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Numerical efficiency assessment of the lattice Boltzmann model for digital nano-porous rock applications

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ABSTRACT

Study of transport properties of low permeable sedimentary clay formations is of growing interest in exploration of non-conventional resources, and for long term radioactive waste repositories where these formations play the role of a natural shield which prevents the spreading of radioactive materials in the environment. Recent advances in imaging techniques allow to obtain 3D volume of compacted clay sample with pixel size of order of few nano-meters which enables us to explore transport properties of these media by means of numerical simulation. In our study, the Lattice Boltzmann Model (LBM) is applied to simulate fluid flow inside the 3*D* image of a compacted illite sample to explore its transport properties. The impact of different image segmentation methods applied to treat the raw data on the numerical results is addressed. Because of the nano-metric pore size, various physical phenomena may influence fluid flow. In this study, we consider the influence of gas slippage effect (the Klinkenberg effect) on the permeability. The numerically obtained results are compared with experimental data obtained for a reconstructed compacted illite sample. If the original geometry is not strongly modified by the applied image segmentation method, the numerically calculated Klinkenberg factor follows well existing trends and provides predictions close to the experimental values.

1. Introduction

The main objective of this study is to improve the understanding of one-phase flow in low permeable porous media by means of numerical simulations performed at the pore scale on 3*D* images of clay samples. This objective is closely related with the increasing interest in low permeable sedimentary formations which are projected to be used as host site for long term radioactive waste repository (Dossier, 2005). Characterized by low permeability, these media can serve as a natural barrier against radioactive materials. During the storage phase, indeed, a certain amount of gas (mostly hydrogen) will be released due to corrosion of iron components of the facility. Increased gas pressure can cause gas migration through the highly water saturated sedimentary material and even affect the geometry of the pore space modifying transport properties of the clay. Therefore, a good understanding of this complex process is of high interest.

Depending on hydrodynamic conditions, various transport mechanisms participating to gas migration can be in action, separately or together (Cuss et al., 2014; Marschall et al., 2005). Thus, gas diffusion can be favoured, and the dissolved gas will be transported by advection and diffusion (Bardelli et al., 2014). Conversely, for sufficiently high pressures, gas percolates through the water saturated clay and is transported by continuous visco-capillary flow or small bubble migration. The excess of gas pressure can lead to the dilatation of existing and creation of new pathways (Cuss et al., 2014; Davy et al., 2013; Harrington et al., 2012; Pazdniakou and Dymitrowska, 2018). Due to nano-metric pore size, however, specific hydrodynamic features need to be considered.

The clayey material has a complex porous structure with the total porosity ranging from 10% to 40% (up to 50% for bentonite), most of which is associated with pores smaller than 100 nm (Gaboreau et al., 2016; Marschall et al., 2005). If gas pressure is not sufficiently high, the mean free path of gas molecules λ can be significant when compared to the pore size H causing the gas slippage effect. The intensity of gas rarefaction effect is characterized by the Knudsen number Kn

$$\mathrm{Kn} = \frac{\lambda}{H} \tag{1}$$

The continuous flow regime corresponds to $\mathrm{Kn} < 0.001$; the slip flow is associated with $0.001 < \mathrm{Kn} < 0.1$; the transitional flow regime corresponds to $0.1 < \mathrm{Kn} < 10$, and the free molecular flow is related to $\mathrm{Kn} > 10$

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(Guo and Shu, 2013; Mitra and Chakraborty, 2011). For the description of slip flow, the Navier–Stokes equations still can be used together with a slip boundary condition. At the macroscopic scale, the gas slippage effect is manifested in the increased gas permeability K, which is known as the Klinkenberg effect (Klinkenberg, 1941) and historically expressed as

$$K = K_0\left(1 + \frac{b}{P_m}\right) \tag{2}$$

where K_0 is the absolute permeability, b is the Klinkenberg factor related to the medium properties, and P_m is the mean gas pressure.

Recent advances (Gaboreau et al., 2016; Song et al., 2015) in digital rock imaging improved the understanding of the complex hierarchical pore space structure of sedimentary clays. In absence of micrometric fractures, most of the interconnected pores are of nanometric size. The access to the high resolution digital images of real clay samples obtained by FIB-SEM (Focused Ion Beam Scanning Electron Microscope) (Gaboreau et al., 2016), or at the lower scale by Transmission Electron Microscopy (TEM) if the meso-pores are not connected Davy and Adler (2017), provides the opportunity to perform numerical simulations of fluid flows, in order to better understand the transport properties of these low permeable porous media. Various numerical methods can be employed to calculate capillary pressure, absolute and relative permeabilities. In our study, we focus on using the lattice Boltzmann method (Chai et al., 2010). Originally derived as a generalization of lattice gas automata (LGA), the LBM can be also obtained by discretizing the continuous Boltzmann equation in space, time, and particle velocity space. Unlike the classical Computational Fluid Dynamics (CFD) methods, the LBM describes fluid state by the probabilistic particle distribution function. The model was successfully applied to simulate single- and multiphase flow inside the 3D images of porous media (Hassine et al., 2017; Benioug et al., 2017; Dymitrowska et al., 2014; Pazdniakou and Adler, 2013). The gas slippage effect was introduced later by adopting an appropriate solid-fluid boundary condition. Different formulations have been derived for this purpose based on the pure diffuse reflection (Ansumali and Karlin, 2002), its combination with the specular reflection (Tang et al., 2005) or with the bounce-back boundary condition (Chai et al., 2010), and a combination of the bounce-back with the specular reflection (Succi, 2002).

Up to now, however, the use of these boundary conditions is limited to simplified and well discretized geometries (e.g., capillary tubes) with the notable exception of the recent application by Zhao et al. (2016) to 3D digital rocks but without comparison to experimental permeability data. However, challenges still remain to gain reliability in predicting transport properties of such nanoporous materials using Digital Rock Physics (DRP) measurement. First, in spite of the increasing technological advances, it is still unclear whether the spatial resolution available by 3D microscopic imaging techniques (X-ray tomography, FIB-SEM, BIB-SEM (Broad Ion Beam Scanning Electron Microscope),...) is sufficient to properly capture rock surface features (pore curvature, roughness) that may impact the slippage effect for computer-based simulations. In other words, concerns may be raised whether the filtering process conducted for measuring integrated properties such as permeability possesses sufficient imaging-based microscale information in the presence of slip flow. In adddition, even if the solution of LBM model with slip flow boundary condition has been validated rigorously against fluid flow solution through a parallel-wall uniform fracture or Poiseuille tube flow, applicability to 3D complex pore geometry with non-uniforme pore throats (*i.e*, with spatially variable Knudsen number) needs to be assessed. The present work aims at addressing these issues.

Our ultimate objective is to explore the capability of the LBM to predict the transport properties of real nano-porous media and confront them to experimental data. An artificial clay material, initially imaged in 3D by Gaboreau et al. (2016) will be considered for this purpose. It must be noted that, with the present computational resources, it is not possible to treat the whole image of the sample accounting for all pore scales from micro- to nano-metric. Therefore, we are going to work with a selected sub-sample insuring the pore space connectivity. The sensitivity of the numerical methods to the geometry resolution is also investigated. To the best of our knowledge, this is the very first attempt to tackle this complex issue.

2. Numerical model

The Navier-Stokes equations describing the flow inside the pore-space can be numerically solved by various computational fluid dynamics (CFD) methods such as finite volume method (FVM) or finite element method (FEM). Recently, non-conventional numerical methods such as LBM received a lot of attention for single- and multi-phase flow modelling in porous media (Dymitrowska et al., 2014; Pazdniakou and Adler, 2013). Indeed, compared to conventional numerical methods, they allow to cope naturally with fluid-fluid interface and complex fluid-solid boundary conditions. Also, various physical phenomena can be relatively easily incorporated in the basic LBM. Finally, possessing a high level of intrinsic parallelism, the LBM can easily profit from parallel computing on CPU and GPU clusters, which is important when dealing with prohibitively large samples (Alpak et al., 2018).

2.1. Lattice Boltzmann method

2.1.1. The D3Q19 TRT LBM

The LBM originally appeared as a generalization of LGA in an attempt to overcome some of their difficulties. It was first introduced for a hexagonal lattice with six discrete velocities ($D2Q6$) in 2D space and a face-centered hypercube (FHCH) lattice in 4D space (McNamara and Zanetti, 1988). Later, it was demonstrated that LBM can be derived from the continuous Boltzmann equation by applying a proper discretization (He and Luo, 1997a; 1997b). The method rapidly extended to various lattices, collision operators, and boundary conditions. Now, it is applied to simulate a wide variety of fluid flow phenomena.

In our study, a regular cubic lattice in 3D space with 19 discrete velocities ($D3Q19$) is adopted. In LBM, the state of the fluid at each lattice point $\mathbf{r}$ at a given time step t is defined by the particle distribution function $\mathbf{f} = (f_i(\mathbf{r}, t), i = 1, \dots, Q)$, whose components are associated with discrete velocities $\mathbf{c}_i$. For a given time moment t each $f_i(\mathbf{r}, t)$ defines the probability to find a particle with the discrete velocity $\mathbf{c}_i$ at the location $\mathbf{r}$. The 19 discrete velocities for $D3Q19$ are given by

$$\mathbf{c}_i = \begin{cases} (0,0,0), & i = 1 \\ (\pm c, 0, 0), (0, \pm c, 0), (0, 0, \pm c) & i = 2, \dots, 7 \\ (\pm c, \pm c, 0), (\pm c, 0, \pm c), (0, \pm c, \pm c) & i = 8, \dots, 19 \end{cases} \tag{3}$$

where the velocity $c = \frac{\delta x}{\delta t}$ is defined as a ratio of the lattice step δx and the time step δt. Both the lattice and the time steps are set to 1 for simplicity. The evolution of the particle distribution function is described by

$$f_i(\mathbf{r} + \mathbf{c}_i\delta t, t + \delta t) = f_i(\mathbf{r}, t) - \Omega_i(\mathbf{f}, \mathbf{f}^{eq}) + F_i\delta t \tag{4}$$

where $\Omega_i(\mathbf{f}, \mathbf{f}^{eq})$ is the collision operator, F_i is the discretized body force, and $\mathbf{f}^{eq}$ is the equilibrium distribution. The algorithm can be easily split into two steps, *i.e.*, the calculation of the post-collision distributions in the right part of (4), and the propagation of the post-collision distributions according to the discrete velocities directions.

The collision operator $\Omega_i(\mathbf{f}, \mathbf{f}^{eq})$ describes the evolution of the particle distribution function due to collision between the particles. The most simple collision operator is the Bhatnagar-Gross-Krook (BGK) collision operator (Bhatnagar et al., 1954) which relaxes the particle distribution function to its equilibrium with a single relaxation time. When used with the bounce-back boundary condition, the well known drawback of this operator is the viscosity dependent location of the boundary. The solution to this problem is the multi-relaxation time collision operator