Advances in Water Resources 97 (2016) 1–10

Contents lists available at ScienceDirect

Advances in Water Resources

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

Simulating dispersion in porous media and the influence of segmentation on stagnancy in carbonates

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ARTICLE INFO

Article history:
Received 1 October 2015
Revised 19 August 2016
Accepted 19 August 2016
Available online 25 August 2016

Keywords:
Dispersion
Porous Media
Heterogeneity
Carbonates
Segmentation
Stagnant

ABSTRACT

Understanding the transport of chemical components in porous media is fundamentally important to many reservoir processes such as contaminant transport and reactive flows involved in CO_2 sequestration. Carbonate rocks in particular present difficulties for pore-scale simulations because they contain large amounts of sub-micron porosity. In this work, we introduce a new hybrid simulation model to calculate hydrodynamic dispersion in pore-scale images of real porous media and use this to elucidate the origins and behaviour of stagnant zones arising in transport simulations using micro-CT images of carbonates. For this purpose a stochastic particle model for simulating the transport of a solute is coupled to a Lattice-Boltzmann algorithm to calculate the flow field. The particle method incorporates second order spatial and temporal resolution to resolve finer features of the domain. We demonstrate how dispersion coefficients can be accurately obtained in capillaries, where corresponding analytical solutions are available, even when these are resolved to just a few lattice units. Then we compute molecular displacement distributions for pore-spaces of varying complexity: a pack of beads; a Bentheimer sandstone; and a Portland carbonate. Our calculated propagator distributions are compared directly with recent experimental PFG-NMR propagator distributions (Scheven et al., 2005; Mitchell et al., 2008), the latter excluding spin relaxation mechanisms. We observe that the calculated transport propagators can be quantitatively compared with the experimental distribution, provided that spin relaxations in the experiment are excluded, and good agreement is found for both the sandstone and the carbonate. However, due to the absence of explicit micro-porosity from the carbonate pore space image used for flow field simulations we note that there are fundamental differences in the physical origins of the stagnant zones for micro-porous rocks between simulation and experiment. We show that for a given micro-CT image of a carbonate, small variations in the parameters chosen for the segmentation process lead to different amounts of stagnancy which diffuse away at different rates. Finally, we use a filtering method to show that this is due to the presence of spurious isolated pores which arise from the segmentation process and suggest an approach to overcome this limitation.

1. Introduction

The hydrodynamic dispersion of solute particles in porous media is of great importance in many scientific and engineering applications (Adler, 1992), including ground water pollution, CO_2 sequestration and hydrocarbon recovery. The upscaling of dispersion phenomena from the pore to core scale is complex and a rigorous theoretical description remains an outstanding scientific challenge (Bijeljic and Blunt, 2006). Various numerical methods have been proposed to investigate dispersion at the pore scale. Historically, network modelling has been widely used (Bruderer and Bernabé, 2001; Bijeljic et al., 2004; Bijeljic and Blunt, 2006; Acharya et al., 2007). However, for heterogeneous porous media, such as carbonate rocks, it is very difficult to extract reliable and unique pore networks (Knackstedt et al., 2006). For this reason, direct calculation on three-dimensional pore space images obtained from e.g. micro-CT scanning or Confocal Laser Scanning Microscopy (CLSM) (Shah et al., 2013) has been proposed to avoid the problems associated with network extraction (Ramstad et al., 2012). Coelho et al. (1997) used a finite difference method to solve for the flow and dispersion in unconsolidated bead packs and sandstones. Maier et al. (2000) used a hybrid method, consisting of

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http://dx.doi.org/10.1016/j.advwatres.2016.08.009
0309-1708/

lattice-Boltzmann (LB) simulations to calculate the flow field combined with a random-walk particle-tracking method to simulate dispersion in a sphere pack. They found good agreement with nuclear magnetic resonance (NMR) experiments for both transient and asymptotic dispersion. Kandhai extended this model to include effective diffusion inside porous beads (Kandhai et al., 2002) and found this to lead to stagnant zones which diffuse out over long time-scales. Recently, Scheven et al. (2005, 2007) reported molecular displacement (or propagator) distributions for different rock samples obtained from Pulsed Field Gradient—Nuclear Magnetic Resonance (PFG-NMR) experiments. They observed that the character of the propagator distributions strongly depends on the heterogeneity of the porous medium. Bijeljic et al. (2013), used a Stokes solver for the flow field and a streamline-based algorithm for solute dispersion which included interpolation of the velocity field at the fluid-solid boundary (Mostaghimi et al., 2012; Nunes et al., 2015), and observed agreement with the experimental NMR propagator results (Scheven et al., 2005). Mitchel et al. (2008) improved the analysis of PFG-NMR experiments by correcting for the loss of signal due to spin relaxation and these results have also been compared to propagators calculated from micro-CT images (Bijeljic et al., 2011). The extent of agreement between the calculated and measured propagator distributions is surprising for the carbonate rocks, given that a significant fraction of the porosity in such samples is below the resolution of the CT scan (Crawshaw and Boek, 2013) and therefore excluded from the simulations. Yang, Crawshaw, and Boek (2013) developed a new LB algorithm to calculate both the flow field and solute dispersion in pore space images of different heterogeneity. They quantified the degree of heterogeneity and calculated the fraction of solute particles trapped by integrating over the stagnant peak (Yang et al., 2013). However, it appeared to be difficult to study the diffusive coupling for long time scales in a quantitative fashion. For this reason, we propose here a new hybrid algorithm, using LB simulations to solve the flow field coupled with a streamline-based algorithm for solute dispersion. In addition, we propose a second order velocity-field interpolation scheme for particle advection, which is more accurately able to compute the dispersion of solute in finer features of the pore-space. We observe good agreement with the experimental propagator distributions (Scheven et al., 2005; Mitchell et al., 2008).

Although several of the aforementioned studies have reported quantitative matches with NMR data in the case of the Portland carbonate, the origins of the stagnant fraction of solute in the simulations of flow in this micro-porous rock deserve further consideration. We investigate here the origins of the stagnant peak in transport simulations based on micro-CT data, since the limited resolution of these images cannot have accurately represented micro-porous regions, while the fluid in these regions is included in the NMR data after the correction for spin relaxation effects noted above. Necessarily for such modelling investigations, a segmentation procedure must convert grey-scale microporous regions of the micro-CT image into discrete pore or grain regions. This suggests that unphysical isolated pores could have arisen from this procedure and may cause an artificial stagnancy. To determine whether this hypothesis is sound, we obtained several segmented images of a Portland carbonate sample from the same scan by varying the segmentation parameters, and we demonstrate that this changes the magnitude and transient behaviour of the stagnant peak. Finally, we apply a filtering algorithm to remove isolated pores from the segmented images which enables us to differentiate between (a) small isolated pores containing permanently trapped solute and (b) regions of poorly connected structure whose solute would be expected to diffuse into flowing paths over long time-scales.

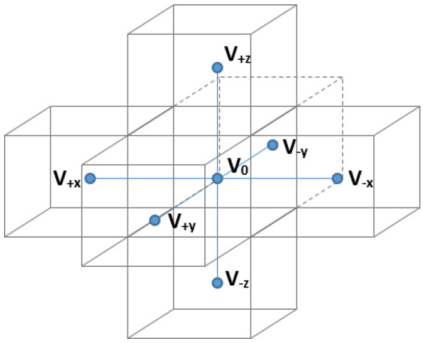

Fig. 1. Centre node velocity vector $\mathbf{V}_0$ and its six nearest neighbours.

2. Method

The simulation is performed on a 3-dimensional Cartesian lattice with nodes marked as either fluid or solid describing the geometry. Fluid nodes are associated with a flow vector which is the solution to the incompressible Stokes flow at the centre of the grid element. This flow-field is computed using the single-phase multiple-relaxation-time (MRT) lattice Boltzmann model (Gray and Boek, 2016).

The stochastic tracer method consists of transporting particles through the domain in two steps. First, a forward integration along the flow vectors describes the advection part, followed by a random-walk step to simulate diffusion by Brownian motion. To derive the second order advection scheme, we interpolate a second order velocity field around each node's flow vector $\boldsymbol{V}_0$ using the 6 neighbouring vectors $\boldsymbol{V}_{\pm x,\,y,\,z}$ (Fig. 1). Generally, these polynomials are written as

$$v^i(x,y,z) = V_0^i\left(a_x^i x^2 + b_x^i x + c_x^i\right)\left(a_y^i y^2 + b_y^i y + c_y^i\right)\left(a_z^i z^2 + b_z^i z + c_z^i\right) \tag{1}$$

where $i = x, y, z$ is the component of the flow vector. The position x, y, z is relative to the centre of the node and the grid spacing is such that the distance between the centres of each neighbour is unity. The coefficients a, b and c are to be determined in terms of the neighbouring vectors.

We may then impose boundary conditions to calculate the 27 advection coefficients for each node. Two of these conditions are

$$v^i(0,0,0) = V_0^i \tag{2}$$

$$v^i(\pm 1, y, z) = V_{\pm x}^i \tag{3}$$

These conditions imply that all the c coefficients are equal to 1, and thus we only need store 18 coefficients for each fluid node.

Expressions for the a and b coefficients for a case without adjoining solid nodes can then be obtained for each component i in terms of the neighbouring vectors. For the x coefficients

$$a_x^i = \frac{V_x^i + V_{-x}^i}{2V_0} - 1 \tag{4}$$

$$b_x^i = \frac{V_x^i - V_{-x}^i}{2V_0} \tag{5}$$

When a neighbouring node is solid, we impose a 0 velocity vector at the boundary, in line with the halfway bounce-back lattice Boltzmann scheme. For a solid at the $+x$ node, the condition is

$$v^i\left(\frac{1}{2}, y, z\right) = 0 \tag{6}$$