Review of methods and applications for incorporating fluid flow in the Discrete Element Method

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ABSTRACT: Since the early 1990s a great diversity of modeling techniques have been developed to combine fluid-flow models with the discrete element method (DEM). These methods have been applied to a broad spectrum of application areas. As fluid flow is a broad topic, no single fluid/DEM coupling method is suitable for all applications. This paper is intended as a top level review of the most common fluid-particle interaction methods.

1 INTRODUCTION

The detailed modeling of fluid flow and coupling in a discontinuous medium, including all effects of local 3D pore geometry, would require great computational effort. In many cases, a detailed and highly coupled approach is unnecessary because approximations can be made, while still capturing the primary mechanisms that operate in the particular case (Itasca 2008). Below, we consider situations with different fluid flow length-scales and processes, and the approaches that might be appropriate to each case.

2 LOW CONCENTRATION OF PARTICLES IN A FLUID

For the case in which particles are simply submerged in a still fluid, the buoyant (submerged) weight of each particle is used. The force is

\[ f = \frac{4}{3} \pi r^3 \rho_f g \]

where \( r \) is the particle radius, \( \rho_f \) is the fluid density and \( g \) is the acceleration due to gravity. This accounts for the effect of the hydrostatic gradient. If particles move independently of each other (i.e., the particles are widely spaced) and they occupy a small fraction of the fluid volume, viscous forces may be applied to each particle to represent the effects of the fluid. Drag force on a spherical particle is given by

\[ f = \frac{1}{2} C_d \rho_f \pi r^2 |\vec{u} - \vec{v}|(\vec{u} - \vec{v}) \]

where \( \vec{u} \) is the particle velocity, \( \vec{v} \) is the fluid velocity and \( C_d \) is a dimensionless drag coefficient. For low Reynolds number flow, \( C_d = 24/Re_p \), where \( Re_p \) is the particle Reynolds number typically taken as

\[ Re_p = 2 \rho_f |\vec{u} - \vec{v}|/\mu, \]

where \( \mu \) is the dynamic viscosity of the fluid. For higher Reynolds number flows, the drag force cannot be determined theoretically; one popular empirical formula is

\[ C_d = \left( 0.63 + 4.8/\sqrt{Re_p} \right)^2. \]
3 LOW CONCENTRATION OF FLUID IN PARTICLE ASSEMBLY

When the total fluid volume is a small fraction of the total pore volume, the fluid usually exists at menisci, held by surface tension at contacts between particles. A special contact law can be used to capture the effects of the fluid. The law will have viscous and cohesive components, the latter being strongly dependent on the relative separation at the contact and the volume of fluid trapped. If there are two fluid phases, a combination of approaches presented in sections 2 and 3 can often be used (e.g., overall submersion in oil with water menisci at contacts). One such contact law is described by Gröger et al. 2003, as the Cohesive Discrete Element Method (CDEM). Applications of this method have included studies of bulk material handling (Katterfeld et al. 2011, Donohue et al. 2011). A contact model has been developed to include inter-particle and particle-wall lubrication forces for fully saturated conditions (Tomac & Gutierrez 2013).

4 IMPERMEABLE PARTICLE ASSEMBLY CONFINED BY A FLUID PRESSURE

A pressure boundary condition can be applied to the surface of a PFC$^3$D model via the shining-lamp algorithm (Potyondy 2012). The shining-lamp algorithm was developed to support models of rock-cutting in which the weight of a column of drilling mud has a strong influence of the mechanical behavior of the rock. With this method, the surface that has the pressure applied is free to deform. The method works by computing a grid of axis-aligned ray intersections with the PFC$^3$D model. The orientation and size of the particle surface area intersecting the “shining lamps” determines the force applied. The ray intersection calculation is updated as the model deforms. Applications of this method have included modeling the influence of drilling mud on rock cutting, the application of constant tectonic overburden stresses in modeling fault systems and the application of constant confining pressure in models of laboratory compression tests (Schöpfer 2013).

5 SATURATED PARTICLE ASSEMBLY WITH WEAK FLUID PRESSURE GRADIENTS

For the case of a saturated medium, when pressure fluctuations are small over distances equal to the mean ball radius (specifically, when \( (r/P) \frac{dP}{dx} \) is small, where \( r \) is particle radius), a continuum flow calculation can be made on a grid with elements larger than the particles. These methods are typically called coarse grid methods (Tsuji et al. 1993, Shimizu et al. 2011). This weakly coupled approach can capture mechanisms such as surface erosion, piping and channeling. Depending on the flow regime one of two methods is typically used.

5.1 Fully saturated, low porosity, low Reynolds number flow

The fluid flow is described by Darcy’s Law,

\[
\vec{v} = \frac{K}{\mu \epsilon} \nabla p
\]

where \( K \) is the permeability; \( \mu \) is the fluid dynamic viscosity, \( p \) is the fluid pressure and \( \epsilon \) is the porosity. The drag force applied to the particles is derived from calculated pressure gradients

\[
f = \frac{4}{3} \pi r^3 \nabla p.
\]

Two-way coupling can be accomplished by determining a local porosity and permeability from the particle positions. Typically, a grid of elements which are larger than the particles is used to determine the porosity and permeability. The Kozeny-Carman relation is widely used to estimate the permeability of a porous material in terms of the grain size and permeability,

\[
K = B \frac{\epsilon^3}{(1-\epsilon)^2} d^2
\]
where $d$ is the grain diameter and $B$ is a geometric constant usually taken as 1/180. The drag forces applied to the particles are derived from the calculated pressure gradients. Thus, the particle code feeds averaged permeability to the continuum code, which then feeds back mean flow-rate vectors and, hence, particle body forces. The ground water flow model of FLAC<sup>3D</sup> can be coupled to PFC<sup>3D</sup> for this type of analysis (Itasca 1999). Applications of this approach include proppant stability in hydraulic fractures (Asgian 1995), wellbore erosion, and ground water flow.

5.2 Partially saturated, variable porosity, laminar-to-turbulent flow

The previous method is limited to low Reynolds number, low-porosity flow where the particles have a small velocity compared to the fluid. These restrictions are relaxed by using a different fluid-flow model and an alternative formulation for the particle drag force. The well known Navier-Stokes equations for incompressible viscous flow can be modified to include the effect of a particulate solid phase mixed into the fluid. The equation becomes,

\[ \rho_f \frac{\partial \vec{v}}{\partial t} + \rho_f \vec{v} \cdot \nabla (\epsilon \vec{v}) = -\epsilon \nabla p + \mu \nabla^2 (\epsilon \vec{v}) + \vec{f}_b \]  

(1)

Where, $\vec{f}_b$ is a volume averaged body force and $\epsilon$ is the porosity of the particle assembly. The conservation of volume becomes,

\[ \frac{\partial \epsilon}{\partial t} + \nabla \cdot (\epsilon \vec{v}) = 0 \]  

(2)

The formulation for particle drag force given in Section 2 is used with an extra term to account for the influence of surrounding particles,

\[ \vec{f}_{\text{fluid}} = \left( \frac{1}{2} C_d \rho_f \pi r^2 |\vec{u} - \vec{v}| |\vec{u} - \vec{v}| e^{-\chi} \right) \epsilon e^{-\chi} \]

where the exponent $\chi=3.7-0.65 \exp\left(-(1.50 \log_{10} R_{ep})^2/2\right)$ (Di Felice 1994). A buoyancy force may also be added to $\vec{f}_{\text{fluid}}$.

This formulation of drag force is accurate and smoothly varying for the practical range of porosity and Reynolds numbers. This formulation gives similar results to Ergun’s equation (Ergun 1955). The force acting on the particles due to the fluid is assigned locally to each particle and is based on the fluid conditions in the fluid element that the particle occupies. A corresponding body force is applied to the fluid as an average over one fluid element (Xu & Yu 1997). The volume of fluid (VOF) method can be incorporated into this approach to model two-phase flow. Applications for this method are: pneumatic conveying, fluidized beds (Kawaguchi et al. 1992), particle settling, filter ageing, porous flow, wellbore sanding, injection into unconsolidated granular media (Zhang & Huang 2011, Zhang 2012), liquefaction (El Shamy 2006), wave loading on river embankments (Herbst et al. 2010), and sediment transport (McEwan & Heald 2001, Drake & Calatoni 2001).

![Figure 1. Schematic of coarse grid fluid coupling scheme. Each fluid element has fluid velocity, a porosity and a body force. The fluid body force is equal and opposite the sum of the individual particle fluid-particle interaction forces.](image-url)
SATURATED, COHERENT PARTICLE ASSEMBLY, WITH STRONG PRESSURE GRADIENTS AND FLOW ALONG NOTIONAL CRACKS.

If the target solid material is of low porosity (i.e., the voids between circular particles are disregarded), the flow pathways may be assumed to consist of parallel-plate flow pipes, or “cracks”, at contacts. The aperture of such pipes may be defined as a function of local particle geometry and deformation. The aperture of this pipe increases when the two contact particles move apart, and decreases when two contact particles are forced together. A pore network structure can be constructed by identifying the domains formed by closed chains of particles as the pore spaces (as shown in Fig. 2(a)). Pressures stored in these domains need to be updated during the fluid calculation, as they act on the surrounding particles as equivalent body forces (Potyondy et al. 1996). This model is also called the DEM/pore network model.

![Figure 2. Schematic of (a) pore network fluid flow model in DEM; and (b) pore pressure and the resultant fluid force to particle force.](image)

For fluid flow, each flow pipe is equivalent to a parallel-plate channel. The flow rate (volume per unit time) in a pipe is given by the Hagen-Poiseuille equation:

\[
q = \frac{a^3 (p_2 - p_1)}{12\mu L_p}
\]  

where \(a\) is the aperture of the flow pipe; \(\mu\) is the dynamic fluid viscosity; \(p_1\) and \(p_2\) is the pressure difference of two neighboring pores; \(L_p\) is the length of the flow pipe.

The solution scheme of the fluid flow calculation is explicit. After a fluid time step \(\Delta t\), the volume change for each pore can be calculated by summing up the change in the pipe flow volume around this pore. In addition, the apparent volume change of the pore domain \(\Delta V\) can be calculated based on the particle movement. The pressure increment \(\Delta p\) at each pore can be updated according to,

\[
\Delta p = \frac{K_f}{V} (\sum_{i=1}^{N} q \Delta t - \Delta V)
\]  

where \(K_f\) is the fluid bulk modulus; \(V\) is the current pore volume; \(N\) is the number of flow pipes around the pore. It should be noted that the apparent volume change \(\Delta V\) can be neglected if one only considers the one-way coupling.

The hydromechanical coupling is realized by data exchanging at predetermined time steps. For each particle, a resultant drag force \(F_{\text{fluid}}\), obtained from integration of the pore pressure on the particle surface, see Figure 2(b), is passed from the fluid calculation to the mechanical calculation. The resultant drag force \(F_{\text{fluid}}\) is then applied to each particle in addition to the unbalanced force which resulted from the mechanical contact forces. By solving Newton’s second law of motion, a new particle position can be determined. The configuration of the pore structure can be updated accordingly. The hydromechanical coupling is reflected in the change in the aperture \(a\) due to mechanical deformation and the addition of the drag forces to the particles.
This DEM/pore network model was applied to study the stress-dependent permeability of sandstone (Bruno 1994, Li & Holt 2002, Li 2002) and the evolution of permeability in heterogeneous granular aggregates during chemical compaction (Zheng & Elworth 2012). Recently the DEM/pore network model has been used to study the hydraulic fracturing and induced microseismicity in competent rocks (Thallak et al. 1991, Al-Busaidi 2005, Zhao & Young 2011, Shimizu et al. 2011) and also in naturally fractured rocks when fractures or joints were predefined (Damjanac et al. 2010, Han et al. 2012, Garcia et al. 2013). In addition to the applications with the bonded particle model, the DEM/pore network model has also been applied to fluid injection into granular media (de Pater & Dong 2007, Zhang 2012, Zhang et al. 2012). As the granular media only has friction force between particles, it is prone to large deformation during the fluid invasion. This application to granular media requires an additional manipulation when a particle-particle contact is broken or created. A pore is spit to form two new pores when a new particle-particle contact is created between two particles belonging to the original pore. Similarly, the two pores are merged to form a new pore when a particle-particle contact shared by these two pores is broken.

6.1 Mechanical incompressible fluid scheme

The mechanical incompressible fluid (MIF) scheme is a new coupled fluid-mechanical method to model the mechanisms associated with hydraulic fracturing (Cundall 2011). One of the drawbacks of the classic DEM/pore-network model, described in Section 6, is the small critical time step required to integrate Equation (4). The MIF scheme has an order-of-magnitude larger critical time step for the fluid calculation. This scheme is applicable to cases where the rock compressibility is much greater than the fluid compressibility. This contrast in compressibility occurs when the discretization length of the discrete elements (the particle size) is large compared to the aperture of the notional cracks. Combining the MIF scheme with inertial density scaling leads to fast solutions of hydraulic fracture problems (Detournay et al. 2013).

7 STRONG PRESSURE GRADIENTS AND LARGE DEFORMATIONS IN THE SOLID PHASE

If the “solid” material breaks up and no longer retains a coherent structure, or if the void geometry changes dramatically, the schemes described in Section 6 break down. If important fluid flow features are occurring on a length-scale smaller than the discrete element particles, the coarse-grid schemes described in Section 5 break down. Examples include (i) slurry flow, in which particles have similar velocity to the fluid: single particles or clumps of particles are, in essence, carried along by the fluid, and (ii) evolving, fluid-driven geological system, such as magma intrusion into brittle or ductile rock. An extreme example is “sand production” in perforation cavities in unconsolidated sandstones, in which the solid matrix of reservoir formation becomes disintegrated, so the mechanical behavior of the solid matrix must be modeled as a dynamic procedure of discrete particle assemblage. In this process, the local interfacial hydro-mechanical physics along the fluid-particle interface is critical to the establishment and collapse of the sand arch (Bratli & Risnes 1981). To model the problems in which the performance of the whole system is dominated by the fluid-particle interaction at the local scale, the fluid flow in the pore space needs to be modeled at the scale smaller than the particle size and the hydro-mechanical interaction along the fluid-particle interface has to be handled explicitly and precisely.

Intuitively, the Navier-Stokes equations may be solved directly using conventional CFD methods, such as finite element, finite volume, finite difference, discrete-vortex, and B-spline methods. These solution methods can be directly coupled to a mechanical discrete element model via the pore space geometry and by applying appropriate fluid interaction forces and moments. Such a coupled solution method would reveal all the details of the flow and fluid-solid interactions, and would give a clear picture of the mechanisms involved. However, the extensive computational load required in automatic mesh generation, solution projection between remeshing episodes, and the cumbersome implementation of integrating fluid forces over the solid make this approach prohibitive (Hu et al. 1992, Johnson & Tezduyar 1997). There
are many methods being proposed to model pore-scale fluid flow. For example, the microscopic methods like molecular dynamics (MD) (Costa & Courat 1995), particle-based macroscopic approaches like smoothed particle hydrodynamics (SPH) (Holmes et al. 2010), mesoscopic fluid solvers such as dissipative particle dynamics (DPD) (Liu et al. 2007) and lattice Boltzmann method (LBM) (Chen & Doolen 1998), and so on. Among them, SPH and LBM seem to have been applied more widely.

Both LBM and SPH are simple to implement and parallelize, and can easily accommodate additional physics. Despite the evident advantage as a meshless, Lagrangian, particle-based method, SPH has the drawback of lacking a solid theoretical foundation and difficulty in treating boundary conditions. Additionally SPH has susceptibility of other problems such as tensile instability and zero energy modes. In contrast, LBM can be proven by mathematical means to recover the Navier-Stokes equations in the compressible fluids at incompressible limit (Chen et al. 1992). The analytical pressure and velocity boundary conditions are also available (Zou & He 1997).

The evolution equations of LBM are as follows:

\[
f_a(x_i, t + \delta t) - f_a(x_i, t) = -\frac{1}{\tau} \left[ f_a(x_i, t) - f_{eq_a}^a(x_i, t) \right]
\]  

(5)

\[
f_{eq}^a = w_a \rho \left[ 1 + 3 \frac{e_a \cdot u}{c^2} + \frac{9}{2} \frac{(e_a \cdot u)^2}{c^4} - \frac{3}{2} \frac{u \cdot u}{c^2} \right]
\]  

(6)

Where \( x_i \) is a physical point in the lattice space; \( e_a \) is the lattice velocity vector; \( \delta t \) is the time step; \( \tau \) is the dimensionless relaxation factor; \( \alpha \) is the discretized direction; \( f_a \) is the particle distribution function (PDF); \( f_{eq}^a \) is the equilibrium distribution function (EDF); \( \rho \) is the density; \( u \) is the velocity vector; \( c \) is the lattice speed; \( w_a \) is a weighting factor.

The basic unit in LBM is \( f_a \), which can be understood as the packets containing many fluid particles. The macroscopic quantities such as density and velocities can be recovered from PDF (e.g., see Chen & Doolen 1992). These fluid packets keep propagating across the lattice (see Fig. 3a) representing fluid domain along the predefined links, i.e., the left side of Equation (5). The incoming fluid packets from different links collide with each other when they meet at the lattice node, i.e., the right side of Equation (5). The collision follows a special rule such that the system is relaxed towards to \( f_{eq}^a \) given by Equation (6).

![Figure 3](image-url)

Figure 3. (a) Two-dimensional, nine-velocity (D2Q9) LBM model; (b) concept of fluid particle interaction in LBM-PFC coupling system.
The LBM is capable of producing accurate solutions when applied to solve various fluid dynamics problems (Chen & Doolen 1998, Han 2012). When solid particles are present, the fluid solid interaction along the fluid-particle interface can be precisely captured using momentum transfer principle. Two fluid-solid interaction schemes that are based on momentum transfer principle are often used in LBM-DEM implementation, i.e., momentum transfer algorithm developed by Ladd (1994) and immersed boundary scheme proposed by Noble et al. (1998). The fundamental idea of momentum transfer is to bounce back the non-equilibrium distribution portion in the normal direction and enforcing no-slip condition in the shear direction when fluid packets hit the boundary of solid particles. At the same time, the changed momentum of fluid packets are converted into forces and moments and applied to the solid particles (see Fig. 3b). The immersed boundary method was introduced by Peskin (1972) in modeling the coupling between the blood flow and muscle contraction in a beating heart. The distinguished feature of the method is that the fluid is performed on a Cartesian mesh in which the geometry of immersed objects is not conformed. The effect of the boundary of the immersed objects on the fluid flow is considered through formulating a novel procedure (Mittal & Iaccarino 2005). In the immersed boundary scheme proposed by Noble for LBM, the overlap of the associated area/volume of lattice and solid particle is used to modify the collision phase of LBM and evaluate the fluid-imposed forces and moments on the solid particle (Noble et al. 1998). The application of LBM-DEM in solving many fluid-particle interaction problems indicates that this coupling scheme is very accurate (Han 2012, Han & Cundall 2012). It is interesting to notice that the computational expenses of LBM in solving fluid-solid interaction appear to be comparable to that of SPH. For instance, numerical tests indicate that 20-30 fluid particles (in SPH) or lattice nodes (in LBM) are required to span a pore throat of porous media in order to precisely calculate the fluid drag coefficient (Holmes 2010, Han & Cundall 2011).

LBM has been implemented and coupled with DEM by many research groups. The example applications include modeling particulate suspensions (Ladd 1994), particle transport in turbulent flow (Feng et al. 2007), near wellbore mechanics (Cook et al. 2004a, b), sand production in perforation cavities (Han & Cundall 2012), etc.

8 CONCLUDING REMARKS

The interaction between fluid flow and solid particles, granular materials, and porous rocks is a vast and complex topic. The discrete element method is well suited to studying the mechanical behavior of these systems. This paper has discussed a series of real-world fluid particle systems and methods to model them with DEM. Since the early 1990s these methods have increased in complexity and accuracy. As modeling requirements become more demanding in the future new methods will need to be developed to address them. Future trends in DEM/fluid modeling include combining the methods discussed here in different spatial regions, multi-scale methods, and application to high pressure compressible flows.

REFERENCES


