Advances in Water Resources 47 (2012) 31–42

Contents lists available at SciVerse ScienceDirect

Advances in Water Resources

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

Numerical analysis of solute transport in variably saturated bimodal heterogeneous formations with mobile–immobile-porosity

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ARTICLE INFO

Article history:
Received 3 October 2011
Received in revised form 3 May 2012
Accepted 10 May 2012
Available online 3 July 2012

Keywords:
Spatial heterogeneity
Solute transport
Unsaturated flow

ABSTRACT

Considering flow and transport in three-dimensional, variably saturated, composite bimodal heterogeneous formations, the main purpose of this study was to extend the previous analyses [37], restricted to the one-region case in which the entire water-filled pore space is mobile, to the two-region case in which part of the water-filled pore space of each of the sub-soils of the composite formation is stagnant, and to investigate the effect of the interaction between the mobile and the immobile regions on solute transport in these formations. Following Russo [37], formations with fine- and coarse-textured embedded soils (FTES- and CTES-formations, respectively), were considered in the analyses. Main results of the present study suggest that mass exchange between the two regions masks features of the transport that exist in bimodal, one-region flow domains, related to characteristics of the unsaturated hydraulic conductivity in variably saturated bimodal, heterogeneous formations. In particular, the crossover behavior (i.e., that under relatively wet conditions, solute spread is larger in the FTES-formations than in the CTES-formations, while the opposite occurs under relatively dry conditions) characterizing one-region, bimodal flow domains disappears in two-region, bimodal flow domains. The latter attributes to the transfer of mass from the mobile region to the immobile region and the extension of the capture zone for the solute particles associated with the fine-textured embedded soil to lower water saturations. Consequently, for both steady state- and transient-flows, as water saturation decreases, the response of the composite formations is essentially independent of the texture of the embedded soil.

1. Introduction

Soil properties relevant to solute transport such as the hydraulic conductivity of near-surface geologic formations often exhibit a considerable spatial heterogeneity ([4,24,39,15,38,42,19], among others) that generally is irregular. Based on experimental evidence (e.g., [39,6,47,38]), it is generally assumed that the heterogeneous formation may be viewed as a single population whose properties follow a unimodal distribution and a two-point spatial covariance with a single, finite length-scale. This assumption may be supported on theoretical grounds, based on the concept of the existence of a discrete hierarchy of length-scales of heterogeneity [9], with disparity between scales. Still, a more general approach is required for the situation in which the disparity between different length-scales is not large enough to neglect the variability on one scale when considering the other.

There are two alternative approaches to deal with situations in which the spatial variability of the formation properties is characterized by a relatively complex correlation structure. The first approach (e.g., [12,31,21,33,34,36,37]), adopted also in the present study, replaces the spatial arrangement of distinct soil materials with a single, composite material whose properties are multimodal but statistically homogeneous. The second approach, the random domain decomposition (RDD) model [53–55] identifies the shape of the soil inclusions and their three-dimensional arrangement probabilistically and results in non-stationary statistics. The first approach, which applies naturally to cases in which the soil materials are not compactly grouped in clusters, has few advantages over the RDD model due to its simplicity [53]. Unlike the RDD model, however, the first approach may not be appropriate when the contrast between mean conductivities of the composite formation exceeds few orders of magnitude.

Based on the first-order, Lagrangian-stochastic analysis of vadose-zone transport [34,35], Russo [37] invesigated the effect of the embedded soil's texture and the mean pressure head (i.e., mean water saturation), on solute transport in steady-state flows in these formations. Two distinct variably saturated composite formations consisting of relatively low-conductive, fine-textured embedded soil with appreciable capillary forces, and high-conductive, coarse-textured embedded soil with relatively weak capillary forces (will be termed hereafter as FTES- and CTES-formations, respectively), were considered in the analyses. The main results

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http://dx.doi.org/10.1016/j.advwatres.2012.05.017

of the first-order analyses, confirmed by three-dimensional numerical simulations for more realistic conditions [37], suggested that features of solute transport in variably saturated, heterogeneous bimodal FTES and CTES formations exhibit a crossover behavior attributed to the concave nature of the unsaturated hydraulic conductivity in these formations.

This crossover behavior means that under relatively wet conditions solute spread is larger in the FTES-formations than in the CTES-formations, while the opposite occurs when the formation is relatively dry. Furthermore, the results of the numerical simulations [37] suggested that also under transient, non-monotonous flows, the difference between the responses of the FTES-formations and the CTES-formations decreases substantially, similar to the situation in steady state flows associated with intermediate water saturations corresponding to the mean pressure head at which the crossover occurs.

The analyses of Russo [37], which, considered bimodal formations associated with relatively small volume fraction of the embedded soil, are restricted to limited-contrasts situations; furthermore, the analyses focused on the case in which the entire water-filled pore space is mobile, will be termed hereafter as the one-region case. Near-surface formations, however, may exhibit complex-structured features such as clay soils comprised of aggregates of small-diameter particles [56,18,14], or sandy soils in which the individual sand particles comprising the formation have non-zero porosity [2].

In these circumstances, the water-filled pores between the soil aggregates and/or the sand particles are viewed as channels through which relatively rapid water flow and solute transport may take place. In turn, the soil aggregates and/or the sand particles are typically viewed as regions within which the water-filled-pore-space is essentially stagnant and may exchange solute with the mobile water region by a rate-limiting diffusion process (e.g., [7,52,28,51,40]). The latter case will be termed hereafter as the two-region case.

Field-scale investigations of solute transport (e.g., the transport of bromacil in transient, vadose zone flow [43] and the transport of bromide in steady state, groundwater flow [20], suggest that the transport in these spatially heterogeneous sites is better quantified by the two-region, mobile-immobile transport model, than by the classical, one-region, convection dispersion equation model. The results of these studies support the significance of the rate-limiting mass transfer between the mobile and the immobile regions occurring in heterogeneous formations.

Considering composite bimodal heterogeneous formations, the present study focuses on the case wherein each of the sub-soils of the composite formation has secondary porosity features (e.g., microporosity) that may give rise to mobile-immobile behavior. Specifically, the main purpose of this study is to extend the previous analyses of flow and transport in variably saturated, one-region, bimodal heterogeneous formations [37] to the case in which part of the water-filled pore space of each of the sub-soils of the composite formation is stagnant, and to investigate the effect of the interaction between the mobile and the immobile regions on solute transport in these formations.

The study will be carried out through a series of detailed numerical analyses of flow and transport in a hypothetical, yet realistic, three-dimensional (3-D) variably saturated, two-region, composite, bimodal heterogeneous flow domain. The approach adopted in the present study, viewed as a "numerical experiment", is an efficient tool for studying processes' mechanism and evaluating the flow system's response to plausible scenarios. At the price of reduced generality it circumvents most of the stringent assumptions of analytical studies, and, facilitates analysis of simplified, yet realistic situations at a fraction of the cost of physical experiments

2. Governing partial differential equations

A Cartesian coordinate system (x_1, x_2, x_3, where x_1 is directed vertically downwards) which coincides with the principal axes associated with the principal components of the hydraulic conductivity tensor, $\mathbb{K}$ is considered here. Taking into account water extraction by plant roots, the Richards equation that governs flow in a rigid, variably saturated 3-D flow domain is:

$$\frac{\partial\theta}{\partial t}=\sum_{i=1}^{3}\frac{\partial}{\partial x_i}\left[K_{ii}\frac{\partial\psi}{\partial x_i}\right]-\frac{\partial K_{11}}{\partial x_1}-S_w \tag{1}$$

where t is time, $\psi=\psi(\underline{x},t)$ is the pressure head, $\theta=\theta(\underline{x},t)$ is the volumetric water content, $K_{ii}=K_{ii}(\psi,\underline{x})$, $i=1,2,3$, are the principal components of $\mathbb{K}$ taken as a symmetrical tensor of rank two with zero off-diagonal components and $S_w=S_w(\underline{x},t)$ is a sink term, representing water uptake by plant roots, given [25,5] as:

$$S_w(\underline{x},t)=-R_e(\underline{x},t)K(\psi,\underline{x})[\psi_r(t)-\psi(\underline{x},t)-\pi(\underline{x},t)] \tag{2}$$

where $R_e(\underline{x},t)$ is the root effectiveness function, ψ_r is the total pressure head at the root-soil interface and π is the osmotic pressure head of the soil solution.

Neglecting solute uptake by plant roots, the equation governing two-region, mobile-immobile transport of a passive solute (tracer) in a variably saturated 3-D flow system is:

$$\frac{\partial(\theta_m c_m)}{\partial t}+\frac{\partial(\theta_{im}c_{im})}{\partial t}=\sum_{i=1}^{3}\sum_{j=1}^{3}\frac{\partial}{\partial x_i}\left\{\theta_m D_{ij}\frac{\partial c_m}{\partial x_j}\right\}-\sum_{i=1}^{3}\frac{\partial(u_i\theta_m c_m)}{\partial x_i} \tag{3a}$$

$$\frac{\partial(\theta_{im}c_{im})}{\partial t}=\gamma(c_m-c_{im}) \tag{3b}$$

where $\theta_m(\underline{x},t)=\theta(\underline{x},t)-\theta_{im}(\underline{x})$ and $\theta_{im}(\underline{x})$ are the mobile and the immobile water contents, respectively; $c_m(\underline{x},t)$ and $c_{im}(\underline{x},t)$ are the resident solute concentrations (expressed as mass per unit volume of the soil solution) in the mobile and immobile regions, respectively; u_i ($i=1,2,3$) are components of the Eulerian velocity vector and D_{ij} ($i,j=1,2,3$) are components of the pore-scale dispersion tensor given [3] as:

$$D_{ij}=\delta_{ij}(\lambda_T|\underline{u}|+D_m)+(\lambda_L-\lambda_T)u_iu_j/|\underline{u}| \tag{4a}$$

where λ_L and λ_T are the longitudinal and the transverse pore-scale dispersivities; δ_{ij} is the Kronecker delta (i.e., $\delta_{ij}=1$, if $i=j$, and $\delta_{ij}=0$ if $i\neq j$); $|\underline{u}|=(u_1^2+u_2^2+u_3^2)^{1/2}$ and D_m is the effective molecular diffusion coefficient in the mobile region, given (Millington and Quirk, 1961) as

$$D_m=D_0\left(\theta_m^{10/3}/\theta_s^2\right) \tag{4b}$$

where D_0 is the molecular diffusion coefficient in water, $\theta_s=\theta_s(\underline{x})$ is the saturated volumetric water content, and $\gamma=\gamma(\underline{x})$ is the first-order mass transfer coefficient representing solute diffusion between the mobile and the immobile regions, calculated for spherical particles [48] as:

$$\gamma=15\theta_{im}D_{im}/r_a^2 \tag{5}$$

where r_a is the average radius of the soil particles, $\theta_{im}(\underline{x})$ is the immobile water content and $D_{im}=D_{im}(\underline{x})$ is the effective solute diffusion coefficient in the immobile region (given by (4b) with θ_{im} replacing θ_m and D_{im} replacing D_m).

Regarding the transport equation (3), it should be emphasized (e.g., [43]) that at the small γ limit, $\gamma\to 0$, there is no mass transfer to the immobile region, i.e., $c_{im}=0$ and (3) reduces to the one-region convection–dispersion equation (CDE) with $c=c_m$ and $\theta=\theta_m$. At the large γ limit, $\gamma\to\infty$, physical equilibrium between