Pore-scale Simulation of Water Patch Formation in Unsaturated Granular Media

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Abstract

In unsaturated granular media, the flow phenomena and patch formation of the liquid involve interactions among different constituent phases, including gas, liquid and solid, and are of significance in geotechnical and geo-environmental engineering, including unsaturated soil mechanics, groundwater remediation and oil production. In this paper, in order to study these multiphase flow phenomena in granular media, we adopted an open-source CFD platform (OpenFOAM, in particular the interFoam solver for considering multiple fluid phases) and implemented the specific material parameters, including the contact angle, density, viscosity and surface tension, which were obtained from corresponding experiments. Inside the pore space, the classic Navier-Stokes equations considering the mass and momentum balance are solved by the Volume of Fluid (VOF) method tracking the temporal and spatial evolution of liquid-gas interfaces. Drainage procedure under different conditions in granular media with specified grain size and porosity have been simulated. It is found that the patch formation phenomena are controlled by capillary force and the wettability of the granular packing, i.e., the surface tension and contact angle, as well as the viscous force, i.e., the viscosity. Finally, the results of direct numerical simulation presented here quantitatively study the laws of water patch formation.

Keywords: multiphase flow, patch formation, computational fluid dynamics, unsaturated granular media.

1. INTRODUCTION

Multiphase flow plays a significant role in soil mechanics and considerable research has been conducted within the past decades. It involves many environmental applications and industrial processes including carbon capture and storage (CCS), enhanced oil recovery, geological disaster, pharmaceutics, mining and food processing (Horgue, Augier et al. 2013, Zhao, MacMinn et al. 2016, Rabbani, Joekar-Niasar et al. 2017). The mechanical properties of granular medium would change noticeably when the liquid phase flows into the pore space (Ma, Mason et al. 1996, Méheust, Løvoll et al. 2002, Moebius and Or 2014). In multiphase flow, the complex interplay between viscosity and density of fluid phases, surface tension, pore size and wettability decides the flow behaviour within the media. However, the quantitative studies of influence factors for water patch formation during drainage processes keep relatively scarce.

Darcy's law is widely employed as a macroscopic description (Ferrari and Lunati 2013, Li, Hanaor et al. 2017). Due to the interaction between capillary, viscous and gravity forces, the flow circumstances might perform a number of intricate phenomena, in which Darcy's law is not satisfying (Ferrari and Lunati 2013). With the recent advancement of computational methods and computing facilities, computational fluid dynamics (CFD) is an appropriate method to study the complex two-phase flow regime, which employs the constitutive relationships and macroscopic models in porous medium. For example, the CFD methods including Lattice-Boltzmann method (LBM) and smoothed particles hydrodynamics (SPH) can be used and calculated efficiently for considering multiple immiscible fluid phases (Bandara, Tartakovsky et al. 2011). Although additional forces are added to model the surface tension and viscosity between different lattice nodes (LB) or particles (SPH), during the dynamics processes of these methods, some problems might be raised. For example, the LBM needs a model calibration but it is case-specific, which makes the parameters more complicated (Ferrari and Lunati 2013, Ferrari, Jimenez-Martinez et al. 2015).

We adopted the direct numerical simulation platform, OpenFOAM, based on traditional CFD, which solves the discretization of the Navier-Stokes equation and allows capturing detailed flow dynamics information in the pore network. In addition, OpenFOAM combines the multiphase flow solver (interFoam) with the interface tracking method (Volume Of Fluid, VOF) based on Eulerian algorithms (Greenshields 2015), which treats the immiscible liquids as a single phase with different properties, for solving complex interface dynamics. In this paper, the two-dimensional direct numerical simulation of drainage processes was preformed on a wide range of wettability condition. The numerical result presented in this work (1) shows the capability of the software OpenFOAM to faithfully reflect the detailed information during water patch formation and (2) demonstrates quantitatively the effect of viscosity, surface tension of wetting and non-wetting phases and wettability of granular medium on the resulting water patch formation. This study shows a first attempt towards a systematically analysis for such multiphase processes, e.g., drainage and wetting, in geomaterials.

1. NUMERICAL MODELLING

1.1. Volume of Fluid method

In traditional fluid dynamics, during the process of solving the Navier-Stokes equation involving computation of the velocity field, it is extremely difficult and computationally expensive to solve moving boundary condition problems. However, the Volume of Fluid (VOF) method employs treatments of two immiscible and isothermal, incompressible liquid phases as a single-fluid phase with different properties including density and viscosity, and the method uses an additional interfacial force replacing the jump condition of liquid-liquid interface (Greenshields 2015). In VOF method, the process of drainage in granular medium can be described as a wetting phase ("defending fluid") replaced by a non-wetting phase ("invading fluid") (Fig. 1). The distribution of fluid phase is described as a characteristic function of the different phases and it is defined as

$$F_x = \begin{cases} 0 & \text{in the non-wetting fluid, nw} \\ 1 & \text{in the wetting fluid, w} \end{cases} \quad . \tag{1}$$

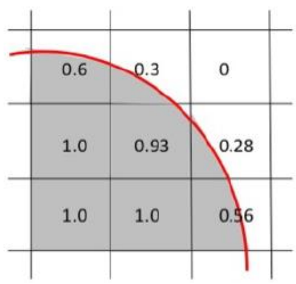

Figure 1. The characteristic function of fluid phase, F, for the coexistence of two immiscible fluids.

The conversation of mass and momentum expresses the dynamic law of fluid phase:

$$\nabla \cdot \mathbf{u} = 0 \tag{2}$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot (2\mu \mathbf{E}) + f_b + f_s \tag{3}$$

where u is the velocity, p the pressure, t the time, f_b all body forces and the rate-of-strain tensor **E**= $\frac{1}{2}(\nabla u+\nabla u^T)$, ρ the density and μ the viscosity,

$$\rho(x) = F(x)\rho_w + (1 - F(x))\rho_{nw} \tag{4}$$

$$\mu(x) = F(x)\mu_w + (1 - F(x))\mu_{nw} \tag{5}$$

and the last term f_s describes the effect of Laplace pressure, i.e., surface tension.

When the above equations compute the velocity field and describe the evolution of the fluid function, the advection equation should be included as

$$\frac{\partial F}{\partial t} + \nabla \cdot (F\mathbf{u}) = 0\ . \tag{6}$$

1.2. Numerical simulation

For a given pore structure, the dynamics during drainage processes depends on the properties of wetting and non-wetting phase. In order to quantify the relative magnitude of viscous and capillary force, we introduced two dimensionless numbers, Bond number and viscosity ratio as:

$$B = \frac{\Delta\rho g a^2}{\gamma} \tag{7}$$

$$H = \frac{\mu_w}{\mu_{nw}} \tag{8}$$

where the typical pore size is denoted as a, wetting liquid density $\Delta\rho$, gravity acceleration g, viscosity of wetting and non-wetting liquid μ_w and μ_{nw} respectively.

The numerical simulation was implemented in an open-source software, OpenFOAM, with a multiphase flow solver interFoam. This solver employs Finite Volume (FV) schemes for the discretization of partial differential equations to calculate multiple immiscible, isothermal and incompressible fluids phases. A mesh generator, snappyHexMesh, is used to automatically generate complex meshes of hexahedral and split-hexahedral cells from triangulated surface geometry in the domain. In this numerical experiment of two-dimensional drainage, the invading fluid displaced a defending fluid, described by VOF method. The dynamics of displacement and morphology of water patch were subjected to the properties of wetting and non-wetting phases. In terms of the specified geometry, the water patch formation depended on wettability of granular medium, capillary and viscous forces (Table 1).

Table 1: Properties of two immiscible liquids used in OpenFOAM

Property	Value
Contact angle (°)	5°~150°
Viscosity of wetting phase (m^2/s)	1.49×10^{-5}, 1.57×10^{-6}, 3.14×10^{-7}, 3.14×10^{-8}
Viscosity ratio, $\frac{\mu_w}{\mu_{nw}}$ (-)	9.49, 1, 0.2, 0.02
Density of wetting phase (kg/m^3)	997
Density of non-wetting phase (kg/m^3)	11.691
Surface tension (N/m)	0.052, 0.042 ,0.032, 0.022
Bond number (-)	7.4×10^{-3}, 9.2×10^{-3}, 0.121, 0.176

A rectangle two-dimensional domain represents the whole domain of drainage, which are filled with the circular obstacles with diameter of 2 mm and throat size of 200 μm (Table 2). The permeability of the granular medium references the Kozeny-Carman as 4.89×10^{-9} m^2. Due to the computational cost, we modelled the granular medium as a 2D 48 circular obstacles. The computational grid and geometry are given in Fig. 2 (a). The initial field of wetting phase is set on the specified cells with the utility as shown in Fig. 2 (b).

Table. 2. Geometrical parameters of the 2D granular medium

Property	Value
Dimensions (mm^2]	25×45.7
Diameter (mm]	2
Number of obstacles (-)	48
Number of cells (-)	114,250
Permeability, k (m^2)	4.89×10^{-9}
Porosity, ∅ (-)	0.649

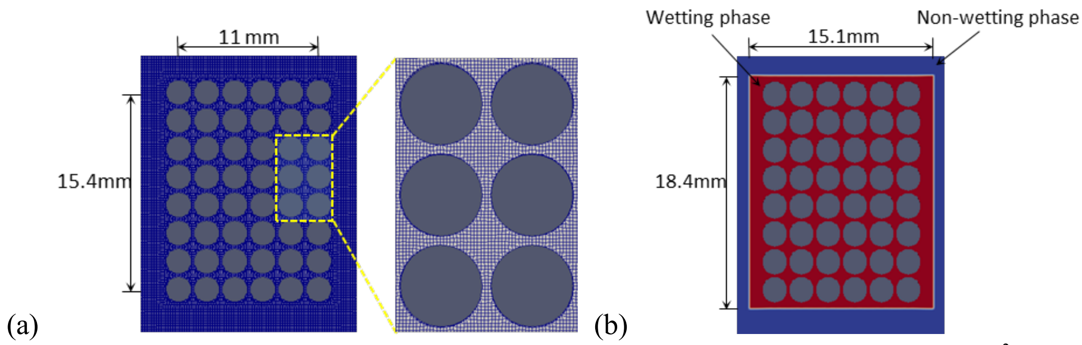

Figure 2: The computational domain: (a) The granular obstacles are arranged in regular array (25×45.7 mm^2; 48 obstacles; particle diameter of 2 mm and throat size of 200 µm). (b) The non-wetting phase (blue) and wetting phase (red).

2. RESULTS AND DISCUSSION

From the saturation state to water patch formation, we repeated several drainage processes by changing viscosity from 1.49×10^{-5} m^2/s to 3.14×10^{-8} m^2/s at the same conditions including density and surface tension, at the Bond number of 0.012. Typical example of the resulting water patch distributions of wetting and non-wetting phases at stable state with different contact angle are shown in Fig. 3.

We calculated the saturation from the stable state under different viscosities condition, which was plotted in Fig. 4 as a function of contact angle. The process of drainage can be divided into three phases: strong-wet, intermediate-wet and strong drainage phases. During strong-wet condition, with the decrease of wettability of solid phase, the pores stay the saturated state. In intermediate-wet condition, the surrounding wetting phase of the granular packing begins to flow out and the residual volume rapidly decreases until approximately the contact angle reaches 110°. Under the drainage condition, due to the strong hydrophobicity of obstacles, the phenomena of liquid trapping occurs noticeably. As a consequence, the saturation of wetting phase has a slight increase. In addition, with the increase of viscosity, overall the saturation increases for the same contact angle.

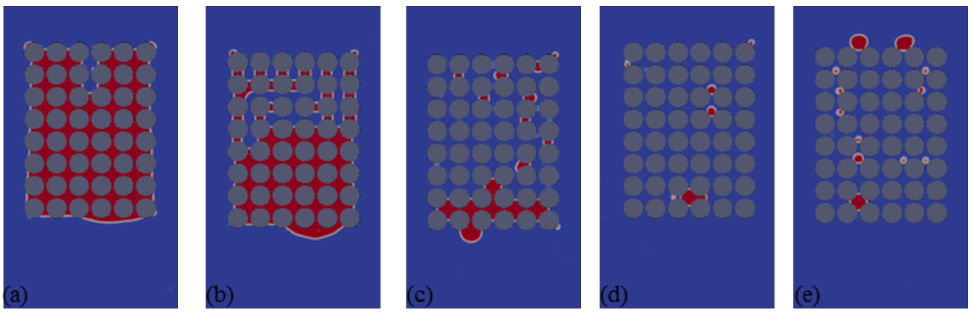

Figure. 3. Numerical results after drainage (kinematic viscosity 3.14×10^{-8} m^2·s^{-1}; surface tension 0.032 N/m) for different contact angle: (a) 30°, (b) 60°, (c) 90°, (d) 120° and (e) 150°.

Moreover, the numerical simulation was repeated by decreasing Bond number from 0.176 to 7.4×10^{-3} to study the effects of weakening the capillary force with respect to gravity force. The saturation of wetting phase was plotted in Fig. 5 as a function of wettability. The results demonstrate that, with the increase of surface tension, the saturation increases significantly as compared to the cases of different viscosity in Fig. 4. This indicates the capillary force has a more important effect on water patch formation than viscous force, indicating the sensitivity of the drainage behaviour to the Bond number, rather than to the viscous ratio, *H*.

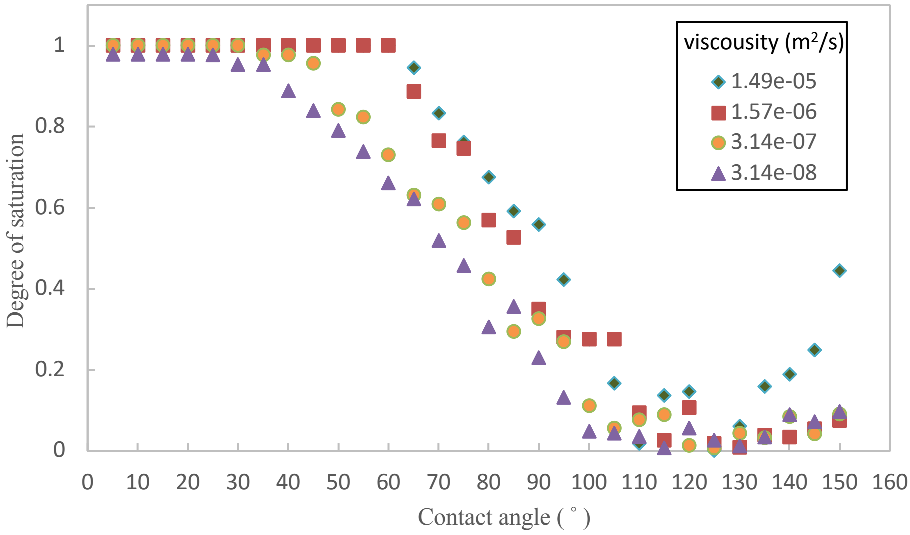

Figure 4. Residual saturation of the different viscosities, as a function of the contact angle.

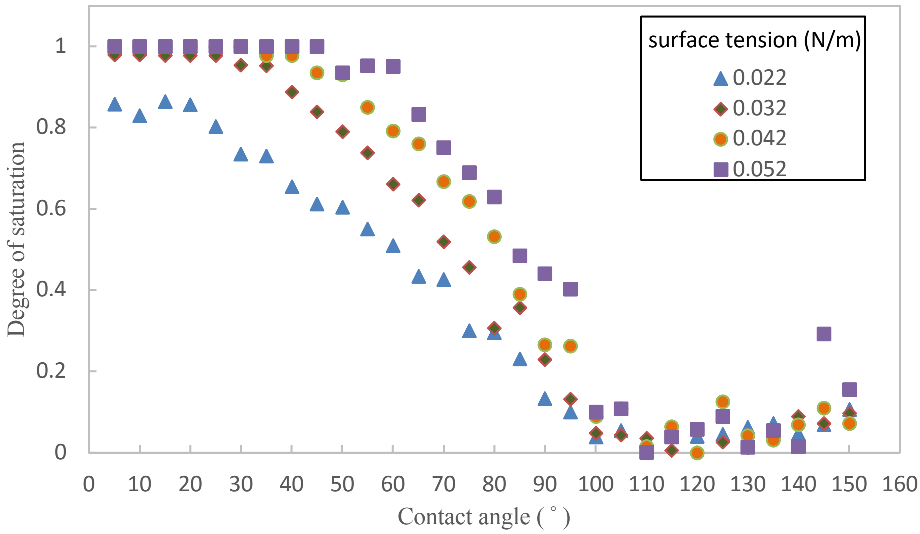

Figure 5. Residual saturation of the different surface tension, as a function of the contact angle.

3. CONCLUSIONS

In this paper, we simulated the water patch formation during the drainage process of saturated granular medium. During the water patch formation, the process can be divided into three regimes: firstly, under the strong-wet phase, with the increase of contact angle, the residual wetting phase in pore space keeps the same quantity; secondly, the saturation decreases drastically under the intermediate-wet condition until contact angle 110° approximately; finally, when under the drainage phase, due to the strong hydrophobic effect, the volume has a slight increase. In addition, the residual volume of wetting phase is subject to viscous and capillary forces. Our simulation results indicate that the drainage process and water patch formation behaviour is more strongly influenced by the surfaces tension, compared with viscosity ratio between the wetting and non-wetting fluids.

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