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Simulation of DNAPL migration in heterogeneous translucent porous media based on estimation of representative elementary volume

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ABSTRACT

When the dense nonaqueous phase liquid (DNAPL) comes into the subsurface environment, its migration behavior is crucially affected by the permeability and entry pressure of subsurface porous media. A prerequisite for accurately simulating DNAPL migration in aquifers is then the determination of the permeability, entry pressure and corresponding representative elementary volumes (REV) of porous media. However, the permeability, entry pressure and corresponding representative elementary volumes (REV) are hard to determine clearly. This study utilizes the light transmission micro-tomography (LTM) method to determine the permeability and entry pressure of two dimensional (2D) translucent porous media and integrates the LTM with a criterion of relative gradient error to quantify the corresponding REV of porous media. As a result, the DNAPL migration in porous media might be accurately simulated by discretizing the model at the REV dimension. To validate the quantification methods, an experiment of perchloroethylene (PCE) migration is conducted in a two-dimensional heterogeneous bench-scale aquifer cell. Based on the quantifications of permeability, entry pressure and REV scales of 2D porous media determined by the LTM and relative gradient error, different models with different sizes of discretization grid are used to simulate the PCE migration. It is shown that the model based on REV size agrees well with the experimental results over the entire migration period including calibration, verification and validation processes. This helps to better understand the microstructures of porous media and achieve accurately simulating DNAPL migration in aquifers based on the REV estimation.

1. Introduction

With the expansion of human activities and the development of the economic society, more and more kinds of dense nonaqueous phase liquids (DNAPLs) have appeared in our daily life. Due to spill-out and other accidents, the subsurface environment is widely contaminated by the released DNAPLs (Essaid et al., 2015; Huang et al., 2015; Liu et al., 2016; Weathers et al., 2016). In the saturated subsurface zone, DNAPLs are usually trapped as residual ganglia and may accumulate in pools above low permeability barriers (Illangasekare et al., 1995). Due to their chemical stability and higher density than water, the released DNAPLs can "sink" and infiltrate through the aquifer (Qin et al., 2007; Liang and Lai, 2008; Liang and Hsieh, 2015). Especially, many compounds in DNAPLs, such as perchloroethylene (PCE) and other polycyclic aromatic hydrocarbons (PAHs) with low solubility, are highly toxic and carcinogenic, which could pose a persistent threat to ecosystem and human health. When DNAPLs come into subsurface environment, their migration and remediation behaviors are crucially affected by the heterogeneities of porous media (such as permeability and entry pressure) (Zheng et al., 2015) and corresponding upscaling problem (Pacheco, 2013; Pacheco et al., 2015). A prerequisite for implementing the groundwater remediation at any DNAPL- contaminated site is the understanding of the heterogeneities and microstructure characteristics such as representative elementary volume (REV) (Brown and Hsieh, 2000; Al-Raoush and Willson, 2005; Al-Raoush and Papadopoulos, 2010; Costanza-Robinson et al., 2011; Wu et al., 2017a) of subsurface porous media.

The heterogeneities and upscaling problem are essential for hydrological research with respect to aquifers (Pacheco, 2013; Pacheco et al., 2015), which has important effect on DNAPL migration in subsurface environment (Wu et al., 2017b). Usually, characterization of porous media and measurement of contaminant migration/remediation are based on high quality laboratory experiments for research (Oostrom et al., 2006; Bob et al., 2008). Natural translucent porous media such as silica sands with different grain sizes can be used to create a variety of mixtures and textures

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similar to natural aquifer media in experiments where the study of DNAPL migration and remediation in these translucent porous media is essential to understanding of aquifer contaminations. Comparing with X-ray measurements and gamma ray radiation, the light transmission visualization (LTV) requires the least specialized equipment (e.g., high energy sources) and is therefore the cost-effective high resolution technique (Niemet and Selker, 2001; Weisbrod et al., 2003; Bob et al., 2008) to quantify the fluid content in translucent porous media. In addition, the porous media has been proven to be fractal objects due to the self-similarity in nature (Pfeifer and Avnir, 1983; Katz and Thompson, 1985; Krohn, 1988). Based on fractal concepts, a number of studies on fractal dimension were carried out to investigate characteristics of porous media (Yu and Cheng, 2002; Yu and Li, 2004; Yu, 2005; Feng and Yu, 2007; Yu et al., 2009; Cai et al., 2010; Li and Yu, 2013). Nevertheless, for two dimensional (2D) translucent porous media (natural translucent silica sands) used in laboratory experiment, critical parameters such as permeability and entry pressure with heterogeneous distribution and corresponding representative elementary volumes (REV) are still hard to derive using single LTV technique or fractal studies. Therefore, a new light transmission micro-tomography (LTM) (Wu et al., 2017a, 2017b) was developed to quantify characteristics of translucent porous media based on previous LTV. Unfortunately, the effect of REV dimension on the simulation of contaminant migration in porous media is not clear yet. The sizes of discretization grid for modeling are usually assigned by reason of computational effort instead of real REV scale in applications, which may cause extra errors in simulation.

This paper focuses on the effect of REV dimension on modeling of DNAPL migration in porous media. Based on the LTM technique newly developed by Wu et al. (2017a, 2017b), the heterogeneous distribution of porosity for 2D porous media is determined. A fractal model of porous media microstructures is then conducted to derive the heterogeneous distributions of permeability and entry pressure. Afterward, a new criterion of the relative gradient error (ε_g^i) is utilized to estimate the REV scales of permeability and entry pressure. To verify the applicability and effectiveness of REV dimension on simulation of contaminant migration in porous media, an experiment of PCE migration in a 2D bench-scale heterogeneous aquifer cell is performed. Different models based on different sizes of discretization grid are used to simulate the PCE migration. Finally, all simulation results are compared with experimental results.

2. Methodology

2.1. Quantification of heterogeneities and REV estimation

Previous LTV method (Niemet and Selker, 2001; Weisbrod et al., 2003; Bob et al., 2008) can be used to quantify the DNAPL saturation in translucent porous media. However, the properties of translucent porous media are unable to be determined by LTV. Fortunately, the LTM method (Wu et al., 2017a, 2017b), as an extension of the LTV (Niemet and Selker, 2001; Weisbrod et al., 2003; Bob et al., 2008), can be utilized to accurately quantify the porosity of translucent porous media, and heterogeneity of permeability and entry pressure. For the sake of completeness, quantification of heterogeneities and REV estimation by the LTM is briefly recapitulated in this section. For more detailed mathematical derivation combined with fractal analysis and porous microstructure, readers can refer to Wu et al. (2017a, 2017b).

2.1.1. Quantification of porosity by LTM

According to Fresnel's law, when light passes through different phases of porous media, the emergent light intensity can be expressed as (Niemet and Selker, 2001; Weisbrod et al., 2003; Bob et al., 2008; Wu et al., 2017a, 2017b):

$$I = CI_0(\Pi_1^{m-1}\tau_j)\, exp\left(\sum_1^m \alpha_i d_i\right) \tag{1}$$

where I is the light intensity after passing through the porous media; C is the correction constant; I_0 is the measured intensity of the light source; τ_j is the transmittance of the interface between compartments i and i+1; α_i is the absorption coefficient of the medium i; d_i is the thickness of compartment i; m is the total number of compartments across the porous media.

If the porous media system includes solid, water liquid and DNAPL, the Fresnel's law can be written as (Niemet and Selker, 2001; Weisbrod et al., 2003; Bob et al., 2008; Wu et al., 2017a, 2017b):

$$I = CI_0\tau_{s,w}^{2k_o}\tau_{w,o}^{2k_oS_{DL}}\, exp(-\alpha_s k_s d_s - \alpha_{DL}k_{DL}d_o) \tag{2}$$

where d_s is the average diameter of solid particles; d_o is the average diameter of pores; k_s is the number of solid particles; k_{DL} is the number of pores saturated by DNAPL; k_o is the whole number of pores; $\tau_{s,w}$ and $\tau_{w,o}$ are the transmittance of the solid-water and water-DNAPL interfaces, respectively; α_s is the absorption coefficient of solid particles; α_{DL} is the absorption coefficient of DNAPL; S_{DL} is the fraction of pores saturated by DNAPL.

If the porous media system only includes solid and water liquid, the Fresnel's law given by Eq. (2) can be simplified as (Niemet and Selker, 2001; Weisbrod et al., 2003; Bob et al., 2008; Wu et al., 2017a):

$$I_s = CI_0\tau_{s,w}^{2k_0}\, exp(-\alpha_s k_s d_s) \tag{3}$$

where I_s is the light intensity after passing through the porous media only includes solid and water liquid.

Consider an infinitesimal element in the 2D porous media saturated by water, of which the corresponding cross-sectional area A_o approaches zero (*i.e.*, $A_o \to 0$). Using the deriving procedure in Wu et al. (2017a), the relationship between porosity (n) and light intensity (I_s) can be obtained:

$$n = \frac{\ln I_s - \beta}{\gamma} \tag{4}$$

where $\beta = ln\left(\frac{CI_0}{e^{\alpha_s d_s L_T}}\right)$, and $\gamma = ln\left(\tau_{s,w}^{\frac{2L_T}{d_0}} e^{\alpha_s L_T}\right)$. Thus, for a particular translucent porous medium, porosity can be directly calculated by determining the values of β, γ in Eq. (4) from the experiment.

2.1.2. Derivation of permeability and entry pressure

In fractal theory, the cumulative islands of special sizes on earth follow the distribution rule $N(B > b) \sim b^{-D/2}$ (Mandelbrot, 1975), where N is the total number of those islands of which area B is greater than b, and D is the fractal dimension of the surface. Fractal theory was applied to study the contact spots on engineering surfaces by Majumdar and Bhushan (1990):

$$N(B \geqslant b) = \left(\frac{b_{\max}}{b}\right)^{D_f/2} \tag{5}$$

where $b_{\max} = g\varphi_{\max}^2$, $b = g\varphi^2$; φ is the diameter of pore size; g is the geometry factor.

The porous media including numerous pores can be considered as the bundle of capillary tubes of different sizes. The capillary tubes in porous media are analogous to the islands on the earth's surface and the contact spots on engineering surfaces. Consequently, the cumulative number of capillary tubes in unit area of porous media follows the power-law relationship (Yu and Cheng, 2002):