Numerical modeling of fluid-particle interaction in granular media

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Abstract Fluid-particle interaction underpins important behavior of granular media. Particle-scale simulation may help to provide key microscopic information governing the interaction and offer better understanding of granular media as a whole. This paper presents a coupled computational fluid dynamics and discrete element method (CFD–DEM) approach for this purpose. The granular particle system is modeled by DEM, while the fluid flow is simulated by solving the locally averaged Navier–Stokes equation with CFD. The coupling is considered by exchanging such interaction forces as drag force and buoyancy force between the DEM and CFD. The approach is benchmarked by two classic geomechanics problems for which analytical solutions are available, and is further applied to the prediction of sand heap formation in water through hopper flow. It is demonstrated that the key characteristic of granular materials interacting with pore water can be successfully captured by the proposed method. [doi:10.1063/2.1302107]

Keywords granular media, fluid-particle interaction, coupled CFD–DEM, single particle settling, 1D consolidation, sand pile, pressure dip

Fluid-particle interaction is accountable for a wide range of complex phenomena relevant to granular materials. Pore fluid in a granular medium may fluctuate or flow under various forces, which could lead to particle motion. This may sometimes be advantageous, such as in the case of sand production in oil reservoir, or become adverse, like in the case of internal/surface erosion of embankment dams and soil slopes which is widely regarded as the major trigger of instability and failure of these structures.[1] While traditional continuum theories of porous media have been limited in many ways towards better understanding the interaction between fluid and particles, a particle-scale modeling approach could provide quantitative characterization of the microscopic behavior of the interaction and could facilitate the establishment of general methods for reliable scale-up, design and control of different particulate systems and processes.[2] A number of collective attempts have been made on the modeling of fluid-particle interaction, among which discrete element method (DEM) plays a key role. In particular, numerical approaches combining the computational fluid dynamics (CFD) and DEM (CFD–DEM) prove to be advantageous over many other options such as lattice-Boltzman and DEM coupling (LB–DEM) method and direct numerical simulation (DNS) coupled DEM (DNS–DEM) in terms of computational efficiency and numerical convenience.[3] The CFD–DEM method has gained some success in application to chemical and mining engineering and powder industries.[2] Meanwhile, there has been a growing interest in the community of geomechanics in exploring the particle-level information on fluid-particle interaction, in sought for key mechanisms and mitigating measures for various geotechnical hazards such as landslide and debris flow. With limited effort being made in this field, this paper aims to develop a coupled CFD–DEM numerical method to model problems relevant to geotechnical engineering.

Following a typical solution procedure, we solve the Newton's equations for the motion of the particle system by DEM, and the Navier–Stokes equation by CFD for the fluid flow, by considering suitable coupling between DEM and CFD.[1,3,4] The key to the coupling between CFD and DEM is a proper consideration of the particle-fluid interaction forces. While the study is focused on granular materials interacting with fluid with relatively low Reynolds number, the interaction forces being considered here include the drag force and buoyancy force only. The expression of drag force $\boldsymbol{F}^{\mathrm{d}}$ for a system of particles in fluid used by Tsuji et al.[4] is employed in this study

$$\boldsymbol{F}^{\mathrm{d}} = \frac{1}{8} C_{\mathrm{d}} \rho \pi d_{\mathrm{p}}^2 \left(\boldsymbol{U}^{\mathrm{f}} - \boldsymbol{U}^{\mathrm{p}}\right) \left|\boldsymbol{U}^{\mathrm{f}} - \boldsymbol{U}^{\mathrm{p}}\right| n^{1-\chi}, \qquad (1)$$

where d_{p} is the diameter of the considered particle, $\boldsymbol{U}^{\mathrm{p}}$ is the velocity of the particle, $\boldsymbol{U}^{\mathrm{f}}$ is the average velocity of a fluid cell, ρ is an averaged fluid density defined by $\rho = \alpha\rho_{\mathrm{w}} + (1-\alpha)\rho_{\mathrm{a}}$, $\alpha = v_{\mathrm{w}}/v_{\mathrm{c}} = 1 - v_{\mathrm{a}}/v_{\mathrm{c}}$, $n = v_{\mathrm{void}}/v_{\mathrm{c}} = 1 - v_{\mathrm{p}}/v_{\mathrm{c}}$. n defines the porosity (void fraction), α is the volume fraction of water phase in a cell, v_{w} is water phase volume, v_{a} is air phase volume, v_{void} is the total volume of air and water phase, v_{p} is the volume of particles occupied in a cell and v_{c} is the total volume of a cell. Evidently, if $\alpha = 1$, the cell will be fully occupied by water. If $\alpha = 0$, it indicates an all-air cell. If $0 < \alpha < 1$, it corresponds to either a cell locating at the air–water interface or there are particles in it. C_{d} and χ depends on the Reynolds number of the

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particle Re_p

$$C_\mathrm{d} = \left(0.63 + \frac{4.8}{\sqrt{Re_\mathrm{p}}}\right)^2,$$
$$\chi = 3.7 - 0.65\exp\left[-\frac{(1.5 - \lg Re_\mathrm{p})^2}{2}\right], \quad (2)$$

where the particle Reynolds number is determined by[1]

$$Re_\mathrm{p} = \frac{n\rho d_\mathrm{p}\left|\boldsymbol{U}^\mathrm{f} - \boldsymbol{U}^\mathrm{p}\right|}{\mu}. \quad (3)$$

The following expression is adopted for the buoyancy force

$$\boldsymbol{F}^\mathrm{b} = \frac{1}{6}\pi\rho d_\mathrm{p}^3\boldsymbol{g}, \quad (4)$$

where $\boldsymbol{g}$ is the gravity constant.

In the coupling CFD–DEM scheme, the fluid phase is discretized with a typical cell size five to ten times of the average particle diameter. At each time step, the DEM code employs a Hertzian contact law in conjunction with Coulomb's friction law and solves the Newton's motion equation of the system to provide such information as the position and velocity of each individual particle. The positions of particles are matched with the fluid cell to calculate relevant information of each cell such as the porosity. By following the coarse-grid approximation method proposed by Tsuji et al.,[4] the locally averaged Navier–Stockes equation is solved by the CFD program for the averaged velocity and pressure for each cell by the InterDyMFoam solver. These obtained average values for velocity and pressure of a cell are then used to determine the drag force and buoyancy force acting on the particles in that cell. Iterative schemes have to be followed to ensure the convergence of relevant quantities such as fluid velocity and pressure. When a converged result is obtained, information of fluid-particle interaction forces will be taken into account for the next step calculation of the DEM part.

Ideally, information on the interaction forces should be exchanged once after each step of calculation for DEM or CFD. This, however, may be computationally extremely expensive in practice. For the problems to be treated in this paper, numerical experience indicates for each CFD computing step, exchange of information after 100 steps of DEM calculation will ensure sufficient accuracy and efficiency. If the time steps for DEM and CFD are sufficiently small, more steps for DEM are normally acceptable.

The CFD–DEM program has been first benchmarked by two classic geomechanics problems where analytical solutions are available: the single particle settling problem and the one dimensional (1D) consolidation problem. In the single particle settling problem, a spherical particle of 1 mm diameter is dropped from 45 mm high from the center of a container with $L \times W \times H = 20$ mm $\times$ 10 mm $\times$ 50 mm. The container

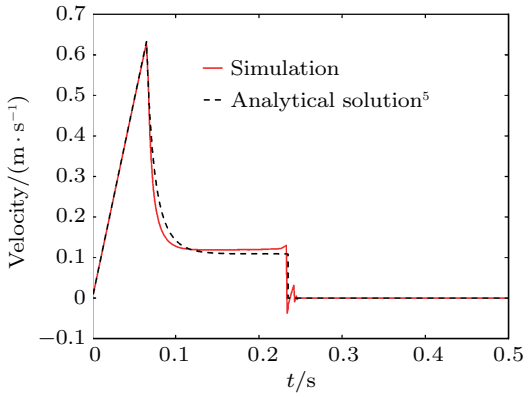

Fig. 1. Comparison of the CFD–DEM predicted particle settling velocity with the analytical Stokes solution for a spherical single particle settling into water.

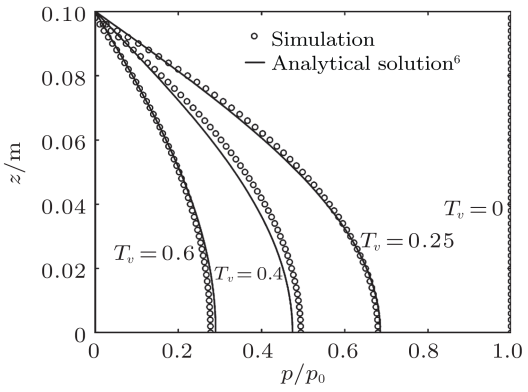

Fig. 2. Predicted dissipation of excess pore pressure by CFD–DEM for the 1D consolidation problem in comparison with Terzaghi's analytical solution.

is half-filled with water. The settling velocity of the particle will be of major interest. In Fig. 1, the predicted settling velocity of the particle dropping from the air and settling into the water of the container is compared with the analytical solution by Stokes[5]. Evidently, the numerical prediction captures well the sharp reduction of velocity when the particle hits the water surface and makes entry into the water ($t = 0.075$ s) and bounces back from the bottom of the container ($t = 0.235$ s). It also agrees well with the analytical solution.

The second benchmark problem is the classical 1D consolidation problem in soil mechanics. Terzaghi[6] has derived a 1D consolidation theory governing the settlement and the dissipation of excess pore pressure in a one-way drained soil layer, which will be employed to benchmark our numerical prediction. A soil column of 100 equal size spheres saturated with water is considered in the simulation of the 1D consolidation problem. All spheres are initially placed at the center line of the column without any overlap. When they are emerged in water, the gravitational force and the buoyancy force are switched on to allow the particles to settle to a hydrostatic state. Once the initial consolidation is fin-

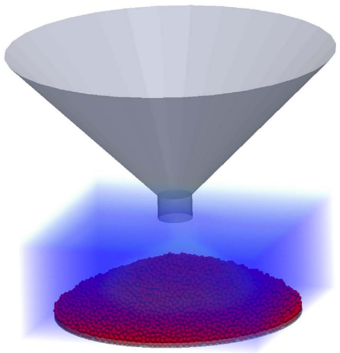

Fig. 3. Simulated process of formation of sand pile into a water container through hopper flow.

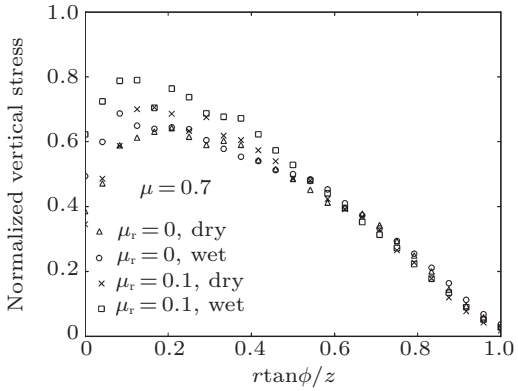

Fig. 4. Predicted vertical stress profile for dry and wet cases, with and without consideration of rolling resistance.

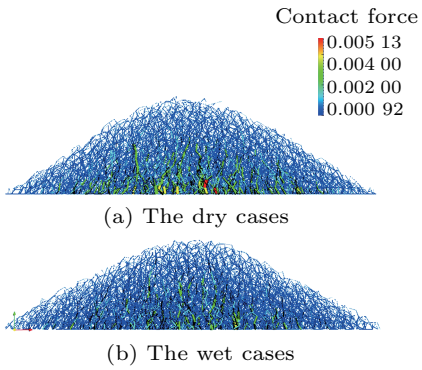

Fig. 5. Comparison of the contact force network in the sand pile.

ished, a surface load is then applied at the top of the column. The simulated dissipation process of normalized excess pore pressure (P/P_0, where P_0 is the surface charge pressure) across the height of the soil column z is presented in Fig. 2, in comparison with the analytical solution by Terzaghi's theory. T_v in Fig. 2 denotes a normalized time used by Terzaghi.[6] The overall predictions are in good agreement with the Terzaghi's analytical solution.

The CFD–DEM program has also been employed to investigate the formation of sand pile in water through hopper flow. Figure 3 presents a snapshot of the simulated process of the hopper flow of particles into water to form a sand pile. In simulating the sand pile problem, we have considered the rolling resistance between particles as well. To ensure the formation of proper sand pile, in particular in the case without rolling friction, a small round baffle is used to bound the receiving panel as can be seen from Fig. 3. The vertical pressure profiles at the base of the sand pile for the different cases are presented in Fig. 4. In this figure, the vertical pressure has been normalized by $\rho g H$, where H is the pinnacle height of the sand pile, g is times by the gravity acceleration, and ρ is the average density of the sand pile. As can be seen, the overall profile of the pressure in the wet cases is slightly higher than the dry cases. The presence of water, however, may moderately reduce the pressure dip as compared to the dry cases. Consideration of rolling resistance may lead to enhanced pressure dip, and the difference is more appreciable in the wet cases than in the dry cases.

Figure 5 further presents a comparison of the contact force network in the sand pile formed in the dry and wet cases (rolling resistance is considered in the both cases). In the dry cases, appreciable inclined orientated strong force chains are observed to form an arch around the centre part of the sand pile which leads to a significant pressure dip. In the wet cases, the force chains are more vertically oriented and this prevent the formation of a strong arch to shield the bottom centre particles which evidently renders the pressure dip less strong as compared to the dry cases.

In summary, a CFD–DEM method has been developed to simulate the fluid-particle interaction in granular materials. The method has been benchmarked by two classic geomechanics problems and has been further applied to the investigation of sand pile formation in water. The numerical results well demonstrate the capability of the CFD–DEM program for particle-fluid system modeling.

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