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Pore-scale simulations of drainage in granular materials: Finite size effects and the representative elementary volume

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ABSTRACT

A pore-scale model is introduced for two-phase flow in dense packings of polydisperse spheres. The model is developed as a component of a more general hydromechanical coupling framework based on the discrete element method, which will be elaborated in future papers and will apply to various processes of interest in soil science, in geomechanics and in oil and gas production. Here the emphasis is on the generation of a network of pores mapping the void space between spherical grains, and the definition of local criteria governing the primary drainage process. The pore space is decomposed by Regular Triangulation, from which a set of pores connected by throats are identified. A local entry capillary pressure is evaluated for each throat, based on the balance of capillary pressure and surface tension at equilibrium. The model reflects the possible entrapment of disconnected patches of the receding wetting phase. It is validated by a comparison with drainage experiments. In the last part of the paper, a series of simulations are reported to illustrate size and boundary effects, key questions when studying small samples made of spherical particles be it in simulations or experiments. Repeated tests on samples of different sizes give evolution of water content which are not only scattered but also strongly biased for small sample sizes. More than 20,000 spheres are needed to reduce the bias on saturation below 0.02. Additional statistics are generated by subsampling a large sample of 64,000 spheres. They suggest that the minimal sampling volume for evaluating saturation is one hundred times greater that the sampling volume needed for measuring porosity with the same accuracy. This requirement in terms of sample size induces a need for efficient computer codes. The method described herein has a low algorithmic complexity in order to satisfy this requirement. It will be well suited to further developments toward coupled flow-deformation problems in which evolution of the microstructure require frequent updates of the pore network.

1. Introduction

Understanding two-phase flow in granular media and the coupling with deformations of the granular skeleton is of great importance in many areas of engineering and science. This includes transfers in soils and associated phenomena such as desiccation cracks, swelling and slopes instabilities, various oil recovery techniques or the extraction of methane hydrates from sea bed sediments. Microscale imaging techniques together with pore scale numerical models are promising tools for gaining insight into the governing mechanisms of two-phase flow in such systems. However, both experimental techniques and computational methods have severe limitations in terms of sample size, which raises questions about possible finite size effects. On the modelling side, this difficulty is amplified when coupled flow-deformation processes are simulated, since time integration implies repeated executions of the flow solver in an ever changing pore geometry, hence even smaller problem sizes to keep computational costs acceptable. The aim of this work is twofold: to introduce a pore-scale method enabling high speed simulation of drainage in dense sphere packings and to evaluate finite size effects in such systems. The case of a deforming skeleton is not explicitly tackled yet, but this work is clearly meant for a step in this direction. For this reason the method has to be compatible with the direct simulation of deforming granular structures.

There are several approaches at different scales available for simulating two-phase fluid flows. Macro-continuum scale models are used in most field-scale applications. They are based on empirical relations describing, namely, capillary pressure – saturation ($P_c - S_w$) curves and their evolution with strain, relative permeability, and effective stress. Such methods have acceptable computational costs for large problems, but the empirical laws therein have well known issues. Namely, hysteretic effects are very difficult to model and an accepted effective stress framework is still missing.

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The micro-continuum scale methods, which include lattice Boltzmann (LB) method, volume of fluid (VOF) method, smoothed particle hydrodynamics (SPH) method and level set method, do not rely on such empirical relations. They are promising approaches for getting accurate results at very small scales and gaining understanding of the phenomena observed at the macroscale. However, they have high computational cost.

Pore-network models introduce an intermediate scale at which pore bodies are identified. They enable the simulation of larger domains compared to micro-continuum models, with much fewer assumptions than the macro-continuum models. They idealise the porous medium as a network of pore bodies connected by narrow throats. Pore-network modelling was pioneered by Fatt (see [1] and companion papers), who derived $P_c - S_w$ curves of primary drainage and computed pore size distributions in a network of interconnected pores. Since then, a number of different researchers have contributed to the current understanding of two-phase flow using pore-scale models. The model we present herein differs from previous pore-network models in some aspects, but the general methodology is very similar.

Many networks are based on regular lattices. Typically, squared lattices with a coordination number of four in two-dimension (2D) or cubic lattices with a coordinate number of six in three-dimension (3D) [2–4]. The shape of the pores have been approached by regular geometries (*e.g.*, cubic [5,6] or spherical [7]) and the shape of the pore throats by cylinders with various cross-sectional shapes (*e.g.*, circular [7,8] or triangular [9]) or with parallel pipes [5,10]. Angular cross sections have been proposed by some authors to reflect the phenomena of corner flow and the crevices occupied by the wetting phase. Statistically representative pore networks of this kind can be generated to represent real porous samples [11–13].

Other work focuses on mapping directly the pore space of real granular materials, a problem pioneered by Bryant and Blunt [14] (see also [15,16]), who constructed a network mapping an experimental specimen of packed mono-sized spheres. As imaging techniques reach smaller and smaller scales [17,18], there is a growing interest in this problem and many pore-network extraction algorithms are being developed. They include the multi-orientation scanning method [19], medial axis-based algorithms [20–22], Delaunay/Voronoi diagram-based methods [14,23], or the method of maximal ball [24,25].

Solving coupled flow-deformation problems similarly requires to map a network directly on a given set of solid particles. Moreover mechanical coupling requires a direct and explicit link between the network geometry and the positions of the solid grains, and the computational cost of updating the network should be kept as small as possible. It makes the Delaunay/Voronoi methods best candidates since they introduce a simple duality between the solid objects and the void space. The very few existing models coupling a pore-network with a deforming material also adopted this methodology (in two-dimensions [26,27], hence mainly qualitative). A three-dimensional pore-scale approach termed *PFV* [28] has been proposed to effectively solve flow problems with a single fluid phase. Therein, the fluid flow was modelled using a pore-scale finite volume scheme (PFV) which shares many features with conventional pore-network methods. The method has proven effective in the context of coupled flow-deformation problems [29–31]. In this paper we propose a new model extending the flow model of [28] to quasi-static two-phase flow, as a first step toward coupling two-phase flow and deformation. Beside accuracy, merits of the model are its computational efficiency and its ability to deal with poly-disperse spheres. The coupling with a deformable solid skeleton will be addressed in future publications.

All the measurements or simulation may be sensitive to the problem size and boundary conditions, but this is particularly true when the said sample is made very small because it has to fit in a tomography apparatus [32] or because the computational resources are limited [33]. This is a source of difficulty for the validation of pore scale methods when some details of an experimental setups cannot be reproduced exactly or are simply not known. Anticipating further works in this direction, the first application of our model – and second part of this paper – is a systematic analysis of size effects and boundary effects in small-sized packings of spheres. The structure of the paper is as follows. In Sections 2 and 3, we first employ a decomposition technique to build the pore-network and we introduce the governing equations of drainage. To accommodate different assumptions and experiment situations, various phase trapping options and boundary conditions are implemented. In Section 4, the model is validated by a comparison with quasi-static drainage experiments. In Sections 5 and 6, repeated simulations of drainage in random packings are reported to study finite size effects. Namely, we discuss the effects of sample size, the statistics of saturation obtained by subsampling, and the role of boundary conditions and aspect ratio on capillary pressure-saturation relationships and phases distribution.

2. Pore-scale network

We consider materials in which the solid phase can be seen as a random dense packing of poly-disperse spheres. Such packings will be generated with the DEM method [34]. The network representation of the pore space is obtained in three dimensions by using the Regular Triangulation method, in which the tetrahedra define pore bodies and the facets correspond to the pore throats. The algorithm follows [28] and it is only briefly summarised hereafter.

Regular Triangulation (also known as weighted Delaunay triangulation or power diagram) generalises the classical Delaunay triangulation to weighted points, where the weight accounts for the size of each sphere [35]. Typical examples are shown in Fig. 1. The dual Voronoi graph of regular triangulation (also known as Laguerre graph or radical Voronoi graph) is based on radical planes and it is entirely contained in the void space. This is an appropriate feature to describe the flow path within the pore space, as opposed to the classical Delaunay/Voronoi graphs (see Fig. 2).

Based on this decomposition, a pore is surrounded by four solid spheres whose centres are the vertices of the corresponding tetrahedron. The volume of the pore body corresponds to the irregular cavity within the tetrahedron (see Fig. 3(a)). The shape of a pore throat is defined by the cross sectional area extending within a tetrahedral facet (Fig. 3(b)). The throat does not enclose any volume, but it will play a key role when defining the entry capillary pressure of an invading non-wetting phase (NW-phase).

Since each pore corresponds to a tetrahedron, it has four neighbours, resulting in a lattice of connectivity equal to four. Relatively similar networks can be found in other models [15,36–38], yet the decomposition techniques therein are restricted to uniform particle sizes by the choice of Delaunay triangulation. Regular triangulation extends the approach to poly-disperse spheres. Its mathematical definition is limited to geometrical arrangements of non-overlapping or moderately overlapping spheres. More precisely the maximum overlap is when the centre of one sphere enters another sphere, in this occurrence the regular triangulation would be undefined. Since repulsive forces at contacts prevent such overlaps when the assembled spheres represent solid grains, the regular triangulation that is adopted is always defined.

3. Drainage model

3.1. Local rules

In the absence of gravity the movement of immiscible phases occurs in different regimes distinguished by the relative contribution of viscous stresses and surface tension. The balance between the two depends on two dimensionless numbers, the viscosity ratio M and

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