Journal of Contaminant Hydrology xxx (xxxx) xxx–xxx

Contents lists available at ScienceDirect

Journal of Contaminant Hydrology

journal homepage: www.elsevier.com/locate/jconhyd

Pore scale modelling of DNAPL migration in a water–saturated porous medium

Khalifa Nsir[a,b], Gerhard Schäfer[a,*], Raphaël di Chiara Roupert[a], Lionel Mercury[b]

[a] Université de Strasbourg, CNRS, Laboratoire d'Hydrologie et de Géochimie de Strasbourg (LHyGeS) UMR 7517, Strasbourg, France
[b] Université d'Orléans, CNRS, Institut de Sciences de la Terre UMR 6113, Orléans, France

ARTICLE INFO

Keywords:
Network model
Porous medium
WRC
DNAPL
Immiscible displacement
Fingering

ABSTRACT

A numerical simulator based on the discrete network model approach has been developed to simulate drainage processes in a water-saturated porous medium. To verify the predictive potential of the approach to simulate the unstable migration of a dense nonaqueous phase liquid (DNAPL) at the pore scale, the numerical model was applied to laboratory experiments conducted on a sand-filled column. The parameters relative to pore body size and pore throat size used in the construction of the equivalent network were derived from discrete grain-size distribution of the real porous medium. The observed water retention curve (WRC) was first simulated by desaturation of the network model. The good agreement of the modelled WRC with the experimental one highlights that the applied approach reproduces the main characteristics of the real pore space. The numerical model was then applied to rate controlled experiments performed on a homogenous sand-filled column to study the gravity-driven fingering phenomenon of immiscible two-phase flow of water and a DNAPL. The numerical results match within 10% based on the standard deviation with the experiments. They correctly reproduce the effect of several system parameters, such as flow mode (upward flow and downward flow) and the flow rate, on the stability of the water/DNAPL front in a saturated porous medium.

1. Introduction

Characterization and quantification of the migration of immiscible liquids in groundwater are topics that have received considerable attention in recent years (Alexandra et al., 2012; Wu et al., 2017). Several studies of two-phase immiscible flows have been motivated by the need to treat spills and leaks of so-called dense nonaqueous phase liquid (DNAPL), which can severely impact the quality of subsurface water supplies (Kueper and Frind, 1989; Birovljev et al., 1991; Fayers and Zhou, 1996; Bettahar et al., 1999). When infiltrating through the saturated zone, migration of DNAPL can result in highly fingered fluid distributions. The occurrence of fingering is caused by flow instabilities due to differences in viscosity and density between DNAPL and water (Khataniar and Peters, 1992; Riaz and Tchelepi, 2006; Essaid et al., 2015; Cheng et al., 2016). These fingers propagate rapidly, causing early breakthrough relative to stable displacement (Brailovsky et al., 2006).

Numerical modelling of DNAPL displacement in water-saturated porous media using continuum models has been performed by many researchers (Zhang and Smith, 2001; Nayagum et al., 2004; Aggelopoulos and Tsakiroglou, 2009; Erning et al., 2012; Kokkinaki et al., 2013; Sleep et al., 2015; Schneider et al., 2015). However, the fingering process in a homogenous porous medium cannot be simulated with these models because they do not explicitly consider the instability behaviour of the DNAPL-water interface.

To overcome this shortcoming, microscopic approaches such as Stokes' solution for flow in single pores with a specified geometry or lattice Boltzmann methods (LBM) have been investigated to reproduce unstable displacement experiments. Kiriakidis et al. (1991) developed a 2D algorithm involving Monte Carlo decision-making, random walks, and principles of percolation theory. This algorithm successfully predicted the three distinct behaviours of immiscible displacement in porous media, such as viscous fingering, stable displacement, and invasion percolation, but the model did not include the gravity term, and gravity fingering was not considered. Ewing and Berkowitz (1998) developed a generalized growth model based on invasion percolation to simulate immiscible displacement in saturated porous media. Even capillary, viscous and gravity forces were incorporated in their 3D algorithm, where viscous forces were expressed stochastically rather than explicitly. Glass et al. (2001) developed a macro-modified invasion percolation (MMIP) model, including also the effects of all 3 forces within the invading phase in a macro-heterogeneous porous medium.

* Corresponding author.
E-mail address: schafer@unistra.fr (G. Schäfer).

https://doi.org/10.1016/j.jconhyd.2018.07.001
Received 22 September 2017; Received in revised form 16 May 2018; Accepted 2 July 2018

The simulated evolving invasion structure during the gravity-destabilized condition matched the experimental distributions quite well. Dong et al. (2011) proposed a LBM model taking into account both wettability and gravity to successfully reproduce flow experiments in Hele Shaw cells. Recently, Liu et al. (2013, 2014, 2015) have developed a Lattice Boltzmann model that was able to simulate the main flow regimes (capillary fingering, viscous fingering and stable displacement). The model was applied to simulate drainage micromodel experiments of the liquid CO_2 displacement of water. The authors obtained a good agreement with the experimental measurements and showed that increasing M (viscosity ratio of non-wetting fluid to wetting fluid) or decreasing the media heterogeneity can enhance the stability of the displacement process.

While the lattice Boltzmann method gives a more rigorous description of different physical processes, it is often limited to relatively simple physical situations or to systems encompassing only a few pores. For this reason, pore-scale networks are often used to describe the flow rate of fluids at the pore scale (Koplik and Lasseter, 1985; Aker et al., 1998; Helge et al., 1999; Jia and Shing, 1999; Laroche and Vizika, 2005).

In pore-scale network modelling, local capillary equilibrium via the Young-Laplace equation is generally used to determine multiphase fluid distribution. A set of rules that describes the appropriate physical processes and arrangements of fluid within each pore is developed and then combined to describe the displacement of both fluids in the system. Macroscopic behaviours of the displacement can then be seen in network models, even though they are not coded explicitly.

Many network models have been developed to study a wide range of displacement processes, including drainage and imbibition (Nordhaug et al., 2003; Singh and Mohenty, 2003; Ferer et al., 2007; Joekar-Niasar et al., 2009; Tørå et al., 2012; Sheng and Thompson, 2013; Bultreys et al., 2015; Kallel et al., 2017). Regular lattice structures are generally used, with pore bodies corresponding to the vertices of the lattice and pore throats connecting the pore bodies. The most important aspects of network models are the dimension and coordination (Gao et al., 2012; Jivkov et al., 2013). For example, trapping is a dominant process in 2D, less important in 3D, and virtually non-existent in 4D (3D + time) and when an above multi-directional pore-network is used (Raoof and Hassanizadeh, 2010). Likewise, networks with high coordination behave quite differently than networks with low coordination. In most early network models, pore space parameters were chosen without reference to a realistic porous medium. Network is equivalent only in a statistical sense to the modelled system. Indeed, they were used to explore network concepts as much as to explore porous media. More modern network models were often built directly from micro-CT scans of the rock, and so they had not only the same pore size distribution but also the same exact structure as the rock they are simulating (Al-Raoush and Willson, 2005; Prodanovic et al., 2007; Dong and Blunt, 2009; Raoof et al., 2010; Bultreys et al., 2015). In these cases, the ability to reproduce physical measurements is excellent. However, if the exact rock type has to be used for the network construction, the application of predictive pore-scale modelling will be severely limited due to the complexity and cost of the methods. More details about the methods for obtaining pore space information, constructing pore networks and the application of pore network models in porous media can be found elsewhere (see Joekar-Niasar and Hassanizadeh (2012) and Xiong et al. (2016)).

By controlling parameters such as pore-size disorder, viscosity, and flow rate, previously developed dynamic pore network models were used successfully to reproduce viscous fingering phenomena exhibited in laboratory studies. Lenormand et al. (1998) developed a dynamic drainage pore network model and used it to simulate corresponding micromodel experiments. Their model reproduces capillary fingering, viscous fingering and frontal displacement regimes for different capillary number and mobility ratio combinations successfully. The largest network that they used in their simulations consisted of 100 × 100 nodal junctions and they presented a relatively limited set of simulation results. Aker et al. (1998) developed a two-dimensional network simulator and used it to characterize the different flow regimes observed in drainage. They introduced a new method that allowed the simultaneous flow of two liquids into one pore and demonstrated that viscous fingering could be reproduced. However, the approach was highly CPU intensive and a 60 × 80 network was the largest lattice that could be considered. In addition, they only presented results before a breakthrough of the injected phase. Singh and Mohenty (2003) developed a dynamic network model providing 3D results consistent with the 2D results of Lenormand et al. (1998). Their simulator could reproduce the displacement front structure and dynamics as function of capillary number and viscosity ratio. Whilst their simulator could produce various displacement regimes, including viscous fingering, the largest system used in their study was a 30 × 8 × 8 network. Tørå et al. (2012) extended the model developed by Aker et al. (1998) by incorporating the dynamics of the wetting layers using an approach similar to Singh and Mohenty (2003). They used this model to study saturation profiles during imbibition and the resistivity index at different capillary numbers. Their numerical results were in good agreement with experimental data from sand packs. The simulations were carried out on one realization of model volume of (4.5 × 1.5 × 1.5) mm^3 consisting of 767 nodes and 1750 tubes.

Most of the previous pore network modelling studies described above were performed in small networks and were followed by a successful benchmarking exercise of the numerical simulations against micromodel experiments. However, the modelling approach is rarely used to simulate such mechanisms at the laboratory core scale. Additionally, very few studies have presented saturation maps after breakthrough under unstable conditions. An integrated effort is needed to connect network models and laboratory tests at the core scale more closely.

The main objective of the present work is to test, at the scale of a few centimetres, the capacity of the pore scale network model developed by Nsir and Schäfer (2010) to capture the gravity-driven fingering observed in our own water-DNAPL drainage system. The model is first applied to predict the water retention curve of the model sand used in the experiment. The comparison of the experimental curve and the one modelled will show whether the used network model reproduces the main characteristics of the real pore space. In a second step, the numerical model is then used to simulate the displacement of water by DNAPL during controlled drainage experiments performed in a 68-cm long glass column filled with the homogenous model sand. The numerical results are compared to the observed physical quantities, such as the distribution of arrival times of the DNAPL/water front at a control section, the DNAPL pressure at the inlet as a function of time, and the DNAPL saturation profile at the end of the displacement experiment.

2. Laboratory experiments on DNAPL migration

Laboratory experiments were conducted on a 68-cm long glass column with an internal diameter of 10 cm. The used porous medium is a medium-sized quartz sand with a mean grain-size diameter of 0.4 mm, a uniformity coefficient of 2.1 and a low fraction of organic content (foc = 0.09%, based on NFT 31–109) (Bohy et al., 2006). The hydraulic properties of the quartz sand, such as its moisture characteristics, were quantified in former studies by Cotel (2008). Trichloroethylene (TCE) was chosen as the DNAPL for the experiments because it is among the most frequently detected contaminants in subsurface environments. At 20 °C, TCE has a density of 1.463 g/cm^3, a viscosity of 0.0056 g/s/cm, and a solubility in water of 1300 mg/L.

The experimental setup was designed to produce a controlled and well-defined injection of TCE in an initially water-saturated homogeneous porous medium. The outlet section of the column was kept at a constant water pressure. A high accuracy peristaltic pump with flow