Advances in Water Resources 92 (2016) 23–29

Contents lists available at ScienceDirect

Advances in Water Resources

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

A transport phase diagram for pore-level correlated porous media

M. Babaei, V. Joekar-Niasar*

School of Chemical Engineering and Analytical Science, University of Manchester, M13 9PL Manchester, UK

ARTICLE INFO

Article history:
Received 24 August 2015
Revised 21 March 2016
Accepted 25 March 2016
Available online 30 March 2016

JEL classification:
100: subsurface hydrology
100.040: pore-scale modelling
100.070: single-phase flow and transport
100.020: numerical model solution approaches

Keywords:
Transport phase diagram
Pore-level correlation
Pore-network modelling
Advection
Dispersion

ABSTRACT

Transport in porous media is often characterized by the advection–dispersion equation, with the dispersion coefficient as the most important parameter that links the hydrodynamics to the transport processes. Morphological properties of any porous medium, such as pore size distribution, network topology, and correlation length control transport. In this study we explore the impact of correlation length on transport regime using pore-network modelling. Earlier direct simulation studies of dispersion in carbonate and sandstone rocks showed larger dispersion compared to granular homogenous sandpacks. However, in these studies, isolation of the impact of correlation length on transport regime was not possible due to the fundamentally different pore morphologies and pore-size distributions. Against this limitation, we simulate advection–dispersion transport for a wide range of Péclet numbers in unstructured irregular networks with “different” correlation lengths but “identical” pore size distributions and pore morphologies. Our simulation results show an increase in the magnitudes of the estimated dispersion coefficients in correlated networks compared to uncorrelated ones in the advection-controlled regime. The range of the Péclet numbers which dictate mixed advection–diffusion regime considerably reduces in the correlated networks. The findings emphasize the critical role of correlation length which is depicted in a conceptual transport phase diagram and the importance of accounting for the micro-scale correlation lengths into predictive stochastic pore-scale modelling.

1. Introduction

Geological media have structure on all length scales, and the scale of a few pores is no exception (Lindquist et al., 2000; Blunt, 2001). For example, based on micro CT imaging Yao et al. (1997) reported that the red sandstone from Vosges Mountains in France exhibits correlation lengths of 17.8 μm, 17.5 μm and 20.6 μm in three orthogonal directions for the porosity measurements variations. For the same sandstone Mees et al. (2003) reported an average correlation length of 27.8 μm. Regarding this inherent nature, if one desires to quantitatively reproduce the trends of macroscopic experimental data, the pore structure characteristics must be accounted for and realistically embodied in the models.

Numerous image analysis studies on natural porous media (see *e.g.*, Wardlaw et al. 1987; Bryant et al., 1993a, 1993b; Knackstedt et al., 1998, 2001; Lindquist et al., 2000; Al-Raoush and Willson, 2005) infer the message that spatial correlations exist at the pore scale between pore body and pore throat sizes. Furthermore, the importance of incorporating the spatial correlations at microscale and their key impact on macroscopic flow properties have been pointed out in a large number of works (see *e.g.*, Jerauld and Salter, 1990; Renault, 1991; Ferrand and Celia, 1992; Ferrand et al., 1994; Blunt, 1997; Rajaram et al., 1997; Knackstedt et al., 2001; Jang et al., 2011).

First we briefly review the literature focused on the effects of correlated pore scale heterogeneity on transport properties and next we present the scope of this work.

1.1. Effects of spatial correlation on transport

Transport in porous media is characterized by dispersion coefficient (D_L) for different pore velocities. Péclet number (Pe), which is the ratio of advective to diffusive transport, is utilized to identify the transport regime in a porous medium. Péclet number by definition is defined as $Pe = vL/D$, where L is the characteristic length scale, v denotes the pore velocity and D is the diffusion coefficient. Typically three different regimes are defined based on the trend between dispersion coefficient and Péclet number:

(a) a diffusion-dominated regime for low Péclet numbers ($Pe < 0.3$), where the relationship $D_L/D_m = 1/F\phi$ holds (Sahimi, 1993), F is the formation resistivity factor and ϕ is the porosity of the porous medium;

* Corresponding author. Tel.: +44 1613064867.
E-mail address: vahid.niasar@manchester.ac.uk (V. Joekar-Niasar).

http://dx.doi.org/10.1016/j.advwatres.2016.03.014
0309-1708/

(b) an advection-dominated regime for large Péclet numbers $Pe > Pe^{crit}$ (representing the so-called mechanical dispersion). For this regime, we have $D_L/D_m \sim Pe$, where Pe^{crit} (200–4000) depends on porous medium structure and increases with increasing heterogeneity (Bijeljic and Blunt, 2006);

(c) a mixed diffusion–advection regime in between the two regimes ($1 < Pe < Pe^{crit}$), an approximate power-law regime with a supra-linear dependency as $D_L/D_m \sim Pe^{\beta}$, holds for this regime. The power-law regime happens when there is an interplay between diffusion and advection. In this regime compared to the other two regimes, the relation between the dispersion and Péclet number is more sensitive to the morphological features of the pore space and heterogeneity.

It is interesting to investigate the effects of geostatistical parameters of pore network on dispersion and transport regimes. The correlation length in pore size distribution is one of several geostatistical parameters of pore network models. The representation of spatially correlated fields by pore scale models to study macroscopic dispersion has been the focus of several studies. Using fractally distributed pore space with long range correlations, referred to as disordered porous media, Sahimi (1993) showed that large scale fluctuations in the velocity field due to the spatial variations of the permeability field is the principal cause of dispersion. He also argued that in order to have predictive models of porous media, the permeability of the throats should be assigned in a correlated pattern compatible in range and type with the available experimental data. Using fractional Brownian motion to represent macroscopic long-range correlations in permeability of rocks, Sahimi (1995) demonstrated that the interplay between the correlated nature of the structure of the media and the transport process can give rise to a rich variety of macroscopic transport regimes absent from uncorrelated systems. Numerous studies emphasized the impact of spatial correlations of “macroscopic parameters” on transport coefficients and solute transport (see *e.g.*, Tsang and Neretnieks, 1998; Moreno and Tsang, 1994; Vogel, 2000; Dentz et al., 2002; Knudby and Carrera, 2005, 2006; Renard and Allard, 2013).

A few works due to Bernabé and Bruderer (1998), Makse et al. (2000), Bruderer and Bernabé (2001), Bruderer-Weng et al. (2004) and Le Borgne et al. (2011) are dedicated to specifically target the effect of “pore-level correlations” on transport regimes. Bernabé and Bruderer (1998) investigated the influence of *pore size variance* on the transport in the 2D networks of cylindrical tubes inclined at 45° to the nominal flow direction. Bruderer-Weng et al. (2004) showed that in statistically isotropic, heterogeneous networks, flow channelling intensifies when normalized standard deviation and correlation length of the radii distribution of the pore throats are increased. Intensification of flow channelling increases the dispersion coefficient. Again for 2D models of pore networks, le Borgne et al. (2011) showed that correlation of the spatial velocity should be explicitly included to represent incomplete mixing in the pore throats.

1.2. The present work

In spite of numerous pore-scale studies elucidating the effects of correlation length on transport properties, a systematic study using “*3D, correlated, irregular and unstructured pore-network modelling*” within the context of advective-dispersive transport with clearly defined correlation lengths is missing. Here, we isolate the effect of pore-scale correlation length on the macroscopic longitudinal dispersion coefficient (D_L) and identify transport regimes for different correlation lengths. As discussed in the previous subsection, Bruderer and Bernabé (2001) and Bruderer-Weng (2004) had previously used 2D pore network modelling to exactly see the effect of heterogeneity and correlation length of pore networks on D_L. However the first work was limited to coefficient of variation of the pore radii distribution and the second work did not study the effect of correlated networks for varying Péclet number regimes. Furthermore, the correlation structure in porosity and velocity has been studied at the pore-scale on micro-CT images of sandstones and carbonates (*e.g.*, Bijeljic et al., 2013a,b; Porta et al., 2015), but as discussed correlation length was an integral part of the micro-CT images and could not be independently varied.

To focus *only* on effects of correlation length, we generate networks with identical topology that resemble statistical and topological properties of natural systems. We also employ identical pore size distributions. Only the spatial distributions of pore sizes are assigned differently so as to have various correlation lengths in the networks. We use pore-network modelling because it allows us to simulate large domains at affordable computational costs. The computational efficiency in the proposed methodology and pore-scale analyses is superior to the direct-image simulation, and this is an important factor because multiple simulation scenarios and realizations for different correlation lengths may be required before a good characterization of transport is presented.

In the following sections, first we present the network generation algorithm, and upscaling of the results from pore to REV (representative elementary volume) scale to obtain the macroscopic dispersion coefficient. Then, we present the results and discuss the effect of correlation length on the longitudinal dispersion at different Péclet numbers and we propose a conceptual transport phase diagram that shows variation of transport regime *versus* the correlation length and the Péclet number.

2. Pore network generation and simulation

The first step in pore network modelling is to construct the topology of the network. We use Delaunay triangulation, Voronoi tessellation and a processing step to trim down the network from the excessive long throats such that a realistic mean coordination number is generated.

For all simulations, the topology of the correlated and uncorrelated networks is identical, *i.e.* the pore body locations and the local coordination number assigned to each pore body are identical in all network realizations. The only difference between the networks is the spatial distribution of pore sizes. The correlated network takes a spatially correlated distribution of pore body sizes, whereas the pore bodies in the uncorrelated network are attributed with random values for pore radii chosen from exactly the same distribution of the correlated network. This algorithm allows us to conduct the direct comparison between the outcomes of the two networks based solely on the magnitude of pore size spatial correlation. An approach similar to the methodology developed by the authors in Leng (2013) is used here. The network generation is conducted in four steps:

Step 1: We randomly populate the space with pore body centre points so that no two points are closer to each other than a minimum threshold value assigned by an input.

Step 2: We generate the correlated fields for the pore body radii using the field generator developed by Nowak et al. (2008). We map the points generated in Step 1 to the field generated in Step 2 to assign the pore body radii. Nowak et al. (2008) used fast Fourier transform based on the spectral density estimation to estimate the spectral density function from a random autocorrelated field. We use anisotropic exponential variogram, $\gamma(h) = \sigma_Y^2(1 - \exp(-|h|))$, for a second-order stationary field of $Y = \ln R$, which R stands for the pore radii, σ_Y^2 is the variance of Y, and $h[--]$ is the (anisotropic) effective separation distance scaled by the correlation length scales λ_i[L], $i = x, y, z$, such that $h = (\sum_{i=1}^{3} h_i^2/\lambda_i^2)^{0.5}$, and