



Solute dispersion under electric and pressure driven flows; pore scale processes



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SUMMARY

Solute dispersion is one of the major mixing mechanisms in transport through porous media, originating from velocity variations at different scales, starting from the pore scale. Different driving forces, such as pressure driven flow (PDF) and electro-osmotic flow (EOF), establish different velocity profiles within individual pores, resulting in different spreading of solutes at this scale. While the velocity profile in PDF is parabolic due to the wall friction effects, the velocity in EOF is typically plug flow, due to the wall charge effects. In this study, we applied a pore network modeling formulation to simulate the velocity field driven by pressure and electric potential to calculate and compare the corresponding average solute dispersivity values. The influence of different driving forces on the hydrodynamic dispersion of a tracer solute is investigated. Applying the pore network modeling, we could capture the velocity variations among different pores, which is the main contribution for the dispersion coefficient. The correlation between pore velocities against pore sizes is found to be different for EOF and PDF, causing different solute dispersion coefficients. The results can provide insight into modeling of electrokinetic remediation for contaminant cleanup in low permeable soils.

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1. Introduction

1.1. Electro-osmotic flow and solute transport

Transport of solutes in porous media can be due to different driving forces such as applied pressure or external electric field (Coelho et al., 1996). External electric field, driving flow of fluid and motion of ions in a porous media, is called electro-osmotic flow which involves various applications. Examples are, chromatography (Chen et al., 2005; Hilder et al., 2000), separation technologies and drug delivery (Fine et al., 2011; Grattoni et al., 2010; Ostergaard et al., 2008), groundwater contaminant removal and concrete desalination (Castellote and Botija, 2011; Kamran et al., 2012). Electro-osmotic flow and transport at the micro scale or single capillary tubes have been well studied (Ghosal and Chen, 2012; Gillespie and Pennathur, 2013; Haria and Lorenz, 2012; Jalili et al., 2012; Rani et al., 2013; Rotenberg and Pagonabarraga, 2013). However, there are very few studies available on the topic of electro-osmosis in porous media, which is indeed an assemblage of several capillary pores connected to each other in a complex manner (Berli, 2007; Brovelli and Cassiani, 2010; Revil and Leroy, 2004;

Revil et al., 2007; Zhu and Papadopoulos, 2012). Accurate field scale modeling of contaminants remediation needs input on various flow and solute transport properties which depends on underlying pore scale process.

At the pore scale, the net excess charge within the electric double layer (EDL) causes fluid flow in the presence of an external electric field. On the other hand, in the case of a pressure driven flow (PDF), fluid–solid interfaces act as a source of friction to slow down the flow. As a result, the variation of flow velocity is smaller for EOF compared to the Hagen-Poiseuille flow established under PDF (Dutta, 2008; Hlushkou et al., 2007, 2005; Wang et al., 2006; Xuan and Sinton, 2007). At a larger scale than a scale of a single pore, solute dispersion is due to the velocity variations among pores with different sizes and mixing at the pore junctions. Larger pores are effective for PDF conditions, while smaller pores contribute the most to the flow for EOF due to the higher specific surface area. Starting from pore scale, Dutta (Dutta, 2008) derived an analytical solution to investigate the effect of pore aspect ratio and electrokinetic radius (ratio of the electric double layer to the pore height or radius) on hydrodynamic dispersion. Both parameters were found to significantly affect the hydrodynamic dispersion under decreasing values of aspect ratio and electrokinetic radius. Revil et al. (2011) investigated the effect of the Stern layer on the transversal dispersion coefficient. They found that transport

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within the Stern layer does not affect the transversal dispersion coefficient.

1.2. Pore scale modeling of hydrodynamic dispersion

Porous media are composed of several, interconnected, capillary pores. By simplifying description of porous media as a network of connected capillaries, the alternative scheme to describe transport through macroscopic porous materials was originally developed by Fatt (1956) to study multiphase flow properties in porous media. Pore network modeling has been extensively used and extended by many researchers in various disciplines, e.g. capillarity and multiphase through porous media (Blunt, 2001; van Dijke and Sorbie, 2002), reactive transport (Varloteaux et al., 2013a,b), mineral dissolution and precipitation caused by CO₂ sequestration (Algive et al., 2012; Nogues et al., 2013; Raof et al., 2012), the streaming potential in geophysics (Bernabe, 1998), and electrokinetic transport through charged porous media (Obliger et al., 2014). Applying conservation equations to different pores located in a network of interconnected capillaries and averaging the results can provide a powerful tool to study electro-osmotic flow and transport behavior in porous media. This approach is utilized in pore network modeling for upscaling of fluid flow and solute transport in porous media (Raof and Hassanizadeh, 2010b; Raof et al., 2010). Within pore network modeling, the pore sizes, which are commonly defined using a log-normal distribution (Acharya et al., 2007), and connectivities between different pores are decided in advance to mimic a specific porous structure. Next, equations governing fluid flow and solute transport are solved within each and every pore providing fluid fluxes and solute concentrations in different pores. Integrating solutions over the network domain, effect of pore structure and pore size distribution on flow and transport in porous media can be investigated (Raof et al., 2013). The average values obtained using pore network, provide macro scale parameters such as porosity, permeability, and hydraulic solute dispersivity.

Equally important to the geometric properties of porous media (i.e., pore sizes) are network topology parameters such as connectivity or coordination number and coordination number distribution (Raof and Hassanizadeh, 2010a). Coordination number is defined as the number of pores connected to a given pore in the network. Using pore network modeling, Vasilyev et al. (2012) studied the effect of pore space topology on solute dispersivity. It was shown that the dispersion coefficient increases by increasing the coordination number.

To simulate distribution of solute within the pore network, first the flow field is calculated. Then, solving mass balance equation for solute concentration in each pore, dispersion coefficient can be derived using the breakthrough curve of solute at the outlet of porous medium or using the solute concentration profile along the domain. Bijeljic and Blunt (2007), using a 2D pore scale model, found that the velocity distribution in neighboring pores affects the solute dispersion significantly under pressure driven flow. They concluded that the velocity variation within neighboring pores is a major cause of dispersion at the lower velocities where diffusive transport of solute are the major transport mechanism compared to advective transport. Dentz et al. (2004) proposed a parameter, β , in truncated power law within the context of the continuous time random walk framework (Berkowitz et al., 2006; Cortis and Berkowitz, 2004), related to the degree of non-uniformity/heterogeneity in porous media which is represented by the ratio of standard deviation of the pore radius to the mean pore radius. They have shown that anomalous dispersion occurs at low values of β for low velocity values. They found that non-Fickian transport occurs at low velocity values, which the extent of spreading and mixing of solute is controlled by the variance of pore throat velocities.

Applying pore scale modeling, Hlushkou et al. (2005) investigated electro-osmotic flow using different packed beds, with regular and random packing. They found that the pore level velocity profile of EOF in porous media is controlled by grain surfaces. The major contribution of velocity variance in porous media originates from the heterogeneity of the porous structure (i.e., particle/pore size distribution) and surface heterogeneities which determines the thickness of EDL. Using the lattice Boltzmann method, Daneyko et al. (2011) explored the importance of pore size distribution and porosity on hydrodynamic dispersion. They found that the relative contribution of the pore size distribution and the porosity to hydrodynamic dispersion remained.

1.3. Objectives

Although solute dispersion under pressure driven flow has been widely studied based on underlying pore scale processes, there is much less knowledge on dispersion under electro-osmotic flow in porous media. In this study, we apply pore network modeling method to investigate how pore structure affects hydrodynamic dispersion under pressure driven and electro osmotic flows. Considering electric osmotic flow under the assumption of thin electric double layer, we compared the resulting solute dispersivity value with those obtained under pressure driven flow. First, the flow field in the three dimensional pore network is calculated, and then the resulting velocities are used to simulate transport of a tracer solute within the pore network. The (macroscopic) dispersion coefficient is calculated using the solute breakthrough curves obtained at the outlet of the pore network. Using this method, we investigated the relation between pore size distribution and solute dispersion, for both EOF and PDF.

2. Numerical formulation

2.1. Physical model

Electro osmosis is flow of fluid induced by the applied external electric field. The electric field drags the ions along the charged solid interfaces, due to the excess charge within the electric double layer (EDL). Transport of ions exerts viscous forces on the fluid in the bulk space to establish flow. The resulting electro-osmotic velocity profile within a single pore is plug shaped with uniform velocity distribution along the pore cross section.

2.2. Flow and transport in a single pore

In the presence of pressure gradients, the excess charges within the electrical double layer, coating the wall surface, is dragged by the fluid flow. The resulting flux causes a passive current which is called a streaming current. According to Onsager's reciprocal principle (Onsager, 1931), the fluid flow and ionic current density in a single pore can be described using the following equations:

$$q = L_{11}\Delta P + L_{12}\Delta V \quad (1)$$

$$I = L_{21}\Delta P + L_{22}\Delta V \quad (2)$$

where q denotes the fluid volumetric flow rate (m^3/s), I is the ion current (A). The L_{ij} coefficients are the coupling terms. In the absence of the pressure difference (i.e., $\Delta P = 0$), the resulting fluid flow is electric osmotic flow; otherwise, it is pressure driven flow when L_{12} is equal to zero under the thin double layer conditions. L_{11} and L_{22} are the hydraulic conductance ($\text{m}^3/(\text{Pa s})$) and electrical conductance (S), respectively. The coupling coefficients for a

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