wen et al., 2009; Wang et al., 2019). In chemistry and biology, sedimentation has been used to measure the size of large molecules where the force of gravity is augmented with centrifugal force in an ultracentrifuge (Schuck, 2000), and deposition plays an important role in chemical reaction involving macromolecule settling as well. Besides these, fluidized bed also depends on particle-laden flow theories (Okasha et al., 2003). In geology, an increased undesired transport and sedimentation of suspended material is called siltation pollution, which acts as a main source of pollution in many rivers (Cohen et al., 1993). Therefore, it is of great significance for researchers to study particle-laden flows at length (Li, 2000; Zhu et al., 2007).

Particles in particle-laden flows are in solid phase, so the trajectories are predicted with Newton’s Law of Motion, and calculation of this part is conducted with discrete element method (DEM) (Cundall and Strack, 1979). As for the fluid phase, the velocity field is solved by Navier–Stokes (N–S) equations, continuity equation and sometimes energy equations. The fluid part is usually calculated by a CFD method such as finite volume method (FVM) (Kim et al., 2001), Finite Difference Method (Fadlun et al., 2000) or Lattice–Boltzmann method (LBM) (Shu et al., 2007; Huang and Wu, 2014). In the meanwhile, the fluid and particles interacts with each other, namely, momentum exchange, so an interface that couples CFD with DEM is required to exchange the information among them after certain time steps. There are two classes of methods to couple CFD with DEM, resolved and unresolved method.

For resolved methods, the mesh size is much smaller than the diameter of the particle. In normal cases the particle should contain at least three computational cells in radial direction, and it is usually recommended to have ten or more cells for convergent results (Hager, 2014). The fluid-structure interaction in resolved modeling is implemented with moving boundary treatment algorithm such as immersed boundary method (IBM) and fictitious boundary method (Walayat et al., 2018). The force that the fluid exerts on the particle is directly integrated. Complex wake-related phenomena such as drafting–kissing–tumbling (DKT) can be well captured (Chang et al., 2011; Gan et al., 2003). However, resolved modeling methods are only suitable for the simulations with few particles, as it is fairly computationally expensive to perform large-scale simulations because of the boundary integration and (dynamic) refined mesh. While for aforementioned applications, there tend to be hundreds of thousands of particles, it is nearly impossible to use resolved methods and chase the boundary of every particle with immersed boundary method, and this is the reason why unresolved methods are more preferred for industrial applications.

In contrast, for unresolved method, mesh size is usually at least three times bigger than the diameter of the particle, and no surface catching methods are required. The computational expense is therefore much less than that of resolved method. The momentum exchange in unresolved method is implemented by empirical drag force models, and accurate prediction of the drag is one of the most challenging problems. Many researchers provided different force models throughout the history. The Syamlal O’Brien drag model is one of the earliest and popular force models and it was derived from a particle settling system (Syamlal and O’Brien, 1989). After that, Richardson did a series of experiments to validate the force model and made some modifications to O’Brien’s model (Richardson and Zaki, 1954). In 1994, Gidaspow combined Wen and Yu’s model (Feng and Yu, 2004) with Ergun equation and developed a model, referred to as Gidaspow model (Gidaspow, 1994). The models discussed above are all based on experiments. However, in 1997, Hill, Koch and Ladd simulated periodic, ordered and random arrays of spherical particles in fluid flow with Lattice–Boltzmann Method and developed a force model, called Hill–Koch–Ladd force
model, and this is the first force model developed by CFD methods in history (Hill et al.,
2001).

During the development of force models in unresolved methods, researchers mostly focus
on the effects of Reynolds number (drag coefficient). Nevertheless, the relative velocity
between particles and surrounding fluid plays an essential role in the calculation of drag
force as well, which is not so popularly studied. In unresolved methods, a grid cell contains
a certain number of particles while the velocity field of the surrounding fluid is considered the
same as the velocity at the cell center. Hence, it is clear that in unresolved methods, the
calculated relative velocities between particles and surrounding fluid are not accurate
enough as the fluid velocity is numerically treated as constant everywhere within the cell,
while physically it can be different. For example, when two particles get very close to each
other such that one particle is in the wake of another particle, this particle will be subject to
the force exerted by the wake of the second particle. Hence the wake effects of moving
particles within the cell are not able to be considered in conventional unresolved methods
and this clearly differs from physics. Therefore how to introduce wake effects in cost-
effective unresolved modeling methods while preserving correct physics is fundamentally
important for particle-laden flows. The present work will focus on solving this problem to
make unresolved method capable of simulating drafting–kissing phenomenon and particle
clustering at moderate Reynolds number in the end.

2. Governing equations and modeling methods

2.1 Governing equations

For the particle phase, Newton’s laws of motion should be satisfied for both of the linear and
angular momentum:

\[ m_j \frac{dU_j}{dt} = -\frac{1}{6} \pi D_j^3 \nu \rho + F_{\text{drag}} + m_j g + \sum F_{p-p} + \sum F_{p-w}, \]  

\[ \mathbf{I}_j \frac{d\mathbf{\omega}_j}{dt} = \sum \mathbf{M}_f + \mathbf{M}_r, \]  

The fluid phase is governed by continuity and momentum equations:

\[ \frac{\partial \alpha_I}{\partial t} + \nabla \cdot (\alpha_I \rho \mathbf{V}_I) = 0, \]  

\[ \frac{\partial}{\partial t} (\alpha_I \rho \mathbf{V}_I) + \nabla \cdot (\alpha_I \rho \mathbf{V}_I \otimes \mathbf{V}_I) = -\alpha_I \nabla \rho - \nabla \cdot (\alpha_I \mu (\nabla \mathbf{V}_I)) - \mathbf{S}_p + \alpha_I \rho \mathbf{g}, \]  

where \( U_j \) and \( \mathbf{V}_I \) are velocities of particle \( j \) and fluid velocity in cell \( I \) (throughout the paper,
“U” stands for particle and “V,” for fluid). \( m_j, D_j \) and \( \mathbf{I}_j \) respectively, are the mass, volume
and rotational inertia of Particle \( j \), \( \rho \) is the ambient pressure, \( \mathbf{g} \) is gravitational acceleration.
\( F_{\text{drag}} \) is the drag force exerted on the particle by surrounding fluid (without pressure
gradient), \( F_{p-p} \) is the particle-particle interaction force and \( F_{p-w} \) is the particle-wall
interaction forces; In our case, Hertz model is adopted to calculate the collision forces, where
normal collision force \( F_n = -K_n \delta_n^{3/2} \) and tangential collision force \( F_l = F_{l0} + K_l \delta_l \), in which
\( K_n, K_l \) are normal elastic constant and tangential incremental stiffness, \( \delta_n \) and \( \delta_l \) are
the displacements, \( F_{l0} \) is the original tangential force considering loading history, and details
can be found in (Renzo and Maio, 2004; Stevens and Hrenya, 2005). $M_t$ is the moment generated by tangential forces exerted by other particles and $M_r$ is the rolling friction torque (Zhu et al., 2007). In momentum equations, $\alpha_I$ is fluid fraction of cell $I$, $\rho$ is density of fluid, $\mu$ is dynamic viscosity of fluid and $S_p$ is the source term governing the momentum exchanges between fluid and particle. Calculation of the source term $S_p$ and particle-fluid interaction force $F_{drag}$ depends on the force model chosen in the simulation.

In present work, we used FVM to simulate the fluid flow, DEM to simulate the movement and collision of particles. The interaction between fluid and particles depends on the modeling methods, either unresolved or resolved.

2.2 Implementation of unresolved methods

In unresolved methods, the fluid force exerting on particles, $F_{p-f}$, is implemented using empirical force models. The source term, $S_p$, is calculated by the sum of $F_{p-f}$ over all the particles within the cell, divided by the cell volume. Implementation of these equations in this work is based on an open source code named CFDEM (Goniva et al., 2012), which couples CFD and DEM methods with both resolved and unresolved methods. For unresolved solvers, codes in CFDEM are developed according to Zhou’s classic work in 2010 (Zhou et al., 2010) which describes the development, theory and force models in unresolved modeling methods of particle-laden flows in details.

A step-by-step implementation of the CFD-DEM unresolved methods is listed as follows (Figure 1):

- Set the initial and boundary conditions for DEM and CFD solvers.
- Solving N–S equation (without source term $S_p$) using FVM to predict the fluid field.
- Get DEM data such as velocities and positions of the particles at initial time step (or latest time step) from DEM solver and determine the ID of their owning cells, and calculate the void fraction of both particle and fluid phase.
- Choose a suitable force model to calculate the drag force on particles and send this information back to DEM solver for the initialization of the next time step.
- Take the sum of the calculated drag forces weighed by particle void fraction as the source term $S_p$ in the N–S equations, and solve N–S equation (with source term $S_p$) using FVM to correct the fluid field obtained in Step 2.
- Continue until the final time step.

Figure 1. Flowchart of the unresolved CFD-DEM coupling
2.3 Implementation of resolved methods

In resolved modeling methods, the fluid force exerting on particles, $F_{p-f}$, is implemented using some kind of boundary-capturing algorithm such as immersed boundary method. In traditional IBM, the boundary (either deformable or not) of a moving object immersed in fluid is often represented by a set of Lagrangian points and the movement of these points describe the movement (with possible deformation) of the object. The immersed object is considered as a kind of momentum force in the N–S equation (term $S_p$ in equation (4)), rather than a real body, which avoids the challenge of generating a body conformable grid.

The present work on resolved modeling is also conducted with CFDEM. As illustrated in Figure 2, the stepwise procedure of FVM-DEM coupling with IBM is as follows.

3. Velocity similarity in particle sedimentation

Similarity exists in many cases in nature and mathematics such as the self-similarity of coastlines, leaves and fractals, as well as different kinds of fields in physics such as fluid field or magnetic field. Among them, velocity similarity is one of the most important similarities and widely exists in different flow patterns. In submerged jet flow, velocity similarity was first experimentally and theoretically studied by Albertson et al. (1948), and they gave a series of laws that the velocity field in the jet should obey quantitatively. Wygnanski et al. (1986) studied the similarity turbulence flow behind a 2D cylinder, airfoil and a flat plate and gave some theoretical analysis. For turbulent flows, Pope (2000) also mentioned that the normalized velocity deficit profile of the wake behind a sphere in fully developed turbulence follows Gaussian distribution, which was also observed in experiment by Uberoi and Freymuth (1970).

In this section, the velocity field in the wake behind a settling particle is numerically investigated using a resolved approach, in which FVM is used to model the fluid flow, DEM is used to simulate the motion and interactions of particles and IBM is used to tackle fluid solid interaction. We will show that the velocity field of a settling particle at moderate Reynolds numbers demonstrates similarity, and this velocity similarity can be analytically expressed as a general scaling law after a series of normalization.

In particle settling, after several simulation steps, it is found that the magnitude of velocity in the main settling direction is much larger than that of the transverse velocity [see Figure 3(b)], thus it contributes the most to the wake behind the settling particle and is of great importance in wake-affected phenomena such as DKT phenomenon or particle clustering. The transverse velocity is one order smaller than the vertical velocity, as shown.

![Figure 2. Flowchart of the resolved CFD-DEM coupling](image-url)
in Figure 3(b), and is easily disturbed by vortices and other small flow features, therefore only the vertical velocity was considered in this work.

In the experiment by Uberoi and Freymuth in 1970, they found the normalized velocity deficit profile of the wake behind a sphere in turbulence can be expressed as \( \exp(-\ln 2\zeta^2) \), where \( \zeta \) is the distance normalized by the diameter of the sphere (Uberoi and Freymuth, 1970). However, we find this formula does not fit well with the velocity profile of the wake behind a settling sphere since in Uberoi and Freymuth’s experiment, the downstream flow is fully developed and the wake length almost remains a constant. During the particle settling process, the wake grows with time. Therefore, it is not suitable to describe the normalized velocity field in the wake with a distance normalized by the diameter of the particle, and instead, we use the length of the wake to normalize the distance. Later on, we will see this approach can describe the velocity scaling law quite well.

In our case, firstly, we have to define the length of wake. As the wake smoothly decays as distance increases, for the moment, we define the boundary of the wake by the velocity contour where velocity magnitude equals to 5 per cent of the velocity of the particle, which will not affect the velocity prediction by the to-be-obtained scaling law.

To estimate the length of the downstream wake, we firstly solve the terminal velocity of a settling particle according to Newton’s second law of force, which is written as:

\[
m \frac{dU}{dt} = (\rho_p - \rho) \frac{\pi}{6} D^3 g - \frac{1}{2} C_d \rho U^2 \rho D S U^2,
\]  

where \( m \) is the mass of the particle, \( U \) is magnitude of the settling velocity of the particle, \( \rho_p \) is the density of the fluid, \( \rho \) is the density of the fluid, \( D \) is the diameter of the particle, \( g \) is the magnitude of gravitational acceleration, \( C_d \) is the drag force coefficient and \( S \) is the projected area of the particle and \( S = \frac{\pi D^2}{4} \).
After some trivial transformation, equation (5) can be written as:

$$\frac{dU}{dt} + \frac{3C_dA\rho}{\pi D^2 \rho_p} U^2 = \frac{\rho_p - \rho}{\rho_p} g.$$  \hspace{1cm} (6)

Comparing equation (6) with the following equation containing the derivative of a hyperbolic tangent function:

$$\frac{dtanh(t)}{dt} + tanh^2(t) = 1,$$  \hspace{1cm} (7)

We can assume that the settling velocity $U = A \tanh(Bt)$, where $A$ and $B$ are to be determined coefficients. Substituting $U = A \tanh(Bt)$ into equation (7), and comparing it with equation (6), coefficients $A$ and $B$ are obtained as:

$$A = \sqrt{\frac{\rho_p - \rho}{\rho_p} g \frac{4D}{3C_d}}; \quad B = \sqrt{\frac{\rho_p - \rho}{\rho_p} g \frac{3C_d}{4D}}.$$  \hspace{1cm} (8)

It should be noted that $A$ is the terminal velocity $U_t$ for particle sedimentation that we endeavor to find. Therefore settling velocity with time is also obtained:

$$U = U_t \tanh(Bt) = \sqrt{\frac{\rho_p - \rho}{\rho_p} g \frac{4D}{3C_d}} \tanh \left( \sqrt{\frac{\rho_p - \rho}{\rho_p} g \frac{3C_d}{4D}} \right).$$  \hspace{1cm} (9)

As such, the wake length of a straight-settling particle can be approximated by the distance that the particle covers during the sedimentation:

$$L = A \int_0^t \tanh Btdt = \frac{A}{B} \ln \cosh Bt = -\frac{A}{2B} \ln \left( 1 - \frac{A^2 \tanh^2 Bt}{A^2} \right)$$

$$= -\frac{2\rho_p D}{3C_d \rho} \ln \left[ 1 - \left( \frac{U}{U_t} \right)^2 \right].$$  \hspace{1cm} (10)

After some trivial transformation, we can get the following expression:

$$\frac{L}{D} = -\kappa \frac{\rho_p}{\rho} \ln \left[ 1 - \left( \frac{U}{U_t} \right)^2 \right].$$  \hspace{1cm} (11)

where $\kappa = \frac{4}{3}$ is an empirical coefficient which is believed to be related to the definition of wake length. In numerical simulations, the boundary of the wake is defined as the velocity contour where velocity magnitude equals to 5 per cent of the velocity of the particle $U$. The obtained formula corresponds well with the simulation results, as shown in Figure 4 (dash line). However, the calculated $\frac{L}{D}$ is a little bit smaller than the simulations results at low settling velocities, a possible explanation is that the viscous layer around the particle makes the wake longer than expected. Therefore, we introduce a corrector to remedy the deviation (solid line):
\[
\frac{L}{D} = -k \frac{\rho_r}{\rho} \ln \left[ 1 - \left( \frac{U}{U_t} \right)^2 \right] - 4.5 \left( \frac{U}{U_t} \right)^2 + 3.825 \frac{U}{U_t} . \tag{12}
\]

It should be noted that, it is highly possible for the downstream wake to be interrupted during sedimentation. If the interruption is not happening right behind the particle, the main flow structure at the trailing edge of the settling particle will still preserve similarity. Based on such assumptions, we use the aforementioned wake length \( L \) to normalize the downstream distance \( Z \) (from the point to the particle’s trailing edge), thus the normalized distance \( z = \frac{Z}{L} \), as is shown in Figure 5. Similarly, the normalized vertical velocity of the fluid along the wake axis \( V_{zn1} \) is normalized by the particle velocity \( U \) as \( V_{zn1} = \frac{V_{z|\tau=0}}{U} \), where \( V_{z|\tau=0} \) is the velocity of fluid along the central wake axis \( Z \).

After the normalization, as shown in Figure 6, the vertical velocities along the central axis of the wake at different Reynolds number stand closely in a Gaussian curve. Thus similar to Uberoi and Freymuth’s Gaussian fitted curve obtained from experiment, a new scaling law for vertical velocities is given as:

\[
V_{zn1} = \frac{V_z|_{\tau=0}}{U} = \exp \left( -\beta_1 z^2 \right) , \tag{13}
\]

where \( \beta_1 \) is a coefficient measured as 4.617. As shown in Figure 6, the fitted Gaussian curve can basically describe the velocity profile along the wake axis. For more accurate results, we calculated the difference between the data and the Gaussian curve shown in equation (12), it is found that these small deviations also exhibit similarity in shape, and the only difference is the magnitude. For example, after normalization, \( Corr_3 \) is a two-peak curve [Figure 7(d)], which can be effectively approximated using equation (17).

Hence, after further corrections, the final scaling law is written as:

\[
V_{zn1} = \exp \left( -\beta_1 z^2 \right) \\
+ \left\{ \begin{array}{ll}
(0.0005625Re^2 - 0.01138Re + 0.6636)Corr_1 & 0 \leq Re \leq 100 \\
Corr_2 & 100 < Re < 150, \\
(0.00222Re - 0.239)Corr_3 & 150 \leq Re \leq 200
\end{array} \right. \tag{14}
\]
$$\text{Corr}_1 = (-14.86z + 1.403) \sin (6z - 1.443z^2) \exp (-3.788z),$$  \quad (15)

$$\text{Corr}_2 = 0.174z \cdot \exp \left(-6.263(z - 0.346)^2\right),$$  \quad (16)

$$\text{Corr}_3 = 1.228 \exp \left(-(14.3z - 1.924)^2\right) - 0.52 \sin (6.45z) + 0.438 \sqrt{z},$$  \quad (17)
where $Re$ is the particle Reynolds number defined as $Re = \frac{|U_i - V_i|D}{C_0V_i}$. The first and second correctors only make minor changes on the shape, but the third one are meant to reproduce the little “peak” of the velocity profile close to the trailing edge of the particle, which is actually caused by the vortex and backflow. As Reynolds number continues to grow, the vortex becomes stronger and even sheds from the particle, which makes the velocity profile

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig7.png}
\caption{Normalized vertical velocity along the wake's central axis at different $Re$ (a) and the fitted curves for $V_z|_{z=0}$ when $Re \leq 100$ (b), $100 < Re < 150$ (c) and $150 \leq Re \leq 200$ (d).}
\end{figure}
behind particle unpredictable, and destroys the similarity, thus in our present work, only cases with moderate Reynolds number (up to around 200) are studied.

Obviously, all these correction have a zero value when $z = 0$. The corrected fitted curve can well describe the profile at different Reynolds number, as are shown in Figure 7(a)-(c).

Similarly, the vertical velocity along the wake cross-section can also be normalized. The normalized wake width is defined as $w = \frac{r}{D}$, where $r$ is the distance to the wake axis, as shown in Figure 5. The vertical velocity in the wake cross-section is then normalized as $V_{2n2} = \frac{V_z}{V_z|_r=0}$, where $V_z$ is the velocity of the fluid and $V_z|_r=0$ is the vertical velocity along the wake’s central axis.
After normalization, points stand in series of queues similar to Gaussian error function erf, as is illustrated in Figure 8:

\[ V_{Zn} = \frac{1}{2} [1 - \text{erf}(\beta_z(w - w_d))]. \]  

(18)

In the figure, these series of velocity profiles decay rapidly around \( w_d = \frac{r}{D} = 0.53 \), and that is a distance a little bit farther than the particle boundary \( w_b = \frac{r_{\text{boundary}}}{D} = 0.5 \), which indicates that the wake width just roughly covers the particle diameter. However, the velocity deficit becomes moderate as \( z \) increases, thus the coefficient \( \beta_2 \) drops, and are fitted as (Figure 9):

\[ \beta_2 = 5.8 \exp (-12.4z) + 2.5. \]  

(19)

Since both the normalized velocities along the wake’s central axis and within the cross-section are well-fitted with analytical expressions, the whole velocity in the wake behind a settling particle for small and moderate Reynolds numbers can be described as:

\[ V_Z = V_{Zr=0} V_{Zn} = V_{Zn1} V_{Zn2} U. \]  

(20)
4. A novel velocity corrected unresolved method (VCUM)

In unresolved modeling methods, the velocity field in the FVM cell is considered as a constant equal to the velocity at the cell center when coupled with DEM, making it unable to describe the wake behind a particle. Since the normalized velocity field in the wake is a Gaussian-like distribution, with a sharp velocity drop as the downstream distance increases. When another particle $j$ enters particle $i$'s wake and becomes very close to particle $i$, particle $j$ will be subject to a strong drag force caused by the wake behind particle $i$, leading to phenomena such as DKT and particle clustering, which cannot be simulated by existing unresolved force models yet widely exits in nature and industry.

The velocity similarity in the wake holds true for different circumstances at low and moderate Reynolds number, especially for the close-to-particle region. It is therefore natural to consider correcting the velocity field around a moving particle in unresolved modeling by incorporating this analytical expression of velocity similarity. One problem is how to calculate the wake length in these circumstances. The wake length discussed above is based on sedimentation, which means the initial velocity of the particle is zero or quite small and will eventually reach a terminal velocity. However in reality, a particle can hardly flow in the same direction all the time and the velocity might exceed its terminal velocity due to external forces from the fluid or collision with other particles or walls. If these scenarios happen in natural particle sedimentation, the errors between the calculated velocity and its real velocity will be minute because the particle velocity won't have a prominent change when particles collide into each other in viscous medium after they reaches the terminal velocity, and so is the structure of the wake. If the velocity of the particle exceeds its terminal velocity to a large extend or make a very sharp turn in a few time steps, which of course can hardly happen in natural sedimentation, the wake length model has to be corrected and validated. In this section, only natural sedimentation will be discussed.

To implement the wake into unresolved methods for particle sedimentation, there are few steps to follow:

- Calculate the unit vector of wake direction of particle $i$ as:

$$
W_i = \frac{V_i - U_i}{|V_i - U_i|},
$$

(21)

Where $U_i$ is the velocity of particle $i$ and $V_i$ is the velocity of cell $I$ (Figure 10).

- Calculate the wake length $L_i$ of particle $i$ by the relative velocity between particle $i$ and cell $I$, the diameter of particle $i$, $D_i$, density ratio and the terminal velocity of particle $i$ $U_{ti}$. Thus the wake length vector becomes:

$$
L_i = L_i W_i
= \left\{ -\kappa \frac{\rho_p}{\rho} D_i \ln \left[ 1 - \left( \frac{|U_i - V_i|}{U_{ti}} \right)^2 \right] - 4.5 \left( \frac{|U_i - V_i|}{U_{ti}} \right)^2 + 3.825 \frac{|U_i - V_i|}{U_{ti}} \right\} W_i,
$$

(22)

However, in real application, we will truncate the wake length when the velocity of the particle approaches the settling velocity because the wake structure remains unchanged as the motion of particle becomes stable.
• Search particles in neighboring cells and judge whether they are in the possibly-affected region, a sphere region with a radius equal to the wake length of particle \( i \) at that time step (Figure 11), and if not, terminate the calculation.

• Judge whether particle \( j \) is at the same side with the wake of particle \( i \) (Figure 12) by:

\[
\text{sgn} \left[ (r_j - r_i) \cdot W_{mi} \right] \begin{cases} 
\geq 0 & \text{same} \\
< 0 & \text{different}
\end{cases}
\]

(23)

if particle \( j \) is at a different side, terminate the calculation.

Calculate the relative distance along wake direction \( d_{//} \) and the relative distance perpendicular to the waked \( d_{\perp} \), as shown in Figure 12:

\[
d_{\perp} = \| (r_j - r_i) \times W_{mi} \|,
\]

(24)

\[
d_{//} = \sqrt{\| r_j - r_i \|^2 - d_{\perp}^2},
\]

(25)

• As mentioned before, the width of the downstream wake roughly covers the particle diameter, hence we can use a distance larger than \( w_d D_i \) to judge whether particle \( j \) is in the wake of particle \( i \). In our case, for simplicity, if \( d_{\perp} < D_i = 1.89 w_d D_i \), the calculation proceeds, else aborted.

Figure 10. Relative velocity between particles and its owner cell

Figure 11. Schematics of relative position between neighboring particles and the wake
Drag force exerted on particle $j$ in cell $I$ by the wake generated particle $i$ is calculated by drag force models such as Gidaspow model or modified Hill–Koch model (Benyahia et al., 2006). In these models, the relative velocity between particle $j$ and fluid cell $I$ is originally approximated by $V_I - U_j$. It is noted that as velocity is constant in the cell in conventional resolved methods, it is not possible to reproduce wake effects of particles. Since the velocity field around a settling particle can be analytically expressed in equation (20), it is natural to correct the relative velocity between particle $j$ and fluid cell $I$ as:

$$V^* = V_I + (U_i - V_I) V_{Zn2} V_{Zn1} |_{j\text{-position}} - U_j$$

(26)

However, when particle $j$ is in the wakes of different particles at the same time, the relative velocity will be quite complicated and it is simply estimated by the sum of the velocity vectors for convenience:

$$V^* = (V_I + V_{Zn2} V_{Zn1} |_{r=0}) - U_j = V_I + \sum_{i \in \text{Wake}} (U_i - V_I) V_{Zn2} V_{Zn1} |_{j\text{-position}} - U_j,$$

(27)

Similarity, the particle Reynolds number of particle $j$, $Re_j = \frac{V_j D_j}{\mu}$, is corrected when calculating the drag force coefficient, where $D_j$ is the diameter of particle $j$.

Taking modified Hill–Koch drag model for an example, the drag force is obtained:

$$F_{\text{drag}} = \frac{\pi \beta D_j^2 V^*_r}{6 \alpha_j},$$

(28)

where $\beta$ is an empirical coefficient related to particle void fraction $\alpha_j$ and Reynolds number (Hill et al., 2001). Thus the source term $S_p$ in equation (4) is given as:
\[ S_p = \frac{1}{V_{Cell}} \sum_{ij \in \text{Cell}} \frac{\pi \beta D_i^3 V_i^*}{6 \alpha_i} D(r - r_j), \]  

where \( D \) is a distribution function that distributes the reaction forces on fluid phase at the velocity nodes in staggered Eulerian grids (Hill et al., 2001).

The flow chart of the whole procedure of velocity correction in an unresolved modeling method is shown in Figure 13.

5. Model validation

In this section, the settling process of dual particles and an amount of particles are modeled by the conventional unresolved method and VCUM. The simulation results of dual particle sedimentation are compared with those from resolved modeling of CFD-DEM coupling approach IBM. The implementation of the velocity correction is realized based on the modified Hill–Koch drag model, where the relative velocity between particles and fluid is corrected by using wake’s velocity-similarity. In the following simulation, the particle’s diameter is 0.00165 m, density is 1,500 kg/m³, coefficient of restitution is 0.3, coefficient of friction is 0.5, the size of resolved mesh is around 0.0069 m.

5.1 Settling process of dual particles

Figures 14-16 show the settling process of dual particles simulated with conventional unresolved method, VCUM and IBM. From Figure 14 we can see that the conventional unresolved method without velocity correction can hardly reproduce DKT phenomenon,
and the distance between upper and lower particle almost keep unchanged during the settling process. After the correction, the relative velocity between the upper particle and fluid becomes smaller because of the effect of the wake, thus the resistance force exerted by the fluid is also reduced, making the upper particle chase the lower one. Before the velocity

**Figure 15.**
Snapshots of dual-particle settling obtained using VCUM with velocity correction

*Note:* The drafting–kissing phenomenon is well simulated by present unresolved method with velocity correction

**Figure 16.**
Snapshots of dual-particle settling obtained by IBM

*Note:* The obtained drafting–kissing phenomenon is close to that from the present unresolved method with velocity correction

**Figure 17.**
Qualitative comparison of the distance between two particles obtained by conventional unresolved CFD-DEM with/without velocity correction and IBM
correction, hardly can the upper particle get any closer to the lower one for lack of the wake generated by the lower particle. During the “kissing” stage when the upper particle touches the lower one and stands upon its top, balance of the upper particle becomes unstable and can break easily. However, due to all kinds of disturbances in the fluid field in reality or numerical errors in simulation, the upper particle will falls down very soon after the encounter, as simulated by IBM and the present unresolved method with velocity correction. More importantly, the obtained drafting–kissing phenomenon from the present VCUM (Figure 15) is very close to that from resolved modeling in Figure 17.

The distance between the two particles obtained by conventional unresolved CFD-DEM, VCUM and IBM are qualitatively compared in Figure 19, results from VCUM and IBM are fairly close during drafting and kissing stages, however, it still has difficulties in reproducing the tumbling stage because the upper particle moves out of the wake of the lower particle and the wake produced by particle rotation is also not considered. It is believed that the tumbling phenomena can be reproduced if the velocity similarity of a rotating sphere is studied and added to the model, but this will not be discussed in present work.

Except for accuracy, as shown in Table I, a comparison of the computational time for dual-particle settling between the present VCUM and the resolved method is also

<table>
<thead>
<tr>
<th>Coupling method</th>
<th>Mesh refinement</th>
<th>CPU time</th>
</tr>
</thead>
<tbody>
<tr>
<td>IBM</td>
<td>Around 32,500 cells with dynamic refinement at every step</td>
<td>11,309 s</td>
</tr>
<tr>
<td>VCUM</td>
<td>128 structured cells</td>
<td>218 s</td>
</tr>
</tbody>
</table>

Table I. A comparison of the computational time between the present VCUM and resolved IBM for dual particle settling

Figure 18. Snapshots of sedimentation of a list of particles obtained by conventional unresolved method

Figure 19. Snapshots of sedimentation of a list of particles obtained by VCUM

Note: Clustering is well reproduced
conducted. It is noted that in the resolved coupling, the meshes are dynamically refined as the solid-fluid interface moves. The number of the cells is around 32,500 and it takes over 11,309 s to finish the simulation. In contrast, the present VCUM uses a coarse mesh with 128 structured cells and only takes 218 s. It is clear that compared with IBM, the present VCUM can great save computational cost while obtaining comparable results, which are more physical and reasonable than those from conventional unresolved method.

5.2 Settling process of a column of particles
Figures 18-19 show the simulation results of the settling process of a list of particles. Again, the positions of the particles obtained from conventional unresolved method do not change much, and it is not able to reproduce DKT phenomenon or clustering, but for VCUM, wake-affected phenomena become more observable. If the particle number increases, as are shown in Figures 20 and 21, the series of particles cluster at the front in both cases because of the strong influences exerted by nearby particles, however, the simulation without velocity correction provide a result with a long “tail”, but when the wake’s effect is considered, the clustering phenomenon becomes more conspicuous. Thus we can conclude, our correction can actually make a difference for unresolved simulations.
6. Conclusion
In this paper, a velocity corrected unresolved method is presented to reproduce the wake effects in unresolved simulation of particle-laden flows. We first studied the detailed velocity field around a settling particle with resolved meshes based on FVM-DEM coupling and found the velocity similarity behind a settling particle at moderate number Reynolds numbers. This velocity similarity can be analytically expressed as a general scaling law after a series of normalization, and is then used in unresolved modeling to correct the relative velocity between a particle and surrounding fluid within the wake area. As such, the wake effect of a particle on a neighboring particle within its wake can be considered, and wake-related phenomena such as DKT and clustering can be captured in unresolved modeling of particle-laden flows. To validate this velocity corrected unresolved method (VCUM), the settling process of dual particles, particle list and large amount of particles are comparatively modeled with the conventional unresolved method and VCUM. It is found that different from conventional coupling, the present VCUM can effectively capture wake-related phenomena such as drafting and kissing or particle clustering. Moreover, the obtained phenomenon from present VCUM is very close to that obtained by IBM with much finer mesh. We conclude that the present VCUM can obtain results comparable with those from resolved methods while the computational effort can be significantly reduced.

Similarity of the traverse velocity can also be studied in a similar way, as well as other complicated flow patterns around the sphere, like the flow caused by a rotating sphere. Interestingly, the velocity profile of the wake behind a particle in a fully developed turbulent flow also exhibit similarity even Reynolds number increases, therefore it is possible that similar velocity-correcting treatment can also be introduced to turbulent particulate flows on unresolved meshes. This can be beneficial for unresolved method which is often used in large-scale simulations for industrial problems.

References


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