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Some Considerations on the Modeling of Flow and Transport in Heterogeneous Environments

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ABSTRACT. ***Flow and transport processes occurring in multidimensional heterogeneous environments are particularly challenging to model. Detailed models of these processes, at the scale of the heterogeneity, while feasible and accurate, are very expensive computationally, and upscaled models, based on effective macroscale representations, are often inaccurate, especially where heterogeneity is highly autocorrelated in space, as is the case with macropores. This contribution presents some considerations on modeling of such systems, at both ends of the scale spectrum. In particular, results of detailed simulations (heterogeneity scale) are compared to those of bi-continuum models (macroscale) to identify their potential strengths and shortcomings. Detailed simulations of infiltration, solute transport, and saturated flow, are used for this analysis. In the end, an improved model, that retains some similarity to bi-continuum equations, but is expected to provide more accurate predictions, is presented. The improved model is expected to be flexible enough to remain applicable through a range of subscale features, from isotropic heterogeneity to that which is highly anisotropic and longitudinally autocorrelated.***

Keywords.* *Porous media flow and transport, Heterogeneous environment, Traveling waves, Asymptotic Regimes

Introduction

Accurate modeling of flow and transport processes in porous media, and soil in particular, is important for flood and pollution prevention, the design of efficient irrigation and drainage systems and the design design of earth dams, among others. Where the medium can be assumed homogeneous, classical single-equation approaches are generally considered appropriate. These include the extension of Darcy's (1856) law of water movement in saturated environments to unsaturated media by Richards (1931):

$$C(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}K(h)\frac{\partial h}{\partial x} + \frac{\partial}{\partial y}K(h)\frac{\partial h}{\partial y} + \frac{\partial}{\partial z}K(h)\frac{\partial h}{\partial z} - \frac{\partial K(h)}{\partial z} = \nabla \cdot K(h)\nabla h - \frac{\partial K(h)}{\partial z}$$

where t, x, y and z and temporal and spatial coordinates, h is the moisture potential in the medium, C is its water capacity and K its unsaturated hydraulic conductivity. Similarly, for the dynamics of solute transport, the Convection-Dispersion Equation (CDE) is frequently used in such media (Bear, 1972):

$$\frac{\partial c}{\partial t} = -v_x\frac{\partial c}{\partial x} - v_y\frac{\partial c}{\partial y} - v_z\frac{\partial c}{\partial z} + D_x\frac{\partial^2 c}{\partial x^2} + D_y\frac{\partial^2 c}{\partial y^2} + D_z\frac{\partial^2 c}{\partial z^2} = -v\cdot\nabla c + D\nabla^2 c$$

where c is solute concentration, v is the transport velocity vector and D is the coefficient of dispersion (assumed Fickian and, at right, isotropic).

For heterogeneous media (Figure 1), the above equations are generally considered to apply at the scale at which the heterogeneity occurs. In other words, they can be applied with an explicit spatial description of the heterogeneity field and produce good predictions (Montas et al., 1997a). This approach, while valid, is computationally expensive, and more efficient approaches, that seek effective intermediate-scale description of flow and transport in heterogeneous media, have been the subject of significant research from both deterministic (Shirmohammadi and Montas, 2003) and stochastic (Gelhar, 1993) perspectives. This is particularly important in the case of preferential flow, where the heterogeneity is both highly localized and highly spatially autocorrelated, leading to potentially long-range effects where deviations from single-equation predictions can be observed over large distances (Gish and Shirmohammadi,1991).

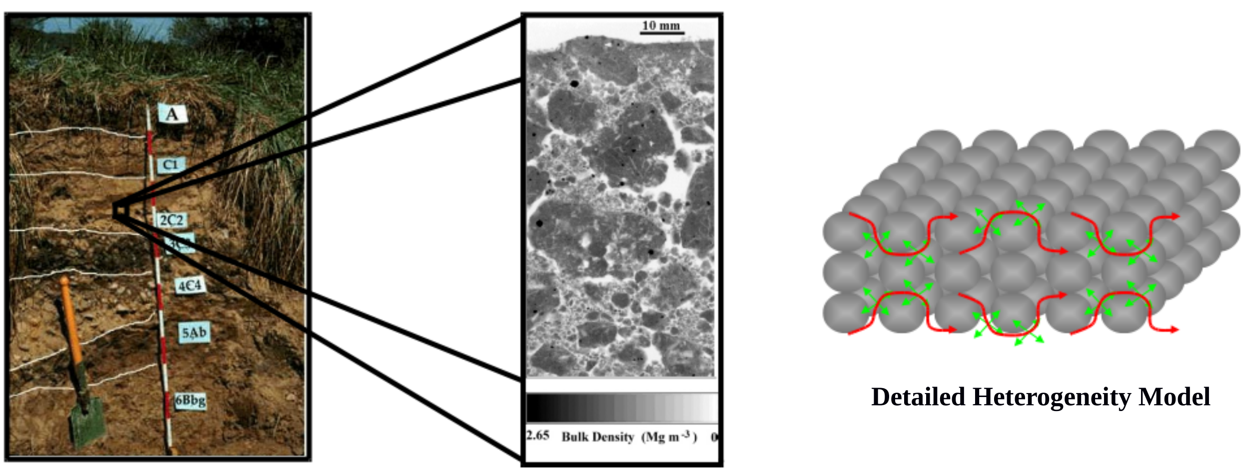

Figure 1. Illustration of Media Heterogeneity in a Soil Profile (left) and in Soil Micromorphology (center), Along with a Detailed Model of Fine Scale Heterogeneity (right).

The bi-continuum, or two-region, model is the most popular approach for simulating flow and transport in heterogeneous media using effective (characteristic, upscaled) properties of the underlying medium. For solute transport under saturated flow conditions, its predictions tend, at large times, towards those of the single equation CDE, which is conceptually satisfactory. The difference between the two models is observed at early times, when the effects of the heterogeneity have not yet been erased by diffusion, and the duration of this period increases with increasing spatial autocorrelation of the heterogeneity (it may therefore be particularly long in cases of preferential flow). Additionally, it has been demonstrated that the bi-continuum model of solute transport is equivalent to the stochastic model of the same process, including nonlocal forms, in the cases of layered and braided heterogeneity (Montas et al., 2000). This helps to place the model on a solid theoretical footing. The model is capable of responding to flow interruptions in the observed manner, with positive and negative concentration spikes in the leading and trailing edges of the effluent, which is not possible with single-equation models (Montas et al., 1997b). One notes also that an analytical solution for the three-region extension of this model exists, albeit subject to two constraints, which can help to verify numerical codes used to solve the model equations in complex environments (Montas, 2003). Finally, we note that a fractional-calculus generalization of the interaction term in the model was used to successfully model nanoparticle-mediated soil remediation (Montas and Shirmohammadi, 2004, 2005).

The bi-continuum model is however not without shortcomings. This manuscript describes some characteristics of flow and transport in heterogeneous media, some results of detailed simulation exercises that illustrate these features, and some of the shortcomings of the bi-continuum model identified by comparison with the detailed simulations. The investigation proceeds dialectically through three processes: 1) infiltration; 2) solute transport under saturated flow, and 3) saturated flow. This order corresponds essentially to the chronological sequence in which these phenomena were investigated by the authors, under the expectation that the model would prove accurate, and, as discrepancies were found, investigations moved from the more complex phenomena (nonlinear unsaturated flow) to the simpler one (saturated flow). This led to the development of a modified model which is presented after the investigative sequence.

Infiltration

Infiltration is the entry of a fluid (here, water) into a porous medium, through its surface, and represents a particular form of unsaturated flow process. Philip (1957) demonstrated that when infiltration occurs with a constant fluid pressure (or head) at the surface of the medium, after an initial development time, the profile of infiltrated moisture content and head propagates downwards without changing shape, much like the traveling waves commonly investigated in nonlinear analysis. At firs thought, it would seem unlikely that such profiles would develop in heterogeneous media. However, Dasse (1965) demonstrated their occurrence experimentally, in an apparatus where two layers of porous materials with different unsaturated conductivities, were arranged vertically, side-by-side, and subjected to constant flux infiltration. Thus, at both ends of the heterogeneity spectrum (homogeneous media and media with perfectly autocorrelated heterogeneity in the principal flow direction) a constant-shape profile develops at large times.

In investigations focused on explicit representation of heterogeneity, Montas et al. (1997c, corrected in Montas 1998) provided computational evidence that constant-shape profiles could arise during infiltration in a Green-Ampt soil with saturated conductivity that varies monotonically in the lateral direction. This was extended to a system similar to that of Dasse, with more realistic unsaturated soil properties, and essentially the same result (Montas et al., 2001). It remains a research topic at this time to verify that such profiles develop during infiltration in soils with arbitrary heterogeneity, what their shape might be, and whether upscaled (intermediate-scale) deterministic and stochastic (eg. Haghighi et al., 2001) formulations predict them.

A bi-continuum version of Richards' equation forms an interesting intermediate-scale model of unsaturated flow:

$$C_1(h_1)\frac{\partial h_1}{\partial t} = -L_{1,2}\left(h_1 - h_2\right) + \nabla\cdot K_1(h_1)\nabla h_1 - \frac{\partial K_1(h_1)}{\partial z}$$
$$C_2(h_2)\frac{\partial h_2}{\partial t} = -L_{2,1}\left(h_2 - h_1\right) + \nabla\cdot K_2(h_2)\nabla h_2 - \frac{\partial K_2(h_2)}{\partial z}$$

where subscripts 1 and 2 refer the two overlapping zones (characteristic sub-media) described by the model and L is an interaction parameter accounting for moisture transfer between the zones. This model was compared to simulations of infiltration with detailed descriptions of the heterogeneity for longitudinal and random variations by Montas (2003) with results shown in Figure 2. Statistics of the bi-continuum predictions are computed from characteristic values for zones 1 and 2 using the method described in Montas et al. (2000). The dynamics of the moisture profile and the statistics of flow in the downwards direction (mean and standard deviations) were found to be well represented by the model. However, the standard deviations of pressures and of flows in the transverse direction were poorly estimated by the upscaled model. The standard deviation of transverse flow is important if the model is coupled to a transport formulation as it determines the magnitude of transverse dispersion to which a solute is subjected. Improvements in the formulation of the model, possibly inspired by similar improvements for saturated flow, as discussed later, would probably be needed to increase its general applicability. The degree to which this model, as well as detailed infiltration simulations, produce a large-time asymptotic infiltration profile, remains to be investigated as well.

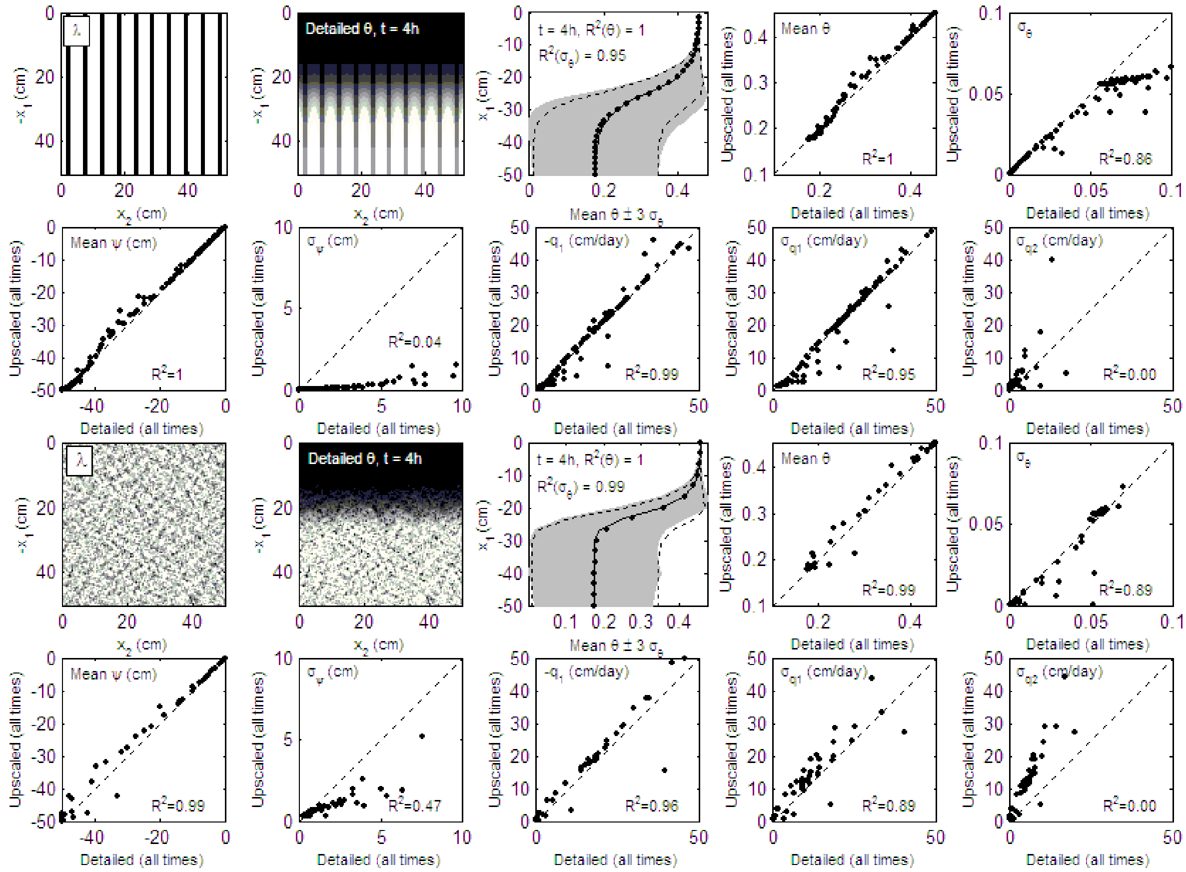

Figure 2. Comparison of Infiltration into a Heterogeneous Medium Modeled in Detail in Two-Dimensions with that Modeled as a One-Dimensional Effective Process by a Bi-Continuum (Upscaled) Model

Solute Transport under Saturated Flow Conditions

The form of the bi-continuum model used to represent solute transport under saturated flow conditions, with mean flow in the x-direction, is essentially:

$$\frac{\partial c_1}{\partial t} = -\frac{L_{1,2}}{f_1}\left(c_1 - c_2\right) - v_{1[x]}\frac{\partial c_1}{\partial x} + D_1 \nabla^2 c_1$$
$$\frac{\partial c_2}{\partial t} = -\frac{L_{2,1}}{f_2}\left(c_2 - c_1\right) - v_{2[x]}\frac{\partial c_2}{\partial x} + D_2 \nabla^2 c_2$$

where subscripts 1 and 2 have the same meaning as in the flow equation presented above, the parameter f represents the fraction of space occupied by each of the two characteristic zones, and [x] indicates a velocity component in the x-direction. The predictions of this model, interpreted statistically, were compared to detailed simulations of transport in media that is either homogeneous, or has one of five different types of periodic hydraulic conductivity heterogeneity (Montas, 2011a). The detailed flowfields of a representative section of each of the 6 transport domains are shown in Figure 3 where lighter shades indicate higher conductivity values and water flows, on average, from left to right. Flow was unidirectional in two of the flowfields (homogeneous and preferential) and multidirectional in the other four. Results of the detailed transport simulations carried out over these flowfields were averaged over Representative Elementary Areas (REAs) of a size equal to one-quarter of a periodic cell (the absolute minimum acceptable as REA). Standard deviations of those concentrations were also calculated over these REAs. The bi-continuum model was applied, with effective characteristic parameters, in two-dimensions, with the same initial conditions as detailed simulations, and its predictions were interpreted statistically, following Montas et al. (2000).

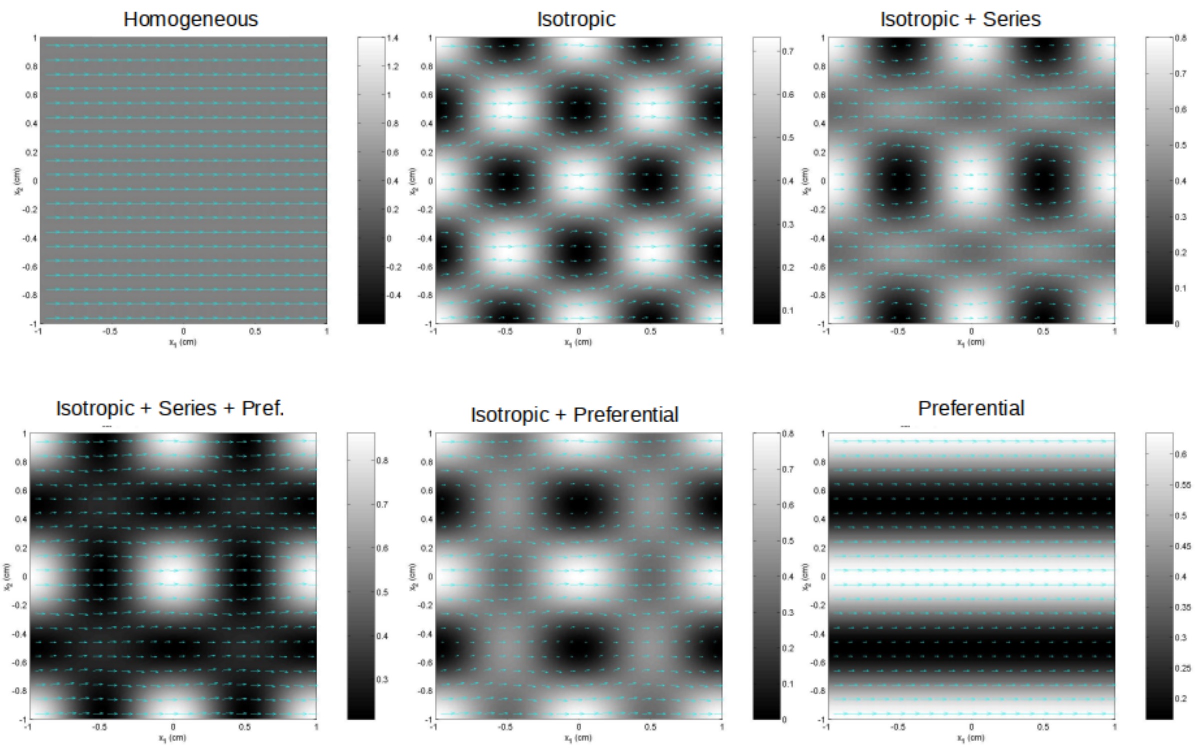

Figure 3. Sections of the Detailed Conductivity Heterogeneity and Associated Flowfields used in Simulations

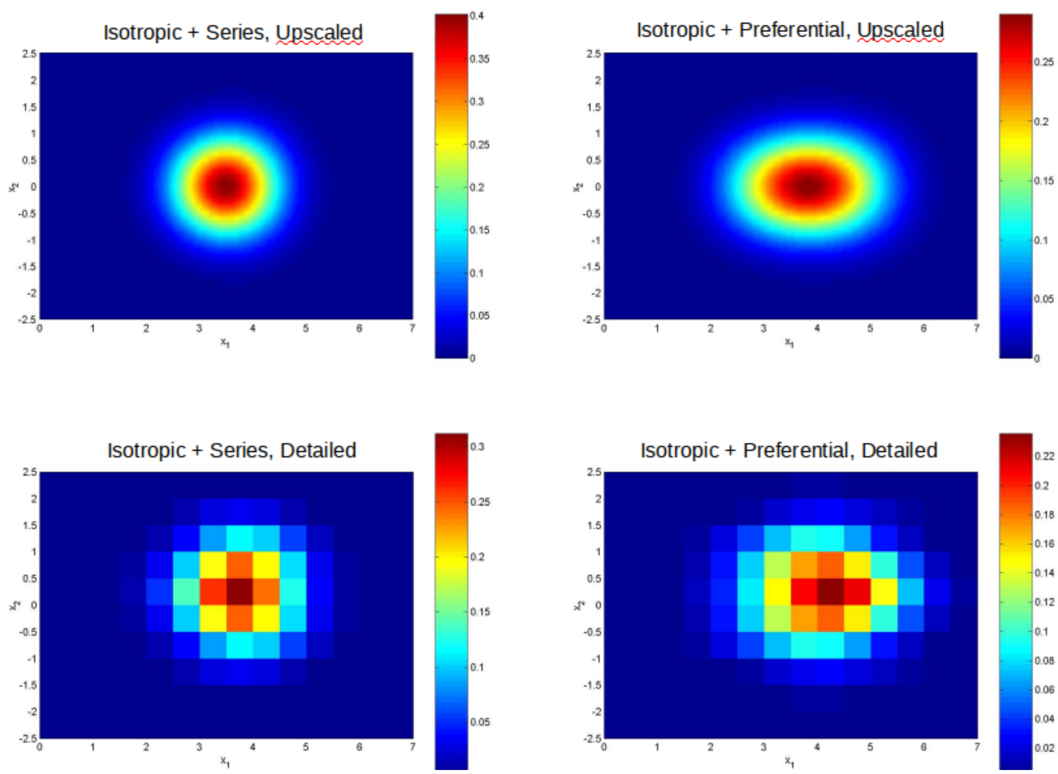

Figure 4. Mean Concentrations at t = 4 hours Obtained by Detailed Simulation and Bi-Continuum Model

The predictions of the mean solute concentration, after 4 hours of transport, by the bi-continuum and detailed model (averaged over REAs), are shown in Figure 4 for two of the multidirectional flowfields. The plumes predicted by both models have moved to essentially the same position, have relatively similar maximum concentration and longitudinal extent (horizontal in the figure) but the lateral (transverse, vertical in the figure) extent of plumes obtained by detailed simulation is larger than that from the bi-continuum model. An analysis of the transverse spreading process suggested that the effective transverse dispersion coefficient used in the bi-continuum model (where macroscopic isotropy was assumed) is in fact one fifth of the value that results from the detailed simulation. As with the infiltration case presented above, this suggests that some description of the transverse variations of flow velocity, that are important to the transverse mixing process, are missing from the bi-continuum model formulation. Incorporating them in the form of an effective transverse dispersion coefficient would see that higher coefficient apply at all times, and would likely negate the benefits of this upscaled formulation, that one hopes would be faithful to the reproduction of the important transition regime, from early-time advection-dominated motion to large-time Fickian transport.

Standard deviations of concentrations obtained with both modeling approaches are shown in Figure 5. Both modeling methods predict that standard deviations are small at the center of the plume and increase away from that point before fading to zero outside of the plume. Detailed simulation results however display a much higher range of standard deviations, especially on the vertical axis that passes through the center of the plume, as compared to the bi-continum model. This means that there is more mixing occurring in those areas, according to the detailed simulation which serves as reference, than predicted by the bi-continuum model. In effect, the spatial distribution of standard deviations has more of a circular, or donut, shape in the reference results, rather than the two-peaked, or eyeballs, shape of bi-continuum predictions. The difference leads to more transverse spreading in the detailed simulations and results from subscale transverse velocities (that average to zero) and are not accurately accounted for in the bi-continuum formulation.

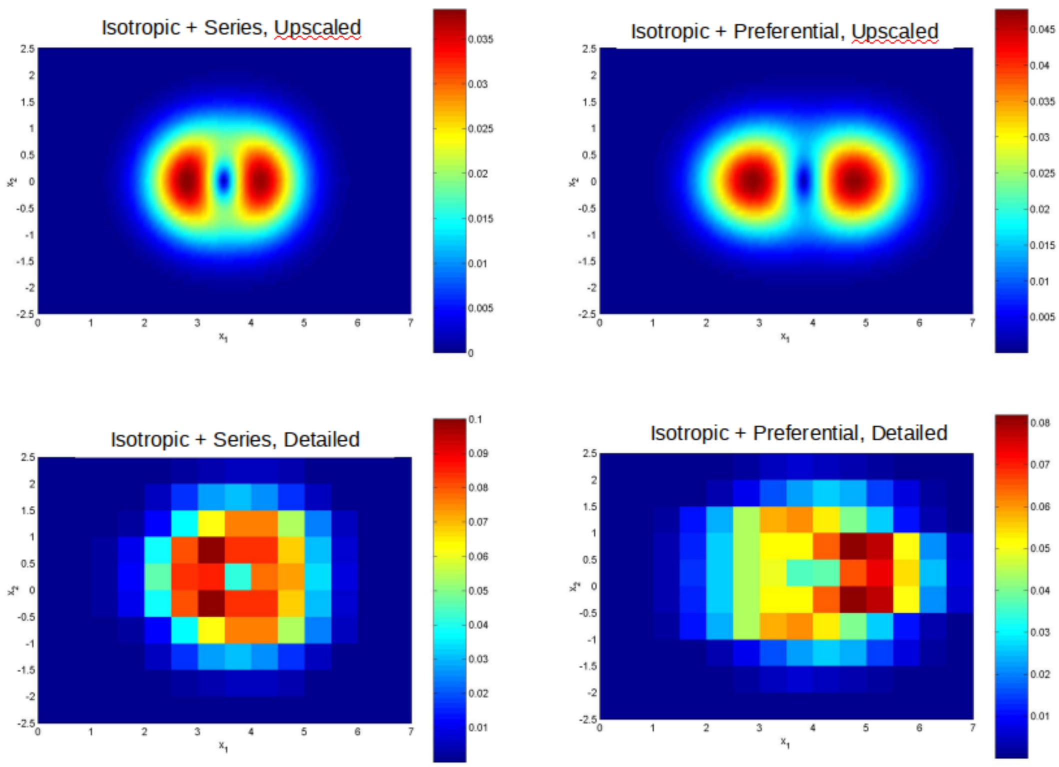

Figure 5. Standard Deviation of Concentrations at t = 4 hours, for Detailed and Bi-Continuum Models

Saturated Flow

The nature of the missing bi-continuum model transverse flowfield component may be investigated with detailed simulations of saturated flow in heterogeneous media, especially where that heterogeneity results in a multidirectional flowfield. Figures 6 and 7 present the results of such investigations for flows that take place in two and three spatial dimensions, with circular or spherical heterogeneities (Montas, 2011b). The two-dimensional flowfields are computed analytically by summing contributions from an array of dipoles (Strack, 1989) while in 3-D they are obtained using a numerical solution technique. In both figures, the detailed flowfields are presented first, followed by the mean-removed flowfield which is obtained by subtracting the mean flow from the detailed flowfield. If one performs such operation with a unidirectional flowfield is a distribution of positive and negative flow velocities, all oriented along the same axis. With multidirectional flowfields however, as shown in the figures, the mean-removed flowfield is characterized by a large number of recirculation cells (apparent vortices) which are the locus of the enhanced mixing process observed in the corresponding media.

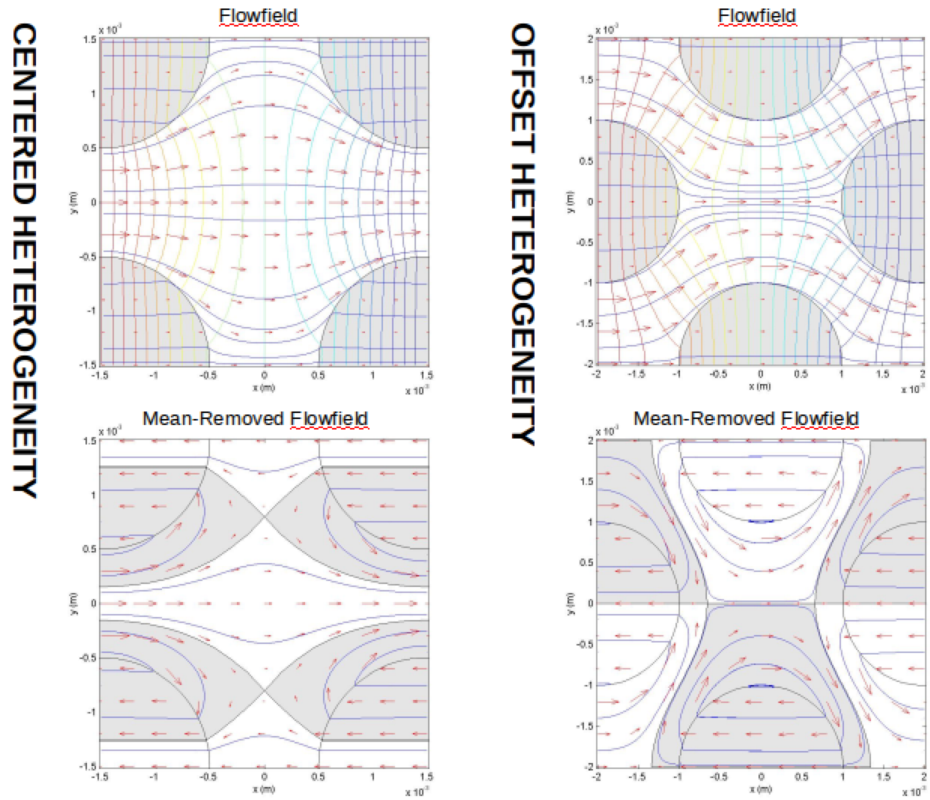

Figure 6. Detailed and Mean-Removed Saturated Flowfields with Two-Dimensional Heterogeneity

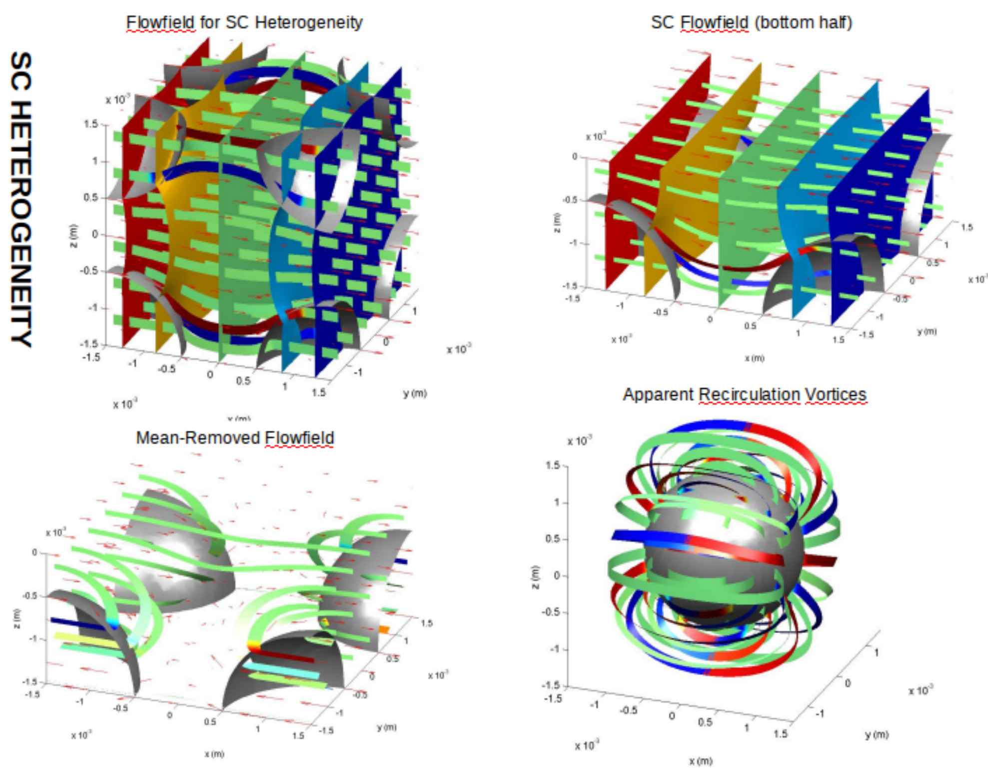

Figure 7. Detailed and Mean-Removed Saturated Flowfields with Three-Dimensional Heterogeneity

For the most part, the formulation of the bi-continuum model implicitly excludes the formation of interzonal advection-driven recirculation patterns. In its more common application, transport velocities in both zones are assumed to be in the same direction, but with different magnitudes. Although one may add a transverse velocity component to each zone, in opposite directions such that the mean transverse transport velocity is zero, this would underlie a description of a rather unrealistic porous medium.

An Improved Solute Transport Model

A model of solute transport under saturated flow conditions that integrates advective recirculation was developed using volume averaging techniques by Montas et al. (2006), for two- and three-dimensional space. The model can equivalently be viewed as the continuous-time limit of a random walk process (depicted in Figure 8) and is equivalently expressible in canonical form (where it is an extension of the bi-continuum model) and in stochastic form. The model needs a minimum of three overlapping zones in two-dimensions and four zones in 3-D. Each such set of zones represents one type of heterogeneous submedium and a highly complex medium, that contains several types of connected heterogeneities, would be represented by some multiple of the base zones. In practice however, it is expected that a single set of 3 (2-D) or 4 (3-D) zones would be used to represent a heterogeneous soil matrix, with the possible addition of one extra zone for preferential flowpaths.

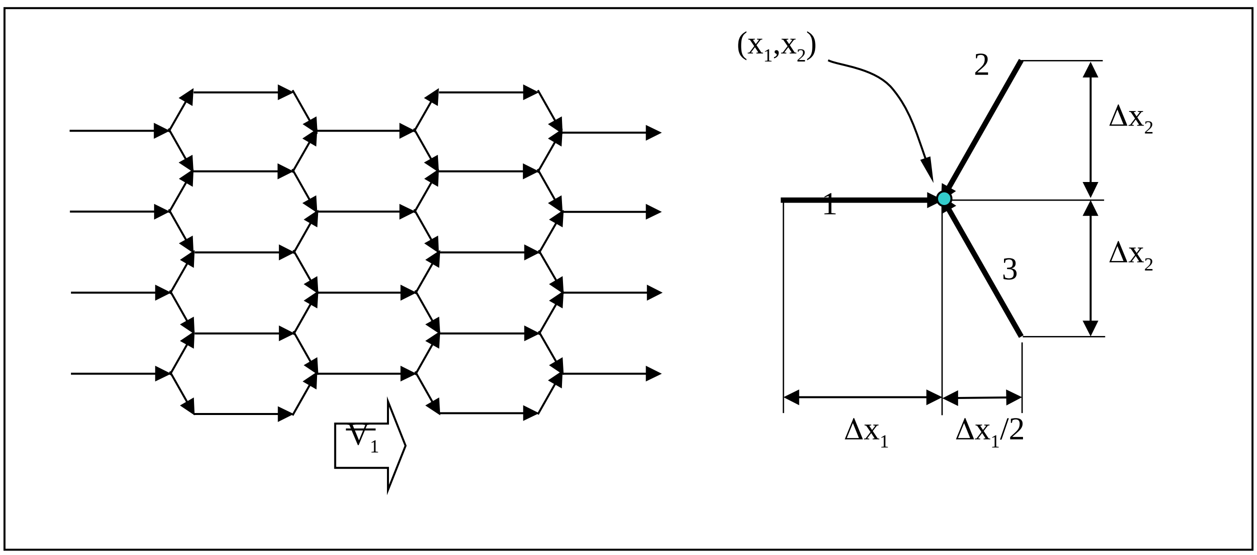

Figure 8. Random Walk Equivalent to the Improved Solute Transport Model in 2-D.

The two-dimensional form of the improved model (for the base case), with mean flow in the x-direction is:

$$\frac{\partial c_1}{\partial t} = -\sum_{i=1}^{3} \frac{L_{1,i}}{f_1}\left(c_1 - c_i\right) - v_{1[x]}\frac{\partial c_1}{\partial x} - v_{1[y]}\frac{\partial c_1}{\partial y} + D\nabla^2 c_1$$
$$\frac{\partial c_2}{\partial t} = -\sum_{i=1}^{3} \frac{L_{2,i}}{f_2}\left(c_2 - c_i\right) - v_{2[x]}\frac{\partial c_2}{\partial x} - v_{2[y]}\frac{\partial c_2}{\partial y} + D\nabla^2 c_2$$
$$\frac{\partial c_3}{\partial t} = -\sum_{i=1}^{3} \frac{L_{3,i}}{f_3}\left(c_3 - c_i\right) - v_{3[x]}\frac{\partial c_3}{\partial x} - v_{3[y]}\frac{\partial c_3}{\partial y} + D\nabla^2 c_3$$

which is very similar to the bi-continuum model except for having an extra zone (there would be 2 extra zones in 3-D) and for including transverse velocities in each zone. Clearly, for the model to be consistent with a mean flow in the x-direction, the mean of transverse velocities has to be zero (as it is also in detailed flowfields) but the main new aspect of the model is that individual zonal velocities are non-zero, representing the fact that subscale transport velocities in this direction are also not uniformly zero. Equations 74 and 105-106 in Montas et al. (2006) provide values for all of the model's parameters in terms of the statistics of the heterogeneous hydraulic conductivity of the porous medium in which transport is taking place, and of the value of the pressure gradient that is driving the flow.

The improved solute transport model has not yet been tested against detailed simulations of transport in heterogeneous media. The inclusion of transverse velocities is however expected to give it increased accuracy when compared to the standard bi-continuum model. To complete the theoretical framework in which it is placed, it will be necessary, also, to develop a multicontinuum model of saturated flow that predicts multidirectional characteristic flow velocities from a unidirectional pressure gradient (possibly using distinct subscale conductivity tensors for each zone) and to then extend this formulation to transient unsaturated flow.

Conclusions

Accurate modeling of flow and transport processes in heterogeneous porous media is crucial to the design of drainage and irrigation systems that are effective and that prevent pollutants from reaching downgradient ecosystems and drinking water supplies. The accuracy of the related models is expected to become increasingly important as climate changes raise the stress levels on our natural resources and more precise designs are required to compensate for its effects without undue costs. Bi-continuum modeling is a popular way to address the deviations, from classical single-equation theories, that are observed in heterogeneous media. The detailed numerical simulations of infiltration and solute transport presented in this manuscript however indicate that this approach has important shortcomings, especially when the media's heterogeneity results in a multidirectional subscale flowfield. An improved version of the bi-continuum model was presented to account for the effects of the transverse advective transport (with zero-mean) evidenced most clearly by the apparent recirculation patterns observed in mean-removed analysis of such flowfields. This model remains to be tested and extended to unsaturated flows, but is expected to provide a new level of accuracy and insights for the modeling of these important phenomena.

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