Advances in Water Resources 114 (2018) 149–163

Contents lists available at ScienceDirect

Advances in Water Resources

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

A hierarchy of models for simulating experimental results from a 3D heterogeneous porous medium

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ARTICLE INFO

Article history:
Received 16 November 2017
Revised 8 February 2018
Accepted 9 February 2018
Available online 10 February 2018

Keywords:
Solute transport
Upscaling
Laboratory experiments
Heterogeneous porous media
Model complexity

ABSTRACT

In this work we examine the dispersion of conservative tracers (bromide and fluorescein) in an experimentally-constructed three-dimensional dual-porosity porous medium. The medium is highly heterogeneous ($\sigma_Y^2 = 5.7$), and consists of spherical, low-hydraulic-conductivity inclusions embedded in a high-hydraulic-conductivity matrix. The bimodal medium was saturated with tracers, and then flushed with tracer-free fluid while the effluent breakthrough curves were measured. The focus for this work is to examine a hierarchy of four models (in the absence of adjustable parameters) with decreasing complexity to assess their ability to accurately represent the measured breakthrough curves. The most information-rich model was (1) a direct numerical simulation of the system in which the geometry, boundary and initial conditions, and medium properties were fully independently characterized experimentally with high fidelity. The reduced-information models included; (2) a simplified numerical model identical to the fully-resolved direct numerical simulation (DNS) model, but using a domain that was one-tenth the size; (3) an upscaled mobile-immobile model that allowed for a time-dependent mass-transfer coefficient; and, (4) an upscaled mobile-immobile model that assumed a space-time constant mass-transfer coefficient. The results illustrated that all four models provided accurate representations of the experimental breakthrough curves as measured by global RMS error. The primary component of error induced in the upscaled models appeared to arise from the neglect of convection within the inclusions. We discuss the necessity to assign value (via a utility function or other similar method) to outcomes if one is to further select from among model options. Interestingly, these results suggested that the conventional convection-dispersion equation, when applied in a way that resolves the heterogeneities, yields models with high fidelity without requiring the imposition of a more complex non-Fickian model.

1. Introduction

In natural geological systems, highly heterogeneous materials are the rule rather than the exception. One approach for representing systems with very high variations of hydraulic conductivity is to represent the field as a set of distinct regions either through hydrofacies mapping (Anderson et al., 1999), through indicator methods (Knudby and Carrera, 2005), or a combination of these two approaches (Bianchi and Pedretti, 2017; Lee et al., 2007). A particular simplification of these models is the case of bimodal (or dual-domain) media, where only two classes of materials are present (e.g., low conductivity *immobile* regions embedded in high conductivity *mobile* regions) (Davit et al., 2012; Fiori et al., 2011; Golfier et al., 2011; Jankovic et al., 2003; Knudby and Carrera, 2005; Molinari et al., 2015; van Genuchten and Wierenga, 1976). Such media can serve as an idealization of a highly heterogeneous but continuous porous medium that has been segmented into *high* and *low* conductivity components so that the total variance of each segment is reduced. The important hydrogeologic role of such representations has been discussed recently by Molz (2015). Low-conductivity (frequently referred to by the terminology *immobile*) regions are often conceptualized as being spherical or ellipsoidal in analytical (Coats et al., 1964; Fernàndez-Garcia and Sanchez-Vila, 2015; Haggerty and Gorelick, 1995; Poley, 1988; Rabinovich et al., 2013), numerical (Bianchi and Pedretti, 2017; Finkel et al., 2016; Lee et al., 2017) and experimental (Golfier et al., 2011; Zinn et al., 2004) investigations. Ellipsoidal or spherical representations

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https://doi.org/10.1016/j.advwatres.2018.02.009

of low-conductivity inclusions have been used extensively both to represent actual structures observed in the field (e.g., Jussel et al., 1994; Murphy et al., 1992), and as a reasonable simplification of low-conductivity regions (Dagan and Lessoff, 2001). The relevance in this approximation has been discussed in detail in Dagan and Lessoff (2001), Janković et al. (2006) (who use ellipsoidal inclusions in their representations), and in the review by Frippiat and Holeyman (2008). In a recent review article on the geological representation of heterogeneity, Eaton (2006, p. 195) discusses such idealizations for situations where the heterogeneity is particularly large by noting

> Composite media approaches, in which different heterogeneous structures of contrasting hydraulic properties, such as inclusions of different shapes, have also been used to quantify flow numerically ... As these methods become more widely understood, and implemented in readily available modeling codes, their application will allow a geostatistical approach to even the most heterogeneous flow systems, a significant advance.

Early investigations of bimodal systems accounted for the influence of immobile regions on transport phenomena by representing the immobile region with a stagnant volume fraction which is coupled to the mobile region with a constant mass transfer coefficient α (Coats et al., 1964; Deans, 1963; Deans and Lapidus, 1960; Rao et al., 1980); this idea has been extended to more general multiple-region models (Carrera et al., 1998; Haggerty and Gorelick, 1995), and models that include convection and dispersion in both regions (Ahmadi et al., 1998; Ginn et al., 2017; Golfier et al., 2007; Goltz and Roberts, 1986; Haggerty and Gorelick, 1995; Haggerty et al., 2000; van Genuchten and Wierenga, 1976). Reviews of much of the literature on this topic have been presented by Cherblanc et al. (2003) and Fernàndez-Garcia and Sanchez-Vila (2015).

For bimodal representation of heterogeneous materials, the spatial domain is usually envisioned as being separated into two components: (1) a connected, high-conductivity medium, and (2) a disconnected low-conductivity medium. Although in some models the low-conductivity medium is assumed to be immobile, in more recent models it is assumed that convective fluxes can exist in the disconnected phase. Because mass transfer occurs between the high- and low-conductivity regions, the resulting model can represent a range of transport behaviors from conventional convection-dispersion, to transport that appears significantly *non-Fickian*. The characteristic times associated with transport in each of the two regions can span a large range if the conductivity variance in the medium as a whole is large. Such differences in transport times can result in asymmetric breakthrough curves and *tailing* (Bianchi et al., 2011; Fiori et al., 2011; Haggerty et al., 2000; Li et al., 2011; van Genuchten and Wierenga, 1976; Zinn and Harvey, 2003). Accurate and economical descriptions of tailing phenomena have been of significant interest in hydrological applications for some time.

The objectives of this paper are (1) to describe a new set of three-dimensional experiments for solute transport in a bimodally-distributed system, and (2) to assess the ability for a hierarchy of decreasingly complex models to adequately represent the breakthrough curves from these experiments. In particular, we are interested in the use of simplified models to simultaneously reduce the complexity (our measure of the complexity is an algorithmic one described in detail below) while maintaining fidelity with the experimental observations.

We analyze the experimental results using two strictly numerical, and two *upscaled* models (Chastanet and Wood, 2008). Each of these models can be described briefly as follows: (1) A fully-detailed (i.e., resolving all heterogeneities fully) direct numerical simulation (DNS) of the entire experimental domain, (2) A fully-detailed, but domain-reduced representation of the experimental system, (3) An upscaled two-region model accounting for transience in the mass transfer process, and finally (4) An upscaled model that assumes that the mass transfer process is roughly quasi-steady (so that the mass-transfer coefficient is a constant). One important feature of this work is that the experimental system has been highly characterized, so all models of the system are in the absence of adjustable parameters. We examine the ability of each of these models to represent the experimental breakthrough curves, and offer some assessment as to how well reduced-complexity models perform as compared to models that represent essentially perfect information (i.e., fully-resolved DNS where the geometrical details are represented explicitly, within the bounds of experimental error).

2. Background and previous work

Bimodally-distributed media have been studied experimentally by a number of researchers; in Table 1 we have summarized the available experimental data (including this work) for both 2- and 3-dimensional systems. We have taken particular care to report only on experiments with bimodally-distributed media and where the experimental conditions were described in sufficient detail as to make the experiments interpretable.

To address the need to capture tailing associated with bimodal media, formally averaged two-region (Whitaker 1999; Frippiat and Holeyman 2008; Li et al. 2011; Golfier et al. 2011) and even multi-region (Davit and Quintard 2015) transport equations have been developed. Although transport phenomena in highly heterogeneous media have been extensively investigated numerically, studies which combine the predictive capabilities of numerical models with experimental validation at the Darcy scale are still somewhat sparse. The most extensively characterized experiments conducted to date in bimodal media are those summarized in Table 1. With only two exceptions (one of which is the work reported here) these experiments were effectively 2-dimensional, and many of them have log-variance of conductivities (σ_Y) that are near unity. The experiments detailed in this paper are unique in that they are conducted in a medium with 3-dimensional heterogeneity, and the variance is more representative of what might be observed in the field ($\sigma_Y = 5.71$).

To help characterize transport phenomena in bimodal porous materials, where the two regions are denoted as the η- and ω-region respectively, Zinn et al. (2004) suggested the definition of three Péclet numbers (as modified by Golfier et al., 2007)

$$Pe_{\omega\omega} = \frac{||\langle v_\omega\rangle^\omega||}{a}\,\frac{a^2}{D_\omega} = \frac{||\langle v_\omega\rangle^\omega||a}{D_\omega} \tag{1}$$

$$Pe_{\eta\omega} = \frac{||\langle v_\eta\rangle^\eta||a}{D_\omega}\,\frac{a}{L} \tag{2}$$

$$Pe_{\eta\eta} = \frac{||\langle v_\eta\rangle^\eta||}{L}\,\frac{L^2}{D_\eta} = \frac{||\langle v_\eta\rangle^\eta||L}{D_\eta} \tag{3}$$

Here, $||\langle v_\omega\rangle^\omega||$ is the magnitude of the intrinsic velocity in the ω-region D_ω denotes the effective diffusivity of the solute of interest (Section 3.3), a is the radius of the inclusion, and L denotes the characteristic distance for gradients of the concentration; conventionally, this is taken as the system length or (when applicable) the solute pulse length. To help with the interpretation of Table 1, we note the following definitions specific to media with heterogeneities segmented into two hydraulic conductivities

$$\bar{Y} = \varphi_\eta \ln(K_\eta) + \varphi_\omega \ln(K_\omega) \tag{4}$$

$$\sigma_Y^2 = \varphi_\eta\left[\ln(K_\eta) - \bar{Y}\right]^2 + \left[\varphi_\omega \ln(K_\omega) - \bar{Y}\right]^2 \tag{5}$$