A Coupled Analysis of Fluid-Particle Interactions in Granular Soils

Analyse couplée des interactions fluide-particules dans les sols granulaires

Zhao J., Shan T.
Department of Civil & Environmental Engineering, Hong Kong University of Science & Technology, Hong Kong

ABSTRACT: Fluid-particle interaction is important to a variety of geotechnical applications. Particle-scale simulation may help to provide key microscopic information towards better understanding of the behavior of granular soils. This paper presents a coupled Computational Fluid Dynamics and Discrete Element Method (CFD-DEM) approach to simulate the fluid-particle interactions in soils. The granular particle system is modeled by solving the Newton's equation of motion by DEM and the fluid (may comprise of both water and air) 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, buoyancy force and virtual mass force between the DEM and CFD computations. The numerical tool has been benchmarked by two classic geomechanics problems for which analytical solutions are available, the single particle settling problem and the one-dimensional consolidation problem. In both cases good comparisons are observed. It has been further applied to the prediction of sand heap formation in water through hopper flow. It is found the pressure dip of vertical stress profile underneath the sand pile appears to be moderately reduced by the presence of water, as compared to the dry case. Characteristics of force chain network in the former case become less heterogeneous.

RÉSUMÉ : L'interaction fluide-particules est de première importance dans un grand nombre d'applications géotechniques. Des simulations à l'échelle de la particule semblent être un moyen pertinent d'améliorer notre connaissance du comportement microscopique des matériaux granulaires. L'article présente une approche couplant Mécanique des Fluides et Modélisation Discrète (CFD-DEM) afin de simuler les interactions fluide-particules dans les sols. Le système granulaire est simulé par résolution des équations du mouvement de Newton par Méthode des Eléments Discrets, et l'écoulement du fluide (gaz et/ou liquide) est simulé par résolution de l'équation de Navier-Stokes moyennée localement. Le couplage CFD-DEM est réalisé par l'intermédiaire des forces d'interaction telles que trainée, poussée d'Archimède, et masse virtuelle. L'outil numérique a été validé sur deux problèmes géotechniques classiques pour lesquels les solutions analytiques sont connues : la chute libre d'une particule unique dans un fluide, et la consolidation unidirectionnelle. Il a ensuite été appliqué à la prédiction de la formation d'un tas de sable dans l'eau après écoulement en trémie. Il apparaît que le déficit de contrainte verticale au centre de la base du tas de sable est modérément réduit en présence d'eau en comparaison avec le cas du sable sec. Il semble également que la présence d'eau homogénéise le réseau des chaînes de forces.

KEYWORDS: Fluid-particle interactions, granular media, coupled CFD-DEM modeling, sand pile, anisotropy.

1 INTRODUCTION

Granular media exist in frequent form of two-phase system with stationary or moving fluids in the pores. The interactions between the fluid phase and the granular particles may play a key role in affecting the overall behavior of the material, which may sometimes work favorably for us, such as in sand production of oil reservoir, but on other occasions may cause generate adverse consequences, such as in the case of internal/surface erosion of embankments and debris flow and slope failures. Conventional approaches considering the coupling between fluid and granular particles have been mainly based on continuum mechanics and mostly phenomenological in nature. They cannot fully account for the microscopic origin of fluid-particle interaction and their impact on the macroscopic behavior of granular media, and have difficulties in dealing with the dynamic interactions between fluid phase and particles as well. This paper presents a micromechanical approach to investigate the coupling behavior in granular materials. In particular, a coupled Computational Fluid Dynamics and Discrete Element Method (CFD-DEM) approach will be developed to consider the coupling. Some interaction forces typical in relevant geomechanics applications are considered in the coupled numerical schemes. The numerical tool will be benchmarked by some classic problems before being applied to the prediction of sandpiling in water.

2 APPROACH AND FORMULATION

The coupled CFD-DEM approach typically solves the following system of equations governing the motions of both particles in the DEM system and the fluid cells in the CFD system

$$\begin{cases} m_i \dfrac{\mathrm{d}\mathbf{U}_i^p}{\mathrm{d}t} = \sum_{j=1}^{n_i^c} \mathbf{F}_{ij}^c + \mathbf{F}_i^f + \mathbf{F}_i^g \\ I_i \dfrac{\mathrm{d}\boldsymbol{\omega}_i}{\mathrm{d}t} = \sum_{j=1}^{n_i^c} \mathbf{M}_{ij} \\ \dfrac{\partial\left(n\rho_f \mathbf{U}^f\right)}{\partial t} + \nabla\cdot\left(n\rho_f \mathbf{U}^f\mathbf{U}^f\right) - n\nabla\cdot\left(\mu\nabla\mathbf{U}^f\right) = -\nabla p - \mathbf{f}^p + n\rho_f \mathbf{g} \\ \dfrac{\partial\left(n\rho_f\right)}{\partial t} + \nabla\cdot\left(n\rho_f \mathbf{U}^f\right) = 0 \end{cases} \tag{1}$$

where the first two equations express the Newton's law of motion which govern the translational and rotational motions of a granular particle i (Cundall and Strack, 1979), while the last two equations are the Navier-Stokes equation and the continuity equation governing the fluid flow which is locally averaged over a specific fluid cell (Anderson and Jackson, 1967). The variables involved in Eq. (1) are explained as follows: $\boldsymbol{U}^p{}_i$ = the translational velocity of the considered particle; ω_i = the translational angular velocities of the particle. $\boldsymbol{F}^c_{ij}$ = the contact force acting on Particle i by Particle j or the wall(s); $\boldsymbol{M}_{ij}$= the torque acting on Particle i by Particle j or the wall(s); n^c_i= the number of total contacts for Particle i; $\boldsymbol{F}^f_i$ = the particle–fluid interaction force acting on particle i; $\boldsymbol{F}^g_i$ = the gravitational force. m_i = the mass of Particle i; I_i = the moment of inertia of particle i. $\boldsymbol{U}^f$ = the average velocity of the fluid cell. n denoting the porosity. ρ_f = the averaged fluid density. p = the fluid pressure in the cell; μ = the averaged viscosity; $\mathbf{f}^p$= the interaction force averaged by the cell volume the particles inside the cell exert on the fluid. $\mathbf{g}$ = the body force vector.

The proposed numerical CFD-DEM approach solves equation system in (1) as follows. The fluid phase is discretized with a typical cell size several times of the average particle diameter. At each time step, the DEM package provides such information as the position and velocity of each individual particle. The positions of all particles are then matched with the fluid cells to calculate relevant information of each cell such as the porosity. By following the coarse-grid approximation method proposed by Tsuji et al. (1993) (see also, Zhu *et al.*, 2007), the locally averaged Navier-Stockes equation is solved by the CFD program for the averaged velocity and pressure for each cell (the flow along individual pore pathways in the mixture will not be modeled by this method). These obtained averaged values for the 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 may have to be invoked to ensure the convergence of relevant quantities such as the fluid velocity and pressure. When a converged solution is obtained, the information of fluid-particle interaction forces will be passed to the DEM for the next step calculation.

Key to the coupling between the CFD and the DEM is the proper consideration of particle-fluid interaction forces. Targeting at geomechanics applications, three interaction forces are considered in this study: the drag force, the buoyancy force and the virtual mass force. The drag force adopts the expression by Di Felice (1994)

$$\mathbf{F}^d = \frac{1}{8} C_d \rho_f \pi d_p^2 \left(\mathbf{U}^f - \mathbf{U}^p \right) \left| \mathbf{U}^f - \mathbf{U}^p \right| n^{1-\chi} \qquad (2)$$

Where d_p= the diameter of the considered particle; C_d= the particle-fluid drag coefficient which depends on the Reynolds number of the particle Re_p where $\mathrm{Re}_p = n\rho_f d_p \left| \mathbf{U}^f - \mathbf{U}^p \right| / \mu$; $\chi = 3.7 - 0.65 e^{-0.5\left(1.5 - \log_{10} \mathrm{Re}_p\right)^2}$. While for the buoyancy force, we employ the following average density based expression

$$\mathbf{F}^b = \frac{1}{6} \pi \rho_f d_p^3 \mathbf{g} \qquad (3)$$

The virtual mass force is considered to reflect the inertia added to a particle accelerating or decelerating in a fluid which may deflect certain volume of the sounding fluid to move through. In this study the following expression of virtual mass force is employed:

$$\mathbf{F}^{vm} = C_{vm} \rho_f V_p \left(\dot{\mathbf{v}}_p - \dot{\mathbf{v}}_f \right) / 2 \qquad (4)$$

Consequently, the three interaction forces add up to the total interaction force considered in the CFD-DEM coupling system

$$\mathbf{F}^f = \mathbf{F}^d + \mathbf{F}^b + \mathbf{F}^{vm} \qquad (5)$$

In computing the interaction forces, a divided void fraction method described in Zhao and Shan (2012a, 2013) is followed to calculate and distribute the forces in the system more accurately.

3 RESULTS AND DISCUSSION

3.1 *Stokes Particle Settling Problem*

The coupled CFD-DEM approach has first been benchmarked by the classic problem of spherical particle settling in water which was treated analytically by Stokes (1844). In the numerical simulation, a sphere is released from the air to a container half filled with water. Detailed model setup and selection of model parameters of the numerical simulation can be found in Zhao and Shan (2012a). Presented in Fig. 1 is the predicted settling velocity of the particle in comparison with the analytical solution derived by Stokes (1844). In the figure, the prediction denoted by "B+D" indicates the simulation only the buoyancy force and drag force were considered (termed as CASE I in the sequel), while the curve denoted with "B+D+VM" was obtained by considering all three interaction forces (hereafter this case will be called CASE II).

As can be seen, both cases of numerical simulations provide reasonable predictions. The particle develops a peak velocity before entering the water at t = 0.065 s. Upon entry into water, it quickly decelerates to a steady terminal velocity at around t = 0.14 s before hitting the bottom of the container and bouncing back. A good accordance is observed between the numerical predictions with the analytical solution for both CASE I and CASE II. There are nonetheless subtle differences between the two cases. When the virtual mass force is considered in CASE II, the deceleration process of the particle during the settling between t = 0.065 s and t = 0.09 s is slightly quicker than in CASE I when it is not considered, which also renders the prediction in CASE II coincides more closely with the analytical solution than CASE I during this stage of settling. This may indicate that the consideration of virtual mass force may reflect the effect of pushing away fluid in front of the particle more reasonably. Meanwhile it is interesting to find the particle in CASE II hits the bottom of the container and bounces back slightly earlier than in CASE I. This is indeed not surprising since the consideration of virtual mass force in CASE II leads to changed velocity field in the fluid than in CASE I which induces slightly smaller drag force during the settling process. While the drag force is found the dominant one in all interaction forces, the overall velocity of the particle in CASE II is hence faster than in CASE I which render the particle to hit the bottom earlier.

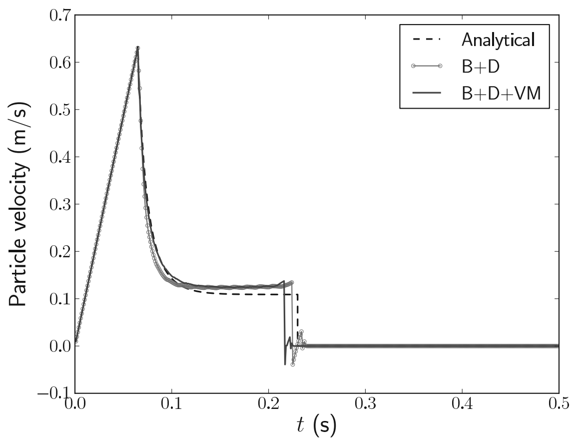

Figure 1. Comparison of the predicted particle settling velocity with the Stokes's analytical solution for a spherical particle settling from air to water (B+D: in consideration of buoyancy force and drag force only; B+D+VM: in consideration of all three interaction forces in Eq. (5)).

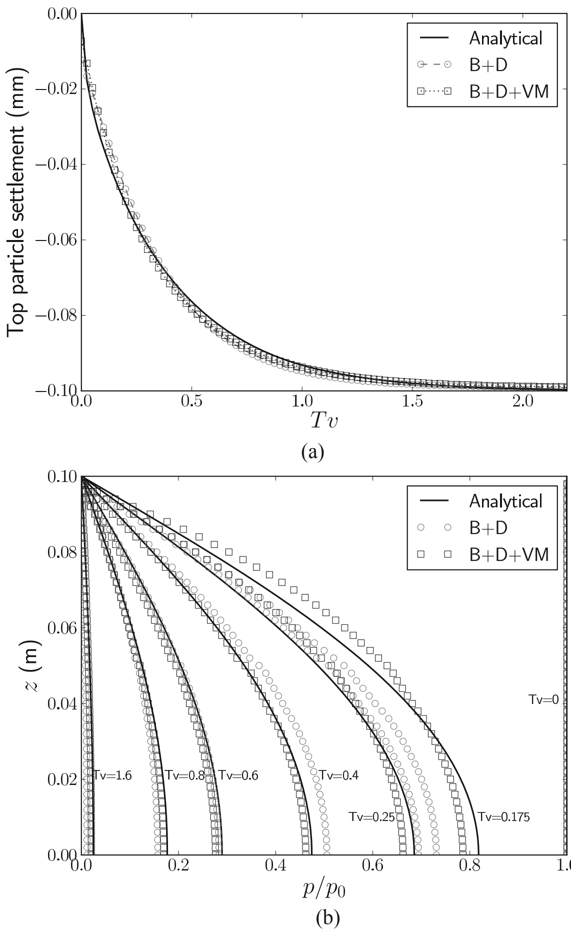

Figure 2. Comparison of the predicted and analytical solutions for 1D consolidation problem on (a) the top particle settlement (b) the dissipation of excess pore water pressure.

3.2 *Terzaghi's one dimensional consolidation problem*

The numerical tool has also been benchmarked by another classic soil mechanics problem, one-dimensional consolidation in a soil layer with one-way drainage, for which Terzaghi (1943) has developed an analytical solution. In simulating this 1D consolidation problem, we consider a soil column comprised of 100 equal size spheres saturated in water. The specific model parameters can be referred to Zhao and Shan (2012a). All particles are initially placed at the centre line of the column without any overlap and are emerged in water. The gravitational force and buoyancy force are then switched on to allow the particles to settle to a hydrostatic state. Once the initial consolidation is finished, a surcharge load p_0=100 Pa is then applied at the top of the column. The predicted settlement of the top particle in the column and the dissipation process of the excess water pressure are presented in Fig. 2, comparing against Terzaghi's analytical solution. As shown in Fig. 2a, the predicted settlement of the top particle in both CASE I and CASE II compare well with the analytical solution. There are some discrepancies, however, in the predicted and analytical solutions for the excess pore pressure. The differences are apparently bigger at the initial stage of the loading. The reason lies in that the analytical solution assumes an instantaneous buildup of the excess pore pressure throughout the column once the surcharge is applied, while the CFD-DEM simulation needs time to build up the whole pore pressure field, which has been discussed in Zhao and Shan (2012a, b). It is also interesting to observe that the predictions by CASE II appear to be more consistent with the analytical solution than by CASE II. This indicates that more realistic prediction can be made by considering the virtual mass force.

3.3 *Application: sandpiling in water*

The two benchmarking problems presented above show that the coupled CFD-DEM tool is capable of providing reliable predictions on the fluid-particle interactions for geomechanics-relevant problem. In this subsection, it is further applied to the prediction of the behavior of sandpiling in water. The piling of granular media is commonplace in many engineering branches and industries, such as the open stockpiles in agriculture, chemical engineering and mining industries. The angle of repose and the stress distribution in a sand pile is a focus of research in the community of both engineering mechanics and physics. In particular, the pressure minimum in the vertical stress profile of the base of a sand pile has been an interesting phenomenon attracting much attention in granular mechanics. While a dominant body of existing studies on sandpiling has been focused on the case of dry granular materials, relevant research on sandpile formation in an environment of water is rather scarce. This latter case can indeed find useful applications in practice, ranging from silos to road and dam constructions, land reclamation and dredging, mine product and tailing handling. To gain better understanding on the stress transmission in granular piles submerged in water, the CFD-DEM approach developed has been employed to examine the behavior of sandpiling in water (see also Shan and Zhao, 2012; Zhao and Shan, 2013).

The basic setup the simulation is as follows. A uniform packing of 15000 sphere particles are poured from a hopper through a container filled with water to form conical sand piles on a circular receiving panel with a small round baffle at the bottom of the container. Fig. 3a demonstrates the setup and the flowing process of the particles which induces the fluid flow shown by small arrows in the figure. Fig. 3b depicts the final state of a stable sand pile formed on the receiving panel. It is found from the simulation that the repose angle of a sandpile formed in water is very close to that in the dry case.

Fig. 4 presents the pressure dip observed in a sandpile formed in water in comparison with the dry case. As compared to the dry case, the presence of water generally leads to a flattened pressure dip (or reduced relative pressure). Indicative information helpful to explain the pressure dip can be obtained from the contact force network of the sandpile, as is shown in Fig. 5 for both the dry case (upper figure) and the wet case (bottom figure). In the dry case, the strong force chains (thicker columns) show an appreciable orientation with an inward inclination angle of around 70 degrees. This indicates that the weights of the upper particles of the sandpile are transferred to the bottom along these inclined chains rather than along the vertical direction. The bottom center part of the sandpile is hence shielded from supporting the weights, which explains the appreciable pressure dip observed in the dry case. In comparison, in the wet case shown at the bottom of Fig. 5, the contact force chains are more preferably oriented to the vertical direction, and there in no effective shield formed to deflect the upper weight of the sandpile. This naturally leads to a much reduced pressure dip in this latter case.

4 CONCLUSIONS

A coupled CFD-DEM approach has been developed to simulate the interactions between fluid and particle system in granular media. The DEM has been employed to simulate the motions and interactions of particles for the granular particle system, while the CFD has been used to solve the locally averaged Navier-Stokes equations for the fluid flow. The interactions between fluids and particles are considered by exchanging

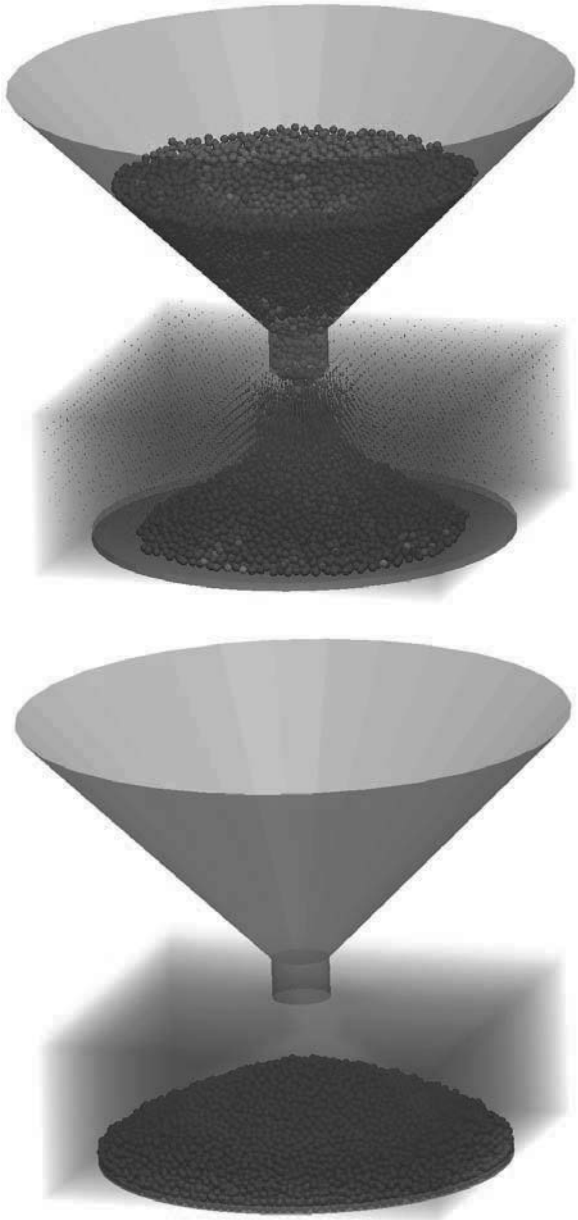

Figure 3. Simulation of sandpiling through hopper flow into a water tank. (a) During the hopper flow; (b) Final stable sand pile.

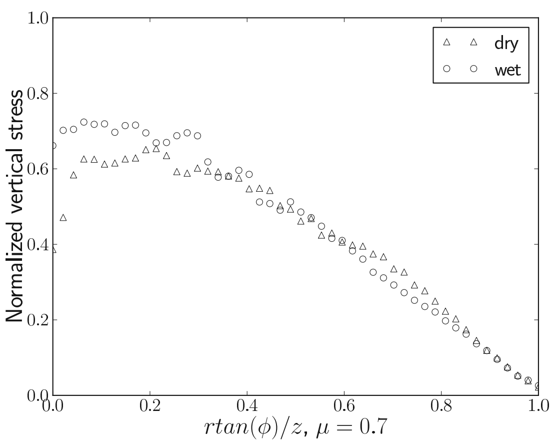

Figure 4. Profile of normalized vertical pressure at the base of sand piles for both the dry and the wet cases.

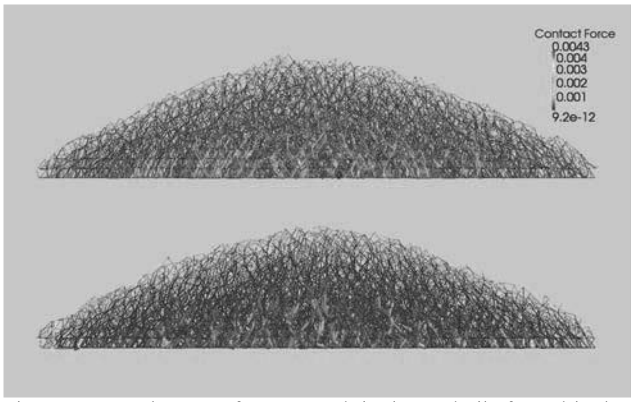

Figure 5. Normal contact force network in the sand pile formed in the dry condition (top) and in water (bottom).

between the DEM and the CFD computations such interaction forces as the drag force, the buoyancy force and the virtual mass force. The coupled numerical tool has been benchmarked by two classic soil mechanics problems and has been further applied to the prediction of sandpiling in water. These examples demonstrate that the proposed method is capable of capturing the main feature of fluid-particle interaction from a microscopic point of view. It is robust and efficient and has the potential to be applied to a wider range of geomechanics problems where fluid-particle interactions are important.

5 ACKNOWLEDGEMENTS

The study was supported by Research Grants Council of Hong Kong (through GRF *622910*).

6 REFERENCES

Anderson T.B. and Jackson R., 1967. Fluid mechanical description of fluidized beds. Equations of motion. *Industrial & Engineering Chemistry Fundamentals* 6, 527-539.

Cundall P.A. and Strack O. 1979. A discrete numerical model for granular assemblies. *Géotechnique* 29, 47-65.

Di Felice R. 1994. The voidage function for fluid–particle interaction systems. *Int. J. Multiph. Flow* 20, 153-159.

Shan T. and Zhao J.D. 2012. The role of water on the pressure dip in sand piles. *The 23rd International Congress of Theoretical and Applied Mechanics* (*ICTAM2012*). 19-24 August 2012, Beijing, China.

Stokes G.G. 1844. On the theories of internal friction of fluids in motion and of the equilibrium and motion of elastic solids. *Trans. Cambr. Phil. Soc.* 8(9), 287-319.

Terzaghi K. 1943. *Theoretical soil mechanics*. New York: Wiley.

Tsuji Y., Kawaguchi T. and Tanaka T. 1993. Discrete particle simulation of two-dimensional fluidized bed. *Powder Technology* 77, 79-87.

Zhao J.D. and Shan T. 2012a. Coupled CFD-DEM simulation of fluid-particle interaction in geomechanics. *Powder Technology*, under review.

Zhao J.D. and Shan T. 2012b. Numerical modelling of fluid-particle interaction in granular media. *Theoretical and Applied Mechanics Letters*. In press.

Zhao J.D. and Shan T. 2013. Discrete modeling of fluid-particle interaction in soils. In Yang Q., Zhang J.M., Zheng H. & Yao Y.P. (eds) *Constitutive Modeling of Geomaterials: Advances and New Application, Proceedings of the Second International Symposium on Constitutive Modeling of Geomaterials* (15-16 Oct 2012, Beijing, China). Springer, pp. 297-301.

Zhu H.P., Zhou Z.Y., Yang R.Y. and Yu A.B. 2007. Discrete particle simulation of particulate systems: theoretical developments. *Chemical Engineering Science* 62, 3378-3396.