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On the development and challenges of particulate flow modeling in geotechnical engineering: A review

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ABSTRACT

Flow of combined granular media and fluids is relevant to many industrial applications and natural phenomena, yet, not fully understood. Particulate flow modeling has significantly developed over the past few decades aided by rapid advances in computational resources. This development is mostly in the chemical engineering field, while contributions to geotechnical engineering are still limited. One of the major reasons for such limited contribution is the large-scale nature of geotechnical structures such as earth dams, which is challenging to model given the available computational resources. In this paper, we aim to present a multidisciplinary summary of the existing approaches, modeling tools and outstanding challenges of particulate flow modeling with a focus on geotechnical applications.

RÉSUMÉ

L'écoulement de la combinaison de matériaux granulaires et de fluides est impliqué dans une multitude d'applications industrielles et de phénomènes naturels, et pourtant, ce n'est pas entièrement élucidé. La modélisation de l'écoulement des particules en suspension s'est significativement développée ces dernières décennies à l'aide des avancées rapides des ressources informatiques. Ce développement est surtout présent dans le domaine de l'ingénierie chimique, alors que les contributions en termes d'ingénierie géotechnique restent limitées. L'une des raisons majeures d'une telle limitation est le caractère grande échelle des structures géotechniques comme les digues en terre, qui sont difficiles à modéliser étant donné les ressources informatiques disponibles. Dans ce papier, nous cherchons à présenter un résumé multidisciplinaire des approches existantes, des outils de modélisation et des défis imposants de la modélisation de l'écoulement de suspensions avec un intérêt particulier pour les applications géotechniques.

1 INTRODUCTION

Understanding the mechanics of fluid flow in particular media is critical to solving important engineering problems (e.g., debris flow, soil erosion, liquefaction, and landslides) (Wachs 2019). Aided by rapid advances in computer hardware, particulate flow modeling has significantly developed over the past few decades. The simulation of industrial and phenomenological scale problems at the particle level, however, continues to be challenging as it requires more computational resources than those available for engineers and researchers.

The interest in fluid-granular media interaction is not new to geotechnical engineering. Examples include mechanical analysis of saturated and unsaturated soils, flow through water-retaining earth structures, and rain-driven landslides. Solid-fluid interaction is commonly estimated through macroscale-based constitutive models. These models utilize a simplified form of fluid flow in soils, e.g., Darcy flow, and constitutively link other parameters such as effective stresses and solid skeleton deformation to the flow variables (Schaufler et al. 2013). Such an approach can be appropriate when dealing with quasi-static applications where deformations in the solid skeleton can be neglected. However, when hydrodynamic forces are of significance to the analysis, more complex physics need are required fully resolve the interaction between soil and water and establish proper constitutive models. The major drawback with considering continuum-based analysis is that micromechanics of interest such as the development and evolution of piping or cavity evolution in earth embankments remains not fully understood. On the other hand, performing particulate flow modelling by accounting for the micromechanics of both soil particles and fluid flow can provide a deeper understanding and help improve the existing constitutive models used to capture the response of such applications.

It is notable that most of the major developments in particulate flow modelling were developed in the context of chemical engineering, with a special focus on fluidized beds and pneumatic conveying due to their vast applications. These developments were later incorporated in civil and geotechnical engineering to simulate a variety of phenomena such as liquefaction (Shamy and Zeghal 2005), landslides (Shi et al. 2018), erosion and cavity evolution (Guo and Yu 2017), riverbed erosion and sediment transport (Harada et al. 2019), and debris flow (Shan and Zhao 2014). However, the largest portion of the literature on particulate flow is found, and seemingly continues to be, in the context of chemical engineering. In contrast, civil and geotechnical engineering contribution to the subject is relatively limited. One reason for this limitation is the inherent large-scale nature of geotechnical applications such as earth dams and slope stability, which are computationally expensive to model. It could be argued that applications in chemical engineering are more relevant to particulate flow than geotechnical engineering, however, several geotechnical phenomena such as erosion, debris flow, and liquefaction are strongly relevant to particulate flow modelling and still require in-depth understanding of the underlying dynamics. Indeed, such limited contribution on the side of geotechnical engineering limits the practitioners' accessibility to case studies and models catered to geotechnical engineering, which in turn hinders our understanding of particulate flow in geotechnical-related applications.

2 PARTICLE-FLUID INTERACTION FORCES

One of the most challenging aspects of particulate flow modeling is to accurately estimate the interaction forces and momentum transfer between fluid and solid phases. Such estimation depends on the physical and flow characteristics of solids and fluids as well as the extent, to which, these interaction forces are considered significant. For instance, in particulate flows with little solid concentration, the solid phase is often dispersed and governed by the hydrodynamic forces with a negligible effect of solids on the fluid motion, i.e., one-way coupling. For denser solid concentration, the motion of the solid particles can affect the fluid streams, which is referred to as two-way coupling. In most of the geotechnical applications, the concentration of solids is typically high and requires four-way coupling, that is, accounting for the iterative effect of the changed fluid motion on particles and particle-particle interactions. In two-way and four-way coupling, it is numerically challenging to ensure that Newton's third law of motion is achieved, i.e., the impact of fluid on solids is equal in magnitude to the impact of solids on the fluid in opposite direction.

Although efforts have been made to resolve fluid-particle interactions, this aspect remains not fully understood and the models we have today are based on empirical or semi-empirical relations. This is because the underlying mechanics of such interaction are very complex and depend on many factors such as particle shape, material properties of solid and fluid phases, and the type of coupling considered in the problem. Nonetheless, the existing models have been proven to be robust and can adequately simulate particulate flow with good accuracy. Here, we review some of the particle-fluid interaction forces and how relevant they are to geotechnical engineering applications.

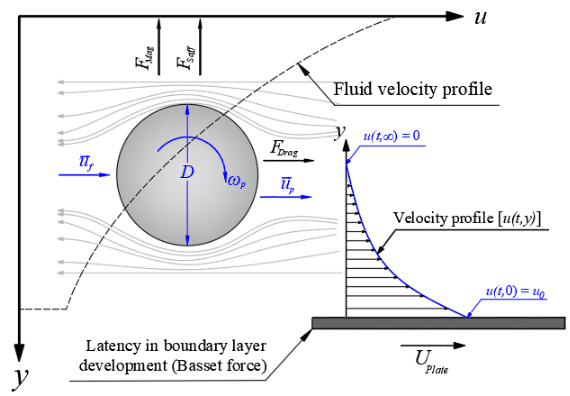

Figure 1. A schematic illustration of particle-fluid interaction forces.

2.1 Drag Force

Drag force is a result of fluid shearing on solid particles due to different velocity of each phase and acts in the direction of the relative velocity between fluid and solid particles (Zhao 2017). This force applies to the surface of the solid particle and is often assumed to be effective at the center of the particle. Early expression for drag force was presented by Ergun (1952) and later corrected by Wen and Yu (1966) and Di Felice (1994) to account for higher solid concentration.

Drag force is always accounted for in particulate flow modeling. The only exception is when one-way coupling of dilute flows with solid concentration is approximately less than 0.1% (Elghobashi 1994). In geotechnical application, where solid concentration is typically larger than 0.1%, the drag force is always considered.

2.2 Pressure gradient force

The difference in pressure across a solid particle induces force that acts over the volume of the particle i.e., buoyancy. For a particle with volume (V_p), the force due to pressure gradient (∇p) acting on that particle ($F_{\nabla p}$) contains two components of hydrostatic and hydrodynamic pressure. As pointed out by Crowe et al. (2012), the hydrostatic pressure component is the buoyancy effect:

$$F_{\nabla p} = \overbrace{-V_p \nabla p_{hydrostatic}}^{buoyancy\ force} - V_p \nabla p_{hydrodynamic} \qquad [1]$$

As can be seen from Equation [1], the force is proportional to the volume of solid particles and the value of the pressure gradient. In geotechnical applications, this force can be very significant, especially the buoyancy component, in submerged solid in quasi-static conditions.

2.3 Virtual (apparent) mass force

The virtual mass force is relevant to the fluid acceleration induced by a solid particle's acceleration and takes effect over the particle volume (Auton et al. 1988). This force can be viewed in the light of the rate of the work needed to change the acceleration of the fluid around a moving particle.

The virtual mass force is most significant in the case of unsteady flows where relative particle acceleration cannot be neglected. From a geotechnical viewpoint, this can be considered in rapid and highly dynamic flows such as debris flow. On the other hand, for quasi-static applications where the unsteadiness of the flow is not considered to be significant (e.g., internal erosion), the consideration of virtual mass forces is not expected to affect the accuracy of the results.

2.4 Lift and time history forces

Other particle-fluid interaction forces can be significant in some specific cases of particulate flow modeling. Examples for these forces include Basset force, which addresses the viscous effect of the fluid on a particle through the time delay in boundary layer development. This delay is a result of the change of relative velocity between the fluid and the particle over time, thus, sometimes referred to as "history term" (Crowe et al. 2012). Other lift forces to be considered are Saffman (Saffman 1965, 1968). and Magnus (Rubinow and Keller 1961) lift forces. Saffman force is induced by fluid velocity gradient across a particle, such that the high velocity on top of the particle contributes to decreasing the pressure, whilst the high pressure at the bottom of the particle (on the side of smaller velocity) drives the particle upward. Magnus force is the lift force induced by a particle's rotational motion. In literature, these forces, along with the virtual mass force, are often neglected in geotechnical applications compared to drag and buoyance forces. The particle-fluid interaction forces are summarized in Table 1.

Table 1. Summary of particle-fluid interaction forces and their significance to geotechnical applications.

Significance to geotechnical applications	Force	Expression	Reference
Significant	Drag	$\boldsymbol{F_d} = \beta(\boldsymbol{u_f} - \boldsymbol{u_p})$ $\beta = \frac{3}{4}\frac{C_d n(1-\alpha)\rho_f}{D}\lvert\boldsymbol{u_f} - \boldsymbol{u_p}\rvert$	Ergun (1952)
		$C_d = \begin{cases} \frac{24}{Re_p}\left(1 + 0.15(\mathrm{Re}_p)^{0.687}\right)\alpha^{-2.65} & Re_p < 1000 \\ 0.44\alpha^{-2.65} & Re_p \geq 1000 \end{cases}$	Wen and Yu (1966)
	Pressure gradient	$\boldsymbol{F_{\nabla p}} = -V_p \nabla p_{hydrostatic} - V_p \nabla p_{hydrodynamic}$	Anderson and Jackson (1967)
Significant in unsteady flows	Virtual mass	$\boldsymbol{F_{vm}} = \frac{\rho_f V_d}{2}\left(\frac{\mathrm{d}\boldsymbol{u_f}}{\mathrm{d}t} - \frac{\mathrm{d}\boldsymbol{u_s}}{\mathrm{d}t}\right)$	Auton et al. (1988)
Insignificant	Basset force	$\boldsymbol{F_{Basset}} = \frac{3}{2}D^2\sqrt{\pi\rho_f\mu_f}\int_0^t \frac{1}{\sqrt{t-t'}}\frac{d}{dt}(\boldsymbol{u_f} - \boldsymbol{u_p})\ dt' + \frac{(\boldsymbol{u_f} - \boldsymbol{u_p})_0}{\sqrt{t}}$	Reeks and Mckee (1984)
	Saffman force	$\boldsymbol{F_{saff}} = 1.61\rho_f\mu_f D^2\lvert\boldsymbol{\omega_f}\rvert^{-\frac{1}{2}}\left[\boldsymbol{u_f} - \boldsymbol{u_p}\right] \times \boldsymbol{\omega_f}$	Saffman (1965, 1968)
	Magnus force	$\boldsymbol{F_{Mag}} = \frac{\pi}{8}D^2\rho_f\left[\left(\frac{1}{2}\nabla \times \boldsymbol{u_f} - \boldsymbol{\omega_p}\right) \times (\boldsymbol{u_f} - \boldsymbol{u_p})\right]$	Rubinow and Keller (1961)

3 NUMERICAL APPROACHES FOR PARTICULATE FLOW MODELING

The governing equations of particulate flows are challenging to solve analytically due to the various nonlinearities associated with it and complex boundary conditions encountered in real problems. Therefore, numerical analysis is conventionally used to solve the set of governing equations. From a numerical point of view, the nonlinear partial differential equations can be solved either using the Eulerian approach or the Lagrangian approach. In the Eulerian approach, the flow variables are viewed as a continuum on a spatially fixed or moving grid and the temporal changes in these variables are tracked locally within each computational cell. In the Lagrangian approach, the trajectory and other flow variables of a fluid or solid particle are tracked overtime for every single particle. Depending on the numerical treatment of both the fluid and the solid phase, particulate flow modeling can be classified into three main categories: (i) Eulerian-Eulerian, (ii) Eulerian-Lagrangian, and (iii) Lagrangian-Lagrangian (Figure 2). Here, we briefly explore the development of different models for particulate flow simulation and their applicability to geotechnical problems.

3.1 Eulerian-Eulerian approach (Two-Fluid Model)

The purely Eulerian approach (Eulerian-Eulerian) essentially depends on averaging the flow variables of solid particles and fluids. The most common type of averaging is volume averaging as the computations are often conducted within a computational cell of a finite volume (Crowe et al. 2012). Early attempts for continuum modeling of particulate flows were presented by Van Deemter and Van der Laan (1961) and Marble (1963) which is often referred to as the “dusty gas equation”. The major drawdown of these models was that they are depended on point values of flow variables with no regard for averaging. This representation is fundamentally flawed because the flow variables can vary significantly to the average control volume considered in the simulation. A later development was presented by Anderson and Jackson (1967). In this model, they proposed an averaging technique to transform the point variables (discrete) to a locally averaged values (continuous) over a volume that is large enough to contain several particles, yet, small compared to the dimensions of the system via a weighting function. This representation became widely adopted and often referred to as the Two-Fluid Model (TFM)

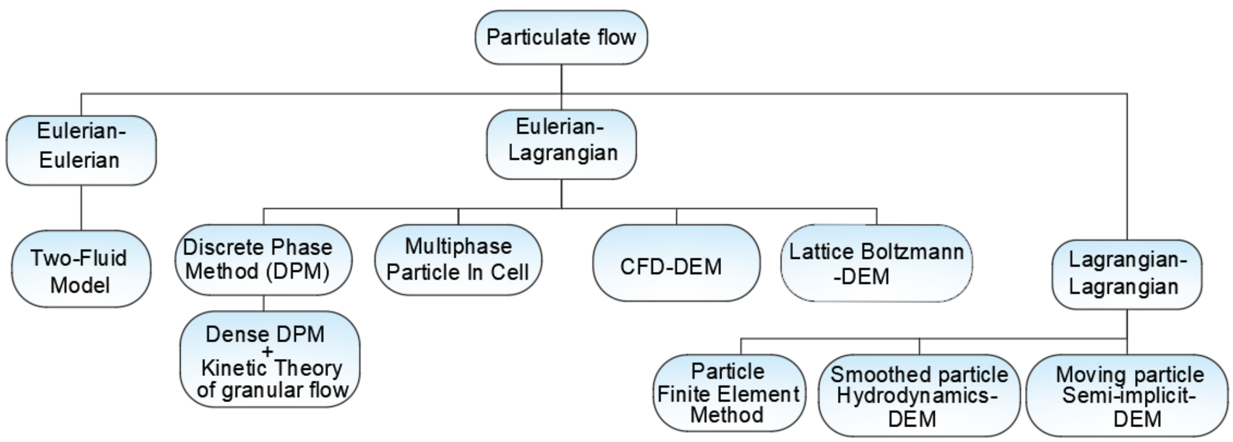

Figure 2. Different approaches and their corresponding models for particulate flow modeling

Although in the TFM both phases are treated as continuum i.e., the particulate nature of the solid phase is not accounted for, the micromechanics of particle-fluid interaction still plays a major role. This role is clear in the estimation of the particle-interaction forces. The interaction forces are considered as cell-averaged values over the computational domain, yet, particle size and shape are needed to calculate these forces. Because the particulate nature is only included implicitly, fluidization and fragmentation due to losing contact between particles cannot be accurately captured. This model has been extensively used in simulating fluidized beds and spouted beds because it is computationally tractable. In geotechnical engineering, however, the TFM has only been recently applied to simulate sediment transport in coastal regions (Chauchat et al. 2017; Cheng et al. 2017)

3.2 Eulerian-Lagrangian approach

In the Eulerian-Lagrangian approach, the motion of the solid particles is tracked using the Newtonian laws of motion. Models presented within this framework include the Discrete Phase Method (DPM) (Vakhrushev and Wu 2013), Dense Discrete Phase Method (DDPM) (Dickenson and Sansalone 2009), the Material Point Method (MPM) (Sulsky and Brackbill 1991) and Multiphase Particle-In-Cell (MP-PIC) (Andrews and ORourke 1996). Among these different approaches, the coupling of the Discrete Element Method (DEM) and Computational Fluid Dynamics (CFD) is by far the most popular approach within the category.

3.2.1 CFD-DEM model

The coupling of the Discrete Element Model (DEM) Cundall and Strack (1979) and Computational Fluid Dynamics (CFD) has been gaining more popularity since it was first introduced by Tsuji et al. (1993). The later model developments were presented to mainly model solid-gas particulate flows in fluidized beds. However, the robustness and solid theoretical grounds of the approach makes it valid for many other applications. For example, it was extensively used in pneumatic conveying modeling (Zhang et al. 2007; Zhou et al. 2014;

Zhou et al. 2016) and food processing (Azmir et al. 2019; Hilton et al. 2013). In geotechnical engineering, the CFD-DEM model was used to model soil liquefaction (Shamy and Zeghal 2005), landslide (Shi et al. 2018; Zhao 2017), erosion and cavity evolution (Guo and Yu 2017). The major drawback of the CFD-DEM model is the high computational cost associated with it. Despite its ability to capture the micro-scale interactions between fluid and solid phases, it takes huge computational resources to perform such computations on a large scale. Hence, phenomenological scale simulations using CFD-DEM have not yet been successfully conducted. Table 2 summarizes the different models used for particulate flow modeling classified by the numerical approach, computational cost, and applicability in geotechnical applications.

Table 2. Summary of particulate flow models and their numerical treatment and computational cost.

Numerical approach	Model	Reference	Applicability in geotechnical engineering	Computational cost
Eulerian-Eulerian	TFM	Anderson and Jackson (1967)	Limited applicability	Low
Eulerian-Lagrangian	DPM	Vakhrushev and Wu (2013)	Not applicable	Moderate
	DDPM +KTGF	Dickenson and Sansalone (2009)	Limited applicability	Moderate
	MP-PIC	Andrews and ORourke (1996)	Limited applicability	Moderate
	CFD-DEM	Tsuji et al. (1993)	Applicable	High
	LBM-DEM	Cook et al. (2004)	Applicable	High
	MPM	Sulsky and Brackbill (1991)	Applicable	Moderate-High
Lagrangian-Lagrangian	SPH-DEM	Potapov et al. (2001)	Applicable	High
	MPS-DEM	Sakai et al. (2012)	Applicable	High
	PFEM	Idelsohn et al. (2004)	Applicable	Moderate

3.3 Modelling tools

In order to carry out particulate flow modelling, the governing equations need to be converted to computer code. It is common that researches construct their own in-house codes such that the applications are tailored for a special case of analysis. However, building and debugging codes can be a time-consuming process and more importantly, optimizing the code may require skillsets that are not available for most of the civil engineers. Thus, a good knowledge of the available computational packages, either open-source or commercial, is essential to facilitate the modelling process and save time and effort. There are specific calibers for selecting the proper modelling tool such as the numerical methods deployed in the package, the robustness of the solver, and the computational efficiency of the solver. While commercial packages are often preferred for use in industrial applications because of the robustness of the solver and the existence of a Graphical User Interface (GUI), they allow for a small room for development. On the other hand, open-source software, despite being less convenient in terms of use, allow for development and implementing different physics of choice.

The modelling tools are seldom discussed in the major reviews on particulate flow modelling (e.g., Deen et al. (2007); van der Hoef et al. (2008); Zhu et al. (2007, 2008)). However, few summaries for the available modelling tools exist in literature within specific contexts such as pneumatic conveying (Ariyaratne et al. 2018), and particulate flow in pipes. Although these reviews are not specifically catered to geotechnical engineering applications, most of the included tools have been successfully used to model geotechnical problems. In Table 3 we present a summary of the available modelling tools for particulate flow modelling. Although the complete features of the computational packages are not reviewed here, the relevant literature in which these packages were used is provided for more information.

4 OUTSTANDING CHALLENGES OF PARTICULATE FLOW MODELLING IN GEOTECHNICAL ENGINEERING

Particulate flow modelling can provide valuable data on several geotechnical applications that cannot be obtained through conventional methods or experiments. However, the computational cost of performing particulate flow computations on a scale that can serve the design and assessment processes is very challenging. In addition to the computational cost, models that can describe complex systems and actual boundary conditions still need to be developed. For example, most of the available literature on particulate modelling in geotechnical engineering use relatively small systems to test the developed models (e.g., Guo and Yu (2017); Shan and Zhao (2014); Zhao et al. (2017)). These small models often contain a small number of particles that can be handled with the available computational resources; moreover, simple boundary conditions. The two most common boundary conditions are periodic boundary conditions and wall boundary conditions. In real-life applications, systems might have boundary conditions of loading, unloading, water draining, phase change, etc. This complexity is not often encountered in chemical engineering applications such as fluidized bed, for which most of the particulate flow models were developed.

More challenges involve dynamic processes related to soils and rocks. In contrast to other applications such as pneumatic conveying and spouted beds, soil particle size can vary significantly in a small sample. Along with size variations, the cohesion between particles, cementing, and fragmentation of a single soil clump can further complicate the dynamics of particulate flow to a great extent. To tackle these issues, constitutive models that account for water existence, whether static or dynamic, need to be developed.

Table 3. Summary of computational packages for particulate flow modeling. The packages marked with (OS) refer to open-source packages and those marked with (CO) are the commercial packages.

method	Solid phase	Fluid phase	Description	Relevant publications
TFM	MFiX® (OS)		Multiphase (solid-fluid) solver based on the TFM model	Fullmer and Hrenya (2018)
	OpenFOAM®(OS) twoPhaseEulerFoam solver		Multiphase (fluid-fluid) solver with the option of KTGF for estimating the stresses in the solid phase	Passalacqua and Fox (2011)
CFD-DEM	PFC3D™ (CO)	OpenFOAM® (OS)	PFC3D code for DEM coupled with OpenFOAM and multi-physics COMSOL for fluid flow	Zhou et al. (2019)
		COMSOL® (CO)		Guo and Yu (2017)
	LIGGGHTS® (OS)	ANSYS Fluent ® (CO)	LIGGGHTS (developed from LAAMPS) for DEM coupled with OpenFOAM	Shan and Zhao (2014)
	EDEM (CO)	ANSYS Fluent ® (CO)	EDEM software for DEM coupled with OpenFOAM and ANSYS Fluent for fluid flow	Sousani et al. (2019)
	MFiX-DEM® (OS)		Multi-phase MFiX code with DEM capability for the particulate solid phase	Bakshi et al. (2018)
	DPMFoam		OpenFOAM solver for multiphase Eulerian-Lagrangian flows	Fernandes et al. (2018)
	ESyS ® (OS)	OpenFOAM® (OS)	DEM solver (ESyS and YADE) combined with CFD solver OpenFOAM	Zhao et al. (2017)
	YADE ® (OS)	OpenFOAM® (OS)		Chen et al. (2011)
SPH	LOQUAT (OS)		Open-source software for SPH in geotechnical applications	Peng et al. (2019)

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