Numerical solutions of moment equations for flow in heterogeneous composite aquifers

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[1] We analyze flow in heterogeneous media composed of multiple materials whose hydraulic properties and geometries are uncertain. Our analysis relies on the composite media theory of *Winter and Tartakovsky* [2000, 2002], which allows one to derive and solve moment equations even when the medium is highly heterogeneous. We use numerical solutions of Darcy flows through a representative composite medium to investigate the robustness of perturbation approximations in porous medium with total log conductivity variances as high as 20. We also investigate the relative importance of the two sources of uncertainty in composite media, material properties, and geometry. In our examples the uncertain geometry by itself captures the main features of the mean head estimated by the full composite model even when the within-material conductivities are deterministic. However, neglecting randomness within materials leads to head variance estimates that are qualitatively and quantitatively wrong. We compare the composite media approach to approximations that replace statistically inhomogeneous conductivity fields with pseudohomogeneous random fields with deterministic trends. We demonstrate that models with a deterministic trend can be expected to give a poor estimate of the statistics of head. *INDEX TERMS:* 1869 Hydrology: Stochastic processes; 1829 Hydrology: Groundwater hydrology; 1832 Hydrology: Groundwater transport; 3210 Mathematical Geophysics: Modeling; *KEYWORDS:* random, stochastic, uncertainty, domain decomposition

1. Introduction

[2] As stochastic hydrology is used to quantify uncertainty in increasingly complicated geological structures, models must accommodate higher levels of material heterogeneity. *Winter and Tartakovsky* [2000, 2002] introduced a composite medium model of groundwater flows to explicitly account for the spatial distribution of multiple materials. A composite medium is a union of disjoint "blocks" made up of internally uniform materials. We use the word block loosely to indicate volumes with arbitrary shapes. Common examples of composite media are layered systems, aquifers that contain inclusions of locally impermeable material, and fractured media. More technically, a composite medium is a bivariate stochastic process depending on (1) the random geometry of the blocks and (2) the statistically homogeneous distribution of hydraulic conductivity within a material block. Highly heterogeneous media can also be represented as statistically homogeneous, but at the cost of large σ_Y^2, the variance of $Y(\boldsymbol{x}) = \ln K(\boldsymbol{x})$, and a mixed distribution that is often multimodal [*Gómez-Hernández and Wen*, 1998; *Rubin and Journel*, 1991; *Rubin*, 1995]. Computationally efficient solutions of stochastic groundwater flow models usually rely on small σ_Y^2. This is true whether the solution method is Monte Carlo simulation or deterministic equations for the moments of pressure head, $h(\boldsymbol{x})$, and Darcian flux, $\boldsymbol{q}(\boldsymbol{x})$. The essence of *Winter and Tartakovsky* [2000, 2002] is that perturbation expansions based on the composite medium approach rely only on small within-block variances of conductivity $\sigma_{Y_M}^2$, where Y_M is the logarithm of conductivity in the Mth material. Thus the individual materials of a composite medium can satisfy the requirements for perturbation expansions, $\sigma_{Y_M}^2(\boldsymbol{x}) \ll 1$, while the overall system may not, $\sigma_Y^2(\boldsymbol{x}) \gg 1$. The composite medium model substitutes the relatively tractable problem of determining the spatial distribution of disjoint blocks of homogeneous material for the difficult problem of dealing with large perturbation variances.

[3] The composite medium model is similar in its goals to the Boolean algorithms used in geostatistical simulations of heterogeneous random fields [*Deutsch and Journel*, 1992]; however, the methods and results are completely different. Moment equations yield explicit expressions for the statistics of head that can be examined qualitatively to understand the general behavior of the averaged flow system. That, of course, is not possible with a simulation-based approach. Several authors have analyzed special classes of composite media. *Matheron and de Marsily* [1980] and *Gelhar et al.* [1979] suppose that the block geometry is known exactly, but the conductivities within blocks are statistically homogeneous random fields. The exchange of mass and momentum between blocks is especially easy to assess in this case since the block geometry is assumed known. The opposite case, where the conductivity of a given material is a known constant, but the block geometry is uncertain, has been investigated by *Levermore et al.* [1986], who considered block boundaries set by a Poisson process, and *Fontes et al.* [1999], who analyzed systems equivalent to porous media composed of two materials. When the difference between materials is the result of a gradual change in the formation of a geological material, it may suffice to model hydrologic variability as a homogeneous process superimposed on a deterministic trend [*Neuman and Jacobsen*, 1984; *Indelman and Rubin*,

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1995; *Li and McLaughlin*, 1991]. In these analyses the logarithm of conductivity is assumed to consist of a known trend added to a statistically homogeneous random process. Since these models assume that the covariance structure of conductivity is the same throughout a porous medium, they do not apply to highly heterogeneous media composed of blocks of different materials.

[4] We formulate the problem of flow through composite media in section 2. Then we investigate perturbation approximations for the first two moments of hydraulic head in section 3. We analyze the relative importance of uncertain geometry and uncertain conductivity in section 4 by comparing special cases in which (1) the block geometry is random, but the hydrogeologic properties of each material are fixed, versus (2) the block geometry is fixed but material properties vary. Finally, we compare the composite medium model to models with deterministic trends in section 5.

2. Problem Formulation

[5] We consider steady state Darcian flow, $\nabla \cdot [K\nabla h] = 0$, in a flow domain (Figure 1) composed of an inner square with random hydraulic conductivity $K(\boldsymbol{x}) = K_2(\boldsymbol{x})$ embedded in an outer square with conductivity $K(\boldsymbol{x}) = K_1(\boldsymbol{x})$. Both conductivities are statistically homogeneous lognormally distributed random fields with corresponding means, $\overline{K}_1 \gg \overline{K}_2$ and variances, $\sigma^2_{K_1}$ and $\sigma^2_{K_2}$. Log conductivities are uncorrelated when they are from different materials, while points within the same block are exponentially correlated,

$$C_{Y_i}(r) = \sigma^2_{Y_i} e^{-r/\lambda_i}, \tag{1}$$

where r is the separation distance within material i and λ_i is the correlation length. To further simplify the presentation, we consider cases where $\sigma^2_{Y_1} = \sigma^2_{Y_2} = \sigma^2$ and $\lambda_1 = \lambda_2 = \lambda$. We set $2a = 12\lambda$. Although we assume that each material is internally homogeneous, we emphasize that the resulting conductivity field is statistically inhomogeneous since its mean, variance, and correlation function are all space dependent.

[6] While the size of the outer square, $2a$, is deterministic, the half-length of the inner square, b, is treated as a random variable to reflect uncertainty about the geometry of such inclusions. For purposes of illustration, we take b to be lognormally distributed, with mean $\overline{b}$ and variance σ^2_b. In our analysis of the flow we impose constant heads on the vertical sides of the outer square,

$$h(0, x_2) = H_1 = 10 \quad h(2a, x_2) = H_2 = 0, \tag{2}$$

while assuming that the other two sides are impermeable. Continuity of both hydraulic head and Darcian flux across the random boundary separating materials completes the mathematical description of the problem.

3. Head Statistics

[7] *Winter and Tartakovsky* [2000, 2002] use a Reynolds decomposition to write $K(\boldsymbol{x}) = \overline{K}(\boldsymbol{x}) + K'(\boldsymbol{x})$ as the sum of an ensemble mean function, $\overline{K}(\boldsymbol{x})$, and a zero-mean random deviate, $K'(\boldsymbol{x})$. Similarly, $h(\boldsymbol{x}) = \overline{h}(\boldsymbol{x}) + h'(\boldsymbol{x})$ with $\overline{h}'(\boldsymbol{x}) = 0$. For steady state flow without sources or sinks, $\overline{h}(\boldsymbol{x})$ can be approximated by closing the averaged flow equation:

$$\nabla \cdot \left(\overline{K}\nabla\overline{h}\right) - \nabla \cdot \overline{\boldsymbol{r}} = 0 \tag{3}$$

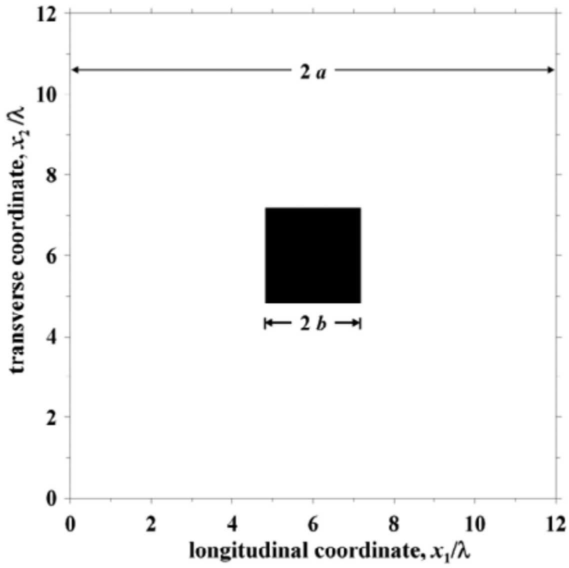

Figure 1. Composite flow domain.

consisting of a deterministic mean flux, $\overline{K}\nabla\overline{h}$, and the mean of a random residual flux, $\boldsymbol{r} = -K'\nabla h'$. Similar techniques lead to approximations for the variance of head.

[8] Solutions of equation (3) require the mean conductivity $\overline{K}(\boldsymbol{x})$ and $\overline{\boldsymbol{r}}(\boldsymbol{x})$. For n_M materials the ensemble mean

$$\overline{K}(\boldsymbol{x}) = \sum_{M=1}^{n_M} \overline{K}_M \, P[\boldsymbol{x} \in M] \tag{4}$$

and variance,

$$\sigma^2_Y(\boldsymbol{x}) = \sum_{M=1}^{n_M} \sigma^2_{Y_M} \, P[\boldsymbol{x} \in M] + \sum_{M=1}^{n_M} \sum_{m=1}^{n_M} \left(\overline{K}_M - \overline{K}_m\right)^2 P[\boldsymbol{x} \in M] \; P[\boldsymbol{x} \in M], \tag{5}$$

can be written in terms of the probability $P[\boldsymbol{x} \in M]$ that the point $\boldsymbol{x}$ is in a unit of material type M. Obviously, $\overline{K}(\boldsymbol{x})$ and $\sigma^2_Y(\boldsymbol{x})$ vary from point to point, so the conductivity field is statistically inhomogeneous.

[9] Equations (4) and (5) also apply when the spatial distribution of materials is ignored, except $P[\boldsymbol{x} \in M]$ is replaced by Q_M, the volume fraction of material M. We call this the "homogeneous model" because it treats the medium as a homogeneous random field (despite the fact that it is not). Usually, $\overline{\boldsymbol{r}}$ is approximated through perturbation expansions based on $\sigma^2_Y(\boldsymbol{x})$, an approach that works well so long as $\sigma^2_Y(\boldsymbol{x})$ is small. Note that σ^2_Y is usually large at every point in the homegeneous model even if component variances $\sigma^2_{Y_M}$ are small. For instance, with the parametrization we are using, the homogeneous version of equation (5) leads to $\sigma^2_Y \approx 20$.

[10] In the absence of a better yardstick we demonstrate the accuracy of our approximations by comparing them to Monte Carlo simulations. The Galerkin finite elements scheme of [*Guadagnini and Neuman*, 1999a, 1999b] is used to solve Darcy's equation with the same boundary conditions and grids as our solutions for the moment equations. We generated 5000 realizations of b on a grid of 3600 square elements (60 rows and

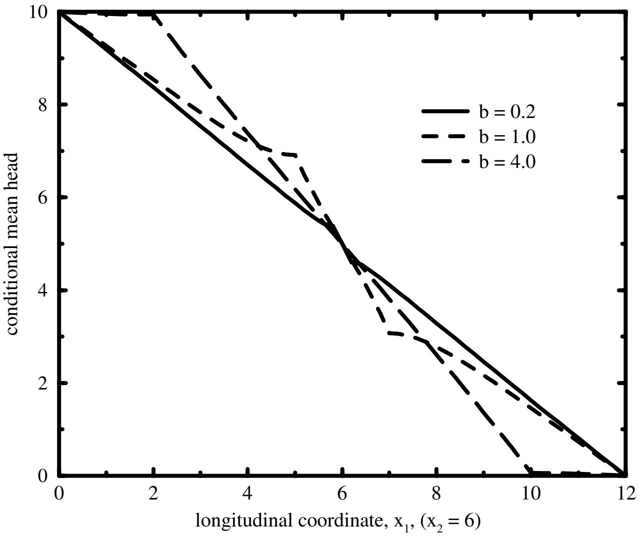

Figure 2. The cross section $x_2 = 6$ of conditional mean hydraulic head $\bar{h}^{[1]}(x_1|b)$, for several realizations of b.

60 columns) of uniform size $\Delta x_1 = \Delta x_2 = 0.2\lambda$ for our Monte Carlo simulations. We prescribed mean $\bar{b} = 1.2\lambda$ and variance σ_β^2 of $\beta = \ln b$. We analyzed the effect of uncertainty in the location of the inner boundary by considering $\sigma_\beta = 0.3$, 0.5, and 1.0, which corresponds to $\sigma_b = 0.36$, 0.64, and 1.6, respectively. For each realization of b we generated 2000 realizations of each of the two random materials on the grid spanning the outer square. We used $\overline{Y}_1 = -4.6$, $\overline{Y}_2 = -13.8$, and $\lambda = 1$ in these simulations. We analyzed the effect of uncertainty in hydraulic conductivity of each material by considering $\sigma_Y^2 = 0.1$ and 1.0. Conditional realizations of our composite media were obtained by superimposing the inner square of the size $2b$ on the outer square. *Guadagnini and Neuman* [1999a, 1999b] noted that a complete stabilization of the Monte Carlo statistics is not necessary for a comparison between the solutions obtained from moment equations and from Monte Carlo simulations to be meaningful. Therefore we limit the number of our Monte Carlo simulations to 5000 for b and 2000 for each of Y_i. Since these 5000 realizations of b fell within 30 discrete classes related to the cell size, we performed a total of $30 \times 2000 = 60{,}000$ Monte Carlo simulations of the flow equations.

3.1. Mean Hydraulic Head

[11] We present our solution for mean hydraulic head as an asymptotic expansion in the conditional log conductivity variance σ_Y^2,

$$\bar{h}(\boldsymbol{x}) = \bar{h}^{(0)}(\boldsymbol{x}) + \bar{h}^{(1)}(\boldsymbol{x}) + O\left(\sigma_Y^4\right), \tag{6}$$

where the superscript denotes terms of the ith order in σ_Y^2. Then, the first-order approximation of mean hydraulic head, $\bar{h}^{[1]}(\boldsymbol{x}) = \bar{h}^{(0)}(\boldsymbol{x}) + \bar{h}^{(1)}(\boldsymbol{x})$, is obtained from

$$\bar{h}^{(0)}(\boldsymbol{x}|b) = K_{g_1} H_1 [G_b(0, 2a; \boldsymbol{x}) - G_b(0; \boldsymbol{x})] \tag{7}$$

$$\bar{h}^{(1)}(\boldsymbol{x}|b) = \sum_{i=1}^{2} \int_{\Omega_i} \nabla G_b(\boldsymbol{y}; \boldsymbol{x}) \cdot \left[\bar{\boldsymbol{r}}_i^{(1)}(\boldsymbol{x}|b) - K_{g_i} \frac{\sigma_{Y_i}^2}{2} \nabla \bar{h}^{(0)}(\boldsymbol{x}|b) \right] d\boldsymbol{y}, \tag{8}$$

where K_{g_i} is the geometric mean of the ith conductivity and G_b is the Green's function corresponding to the fixed boundary b and K_{g_i}. The first-order approximation of the conditional mean residual flux is

$$\bar{\boldsymbol{r}}_j^{(1)}(\boldsymbol{x}|b) = K_{g_j}^2 \int_{\Omega_j(b)} C_{Y_j}(\boldsymbol{x}, \boldsymbol{y}) \nabla_{\boldsymbol{y}} \nabla_{\boldsymbol{x}}^T G_b(\boldsymbol{y}, \boldsymbol{x}) \nabla_{\boldsymbol{y}} \bar{h}^{(0)}(\boldsymbol{y}|b) d\boldsymbol{y}. \tag{9}$$

See *Winter and Tartakovsky* [2000, 2002] for details of the derivation.

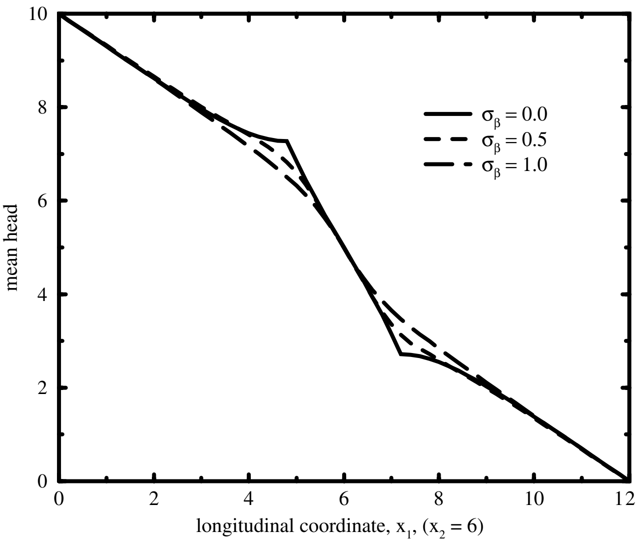

Figure 3. The cross section $x_2 = 6$ of mean hydraulic head, $\bar{h}^{[1]}(x_1)$, for various degrees of uncertainty in the size of the inclusion.

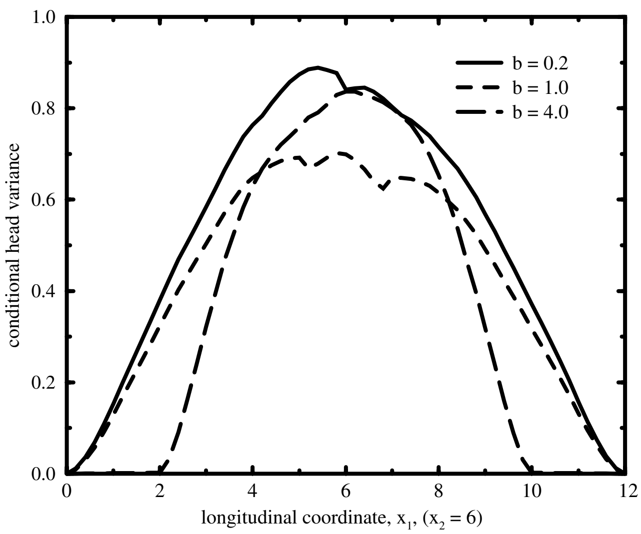

Figure 4. The cross section $x_2 = 6$ of the first-order approximation of the conditional hydraulic head variance, $\sigma_h^2(x_1|b)$, for several realizations of b.

[12] Note that the first-order approximation, $\bar{h}^{[1]}(\boldsymbol{x}|b) = \bar{h}^{(0)}(\boldsymbol{x}|b) + \bar{h}^{(1)}(\boldsymbol{x}|b)$, depends on integrating over domains $\Omega_j(b)$ fixed by conditioning on b. The dependence on b is removed by integrating $\bar{h}^{[1]}(\boldsymbol{x}) = \int \bar{h}^{[1]}(\boldsymbol{x}|b)p(b)db$. We evaluated this integral by means of the law of large numbers,

$$\bar{h}^{[1]}(\boldsymbol{x}) \approx \frac{1}{n_b}\sum_{n=1}^{n_b}\bar{h}^{[1]}(\boldsymbol{x}|b_n) \qquad (10)$$

because we had already generated the large data sets it requires. Taylor series [cf. *Tartakovsky and Winter*, 2001] or other methods can be used to approximate this integral in realisitic cases, where multiple realizations are not available.

[13] We demonstrate an example of such calculations in Figure 2, where the median cross section (x_2 = 6) of the conditional mean head, $\bar{h}^{[1]}(x_1|b)$, is computed by equations (7) and (8) for several realizations of the inclusion's size, b = 0.2, 1.0, and 4.0. The results of Monte Carlo simulations coincide with mean head distribution obtained from our moments equations and thus are not reported in Figure 2.

[14] Figure 3 shows the distribution of mean hydraulic head, $\bar{h}^{[1]}(x_1)$, along the longitudinal cross section x_2 = 6 for several values of σ_β. As before, head distributions obtained from Monte Carlo simulations and from our moments equations are indistinguishable. Hence only the moments equation solution is represented. The effect of uncertainty in the internal boundary on one's ability to estimate hydraulic head is apparent. As σ_β increases, the mean head distribution approaches a straight line that corresponds to the uniform head distribution. *Winter and Tartakovsky* [2002] noted a similar behavior for one-dimensional flow in composite media.

3.2. Hydraulic Head Variance

[15] Similar to evaluating mean hydraulic head, we compute hydraulic head variance in two stages [*Winter and Tartakovsky*, 2000]. First, we evaluate the first-order approximation of head variance conditioned on b,

$$\left[\sigma_h^2(\boldsymbol{x}|b)\right]^{(1)} = -\sum_{i=1}^{2}\int_{\Omega_i(b)} C_{K_ih}^{(1)}(\boldsymbol{y},\boldsymbol{x}|b)\nabla_{\boldsymbol{y}}\,\bar{h}^{(0)}(\boldsymbol{y}|b)\cdot\nabla_{\boldsymbol{y}}\,G_b(\boldsymbol{y},\boldsymbol{x})d\boldsymbol{y} \qquad (11)$$

where the first-order approximation of the cross covariance $C_{K_ih}(\boldsymbol{y},\boldsymbol{x}) = \overline{K_i'(\boldsymbol{y})h'(\boldsymbol{x})}$ is found as

$$C_{K_ih}^{(1)}(\boldsymbol{y},\boldsymbol{x}|b) = -K_{g_i}^2\int_{\Omega_i(b)} C_{Y_i}(\boldsymbol{y},\boldsymbol{z})\,\nabla_{\boldsymbol{z}}\cdot\,\bar{h}^{(0)}(\boldsymbol{z}|b)\nabla_{\boldsymbol{z}}\,G_b\cdot(\boldsymbol{z},\boldsymbol{x})\,d\boldsymbol{z}. \qquad (12)$$

Figure 4 shows the results of this calculation for three realizations of the inner square's size, b/λ = 0.2, 1.0, and 4.0.

[16] Then, we use the law of large numbers to obtain

$$\left[\sigma_h^2(\boldsymbol{x})\right]^{[1]}\approx\frac{1}{n_b}\sum_{b}\left[\sigma_h^2(\boldsymbol{x}|b)\right]^{[1]}. \qquad (13)$$

The resulting hydraulic head variance for σ_β = 0.5 is depicted in Figure 5. Note that our composite media approach produces the local minimum in head variance at the center of the inclusion. This is in contrast with standard, statistically homogeneous models that for similar flow domains would result in the maximum of head variance at the domain center [e.g., *Tartakovsky and Mitkov*, 1999]. A similar effect has been noted when head statistics are

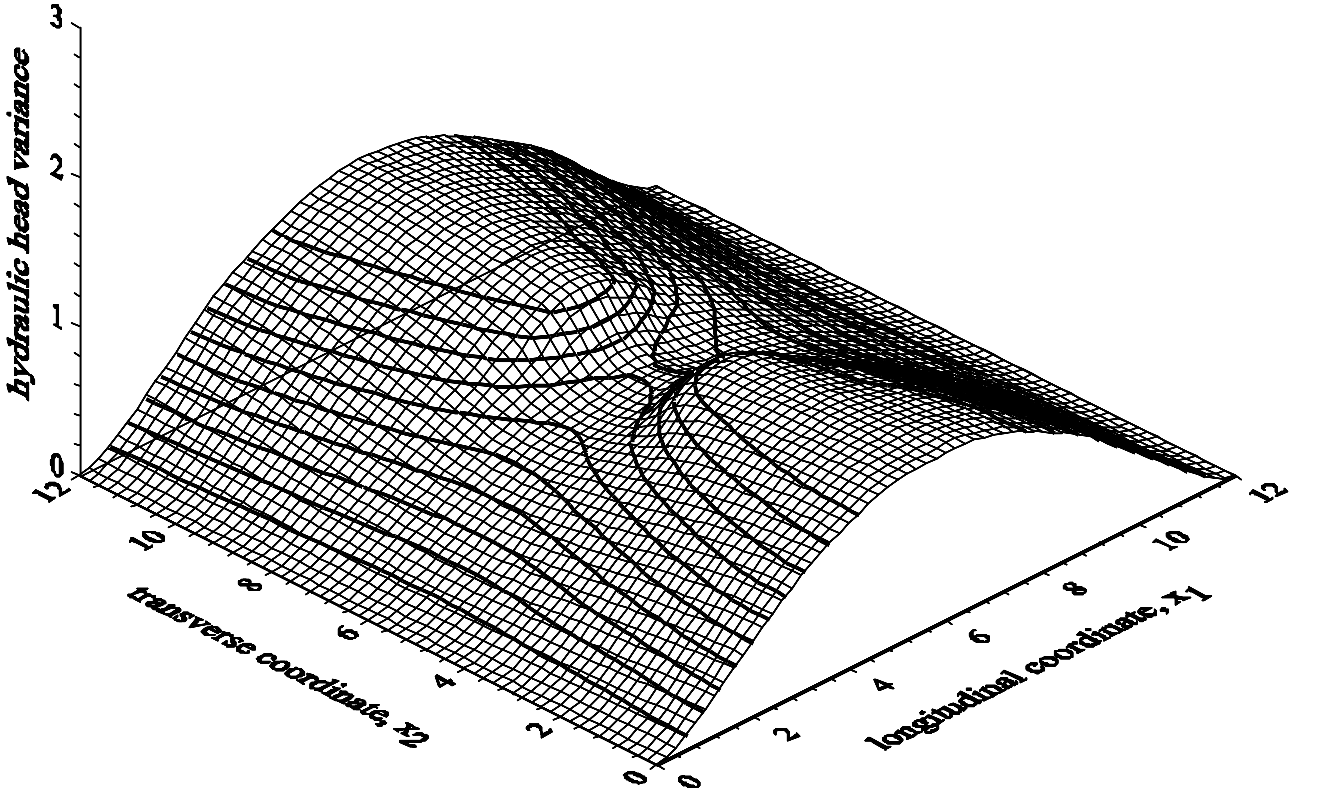

Figure 5. The first-order approximation of hydraulic head variance, $\sigma_h^2(\boldsymbol{x})$, for σ_β = 0.5.

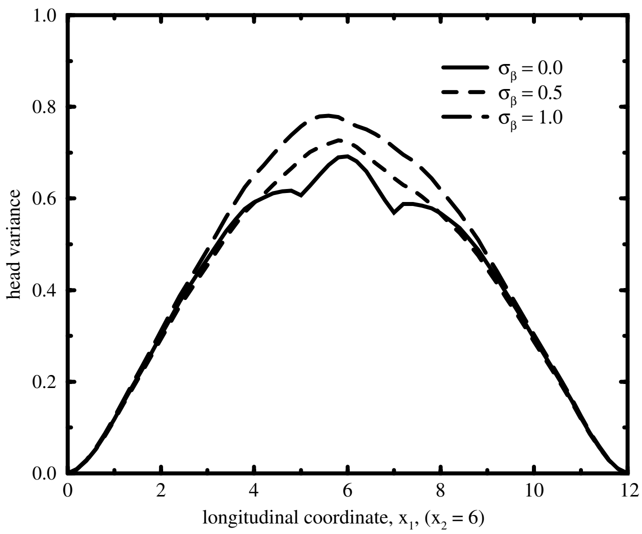

Figure 6. The longitudinal cross section $x_2 = 6$ of the first-order approximation of hydraulic head variance, $\sigma_h^2(x_1)$, for various degrees of uncertainty in the size of the inclusion.

conditioned on local measurements of hydraulic conductivity [*Neuman*, 1997, and references therein].

[17] Figure 6 explores the effects of the uncertain size of inclusions on one's ability to accurately approximate hydraulic head variance. Figure 6 shows the longitudinal cross section, $x_2 = 6$, of the first-order approximation of hydraulic head variance, $\sigma_h^2(x_1)$, for several values of variance of the inner square size. The perfectly known (deterministic) geometry of the inclusion corresponds to $\sigma_\beta^2 = 0$. The increasing degree of uncertainty about the size of the inner square corresponds to a larger value of σ_β^2.

[18] The actual values of head variance depend on a combination of factors: (1) the extent of the conditional inner domain which defines the domain of integration in equations (11) and (12), thus affecting the weight of the conditional conductivity covariance; and (2) the relative (empirical) frequency of realizable inner domain's sizes, which corresponds to the probabilistic weighted average in equation (13). Inclusions whose size has a low probability contribute very little to the total head variance, even though the corresponding conditional variance might be quite large.

[19] The accuracy of the solutions of our moments equations is demonstrated by comparing them with Monte Carlo simulations in Figure 7 for $\sigma_\beta = 1$. This comparison is nearly perfect.

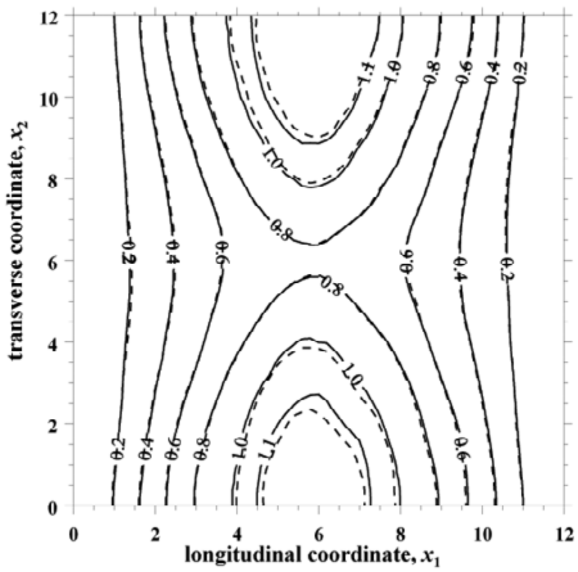

Figure 7. The contour map of the hydraulic head variance computed by the moments equations (solid lines) and by Monte Carlo simulations (dashed lines).

4. Uncertain Geometry Versus Uncertain Conductivity

[20] In this section we compare the relative importance of the two sources of uncertainty for the flow configuration of Figure 1. The case of random boundaries separating media with deterministic properties is conceptually similar to problems considered by *Shvidler* [1986] and *Levermore et al.* [1986]. On the other hand, the conditional simulations in section 3 of this paper serve as an example of flow domains consisting of materials with random properties that are separated by deterministic boundaries.

[21] We start by considering flow where the hydraulic properties of the two materials are deterministic, while the inclusion size is random. Statistics of the hydraulic head distribution were computed by Monte Carlo simulations. The previously generated 5000 values of b were used in the Monte Carlo framework.

[22] We then compare these results with the head statistics obtained for the case where the hydraulic properties of the two materials are random, while the inclusion size is deterministic. We set $b = 1.2$, while using the same conductivity statistics as in the previous section. The resulting head statistics are the same as the conditional statistics for the $b = 1.2$ realization obtained in section 3.

[23] Next we examine the relative effects of each source, geometry or conductivity, of uncertainty. Figure 8 compares the longitudinal cross section at $x_2 = 6$ of mean hydraulic head,

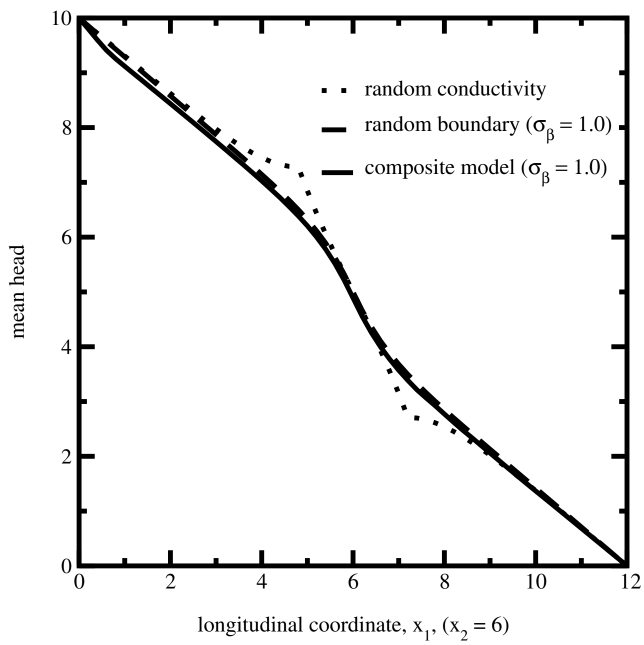

Figure 8. Comparison between the longitudinal cross-section of mean hydraulic head computed for (1) uncertain geometry and uncertain hydraulic conductivities (solid line), (2) uncertain geometry but known conductivities (dashed line), and (3) known geometry but uncertain conductivities (dotted line).

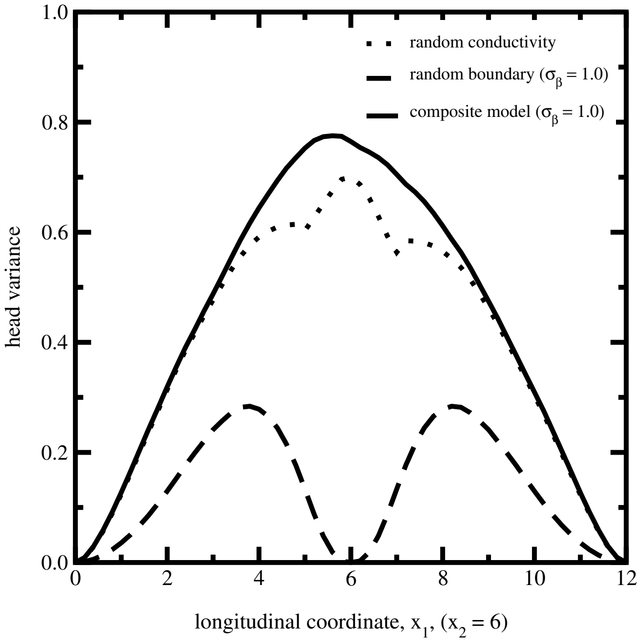

Figure 9. Comparison between the longitudinal cross-section of hydraulic head variance computed for (1) uncertain geometry and uncertain hydraulic conductivities (solid line), (2) uncertain geometry but known conductivities (dashed line), and (3) known geometry but uncertain conductivities (dotted line).

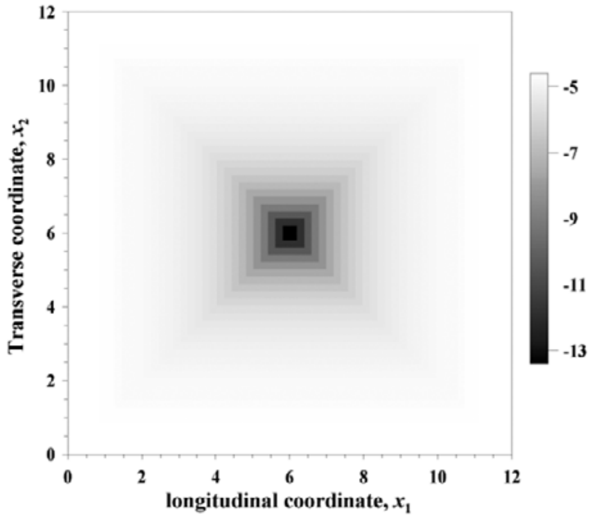

Figure 10. Deterministic trend in log conductivity for Model 2, which is obtained by using local values corresponding to $\sigma_\beta = 1$.

$\overline{h}^{[1]}(x_1)$, resulting from (1) uncertainty in both the inclusion size and hydraulic conductivities, i.e., the full composite media model, (2) uncertainty only in the inclusion size, and (3) uncertainty only in hydraulic conductivities of the two materials. It is clear from Figure 8 that the uncertain geometry smoothes mean head profiles and captures the main features of the mean head estimated by the full composite model.

[24] Uncertainty associated with our head estimators in Figure 8 is quantified by the head variance shown in Figure 9. Both simplified models, when either the boundary is fixed and conductivity is random or when the boundary is random and conductivity is fixed, underestimate the actual head variance of the composite system. This is to be expected since each ignores a source of uncertainty. When the boundary is random but conductivities are fixed, head variance peaks in the region of uncertainty of the boundary location but approaches zero at the domain center, where the probability of being in the inner material is almost 1. Although this model replicates the mean behavior of the composite model almost perfectly, it greatly underestimates head uncertainty. Furthermore, the shape of the variance estimate is qualitatively wrong. On the other hand, the model with the fixed boundary and random conductivity, which failed to replicate the mean behavior of the composite model, provides a better estimate of head variance, both qualitatively and quantitatively. Nonetheless, this model still introduces local minima in the variance at the fixed boundary locations.

5. Comparison With Deterministic Trend Models

[25] Previous attempts to analyze statistically inhomogeneous fields have relied on models with deterministic trends in the mean imposed on a homogeneous random field [e.g., *Neuman and Jacobsen*, 1984; *Rajaram and McLaughlin*, 1991; *Li and McLaughlin*, 1995]. In essence, this type of random field is statistically homogeneous once the mean trend has been removed. The fundamental weakness of such models is that a formation composed of different materials must nonetheless display the same second-order moments at every point. That is at best an approximation. When applied to a layered medium, for instance, the trend model requires the same covariance structure in every layer, a very dubious assumption.

[26] This raises the question of how accurate such approximations are in general. We begin to address this question by comparing head statistics from two different trend models (model 1 and model 2) with that from the composite model. We use the setup in Figure 1 as our test case. In model 1 we represent the trend by a step function, i.e., $\overline{Y} = -4.6$ inside the square inclusion and $\overline{Y} = -13.8$ otherwise. The half-length of the inner square is known and taken to be $b = 1.2$. In model 2 we use our extensive samples of

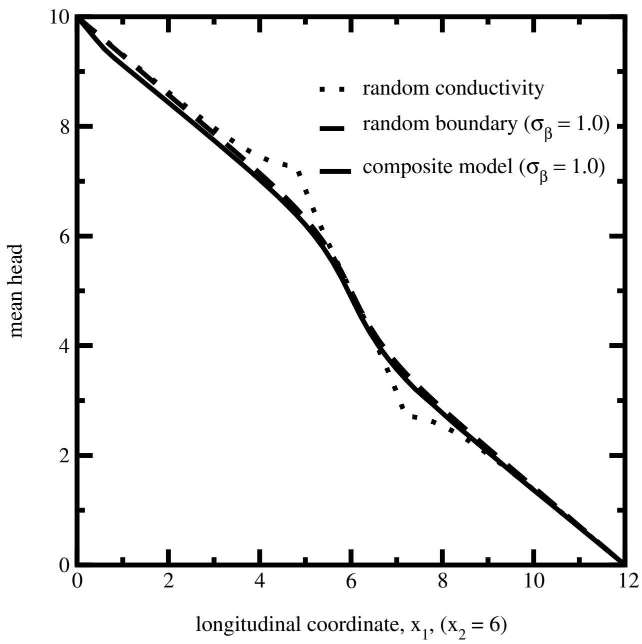

Figure 11. Mean head distributions for our composite media model and for two statistically homogeneous models with deterministic trends.

$Y(\boldsymbol{x}|b)$ and b to compute the sample mean $\overline{Y}(\boldsymbol{x})$, which we then use as a deterministic trend. Note that actually implementing model 2 would require either a large number of realizations from an ensemble of natural porous media or a level of ergodicity, which cannot be justified when the composite model is appropriate, i.e., when we have a statistically inhomogeneous field characterized by uncertain geometry. Clearly, each model is an approximation of the actual field that substitutes a pseudohomogeneous field with deterministic trend for the truly inhomogeneous field.

[27] Figure 10 depicts a two-dimensional image of the resulting $\overline{Y}(\boldsymbol{x})$, obtained by using the local values corresponding to the case with unit variance of the inner square's half-side. Similar plots were obtained for all tested values of the inner domain's size variance.

[28] Figure 11 compares the longitudinal cross-sections of mean hydraulic head, $\overline{h}^{[1]}(x_1)$, at $x_2 = 6$ resulting from our composite model with $\sigma_\beta = 1$ to the models with deterministic trends (models 1 and 2). Both mean head profiles obtained from the deterministic trend models show unrealistically sharp contrasts between regions belonging to different materials. The trend models introduce a level of specificity that is not justified by geometrically uncertain data. The much more linear mean head estimate obtained from the composite model reflects both kinds of uncertainty. This degree of linearity increases with increasing uncertainty in location of the inner material boundary, reflecting the loss of information. It must be stressed that this level of uncertainty cannot be removed by recourse to an arbitrary and almost certainly incorrect deterministic boundary specification.

[29] Figure 12 depicts the corresponding cross section of hydraulic head variance, σ_h^2, for our composite model and for the two statistically homogeneous models with deterministic trends (models 1 and 2). As expected, the pattern of head variance for the homogeneous increment model with trend of $\overline{Y}$ corresponding to model 1 closely resembles the composite model variance conditioned on $b = 1.2$. The discrepancies among the curves can be explained on the basis of equation (1), by taking into account the different spatial patterns of K_{g_i}, log conductivity correlations, and mean hydraulic head gradients.

[30] This preliminary analysis shows that when flow is affected by structural nonstationarity, models with a deterministic trend can be expected to give a poor estimate of the statistics of head. Indeed, trend models provide a false sense of accuracy while instead consistently underestimating the variance of head.

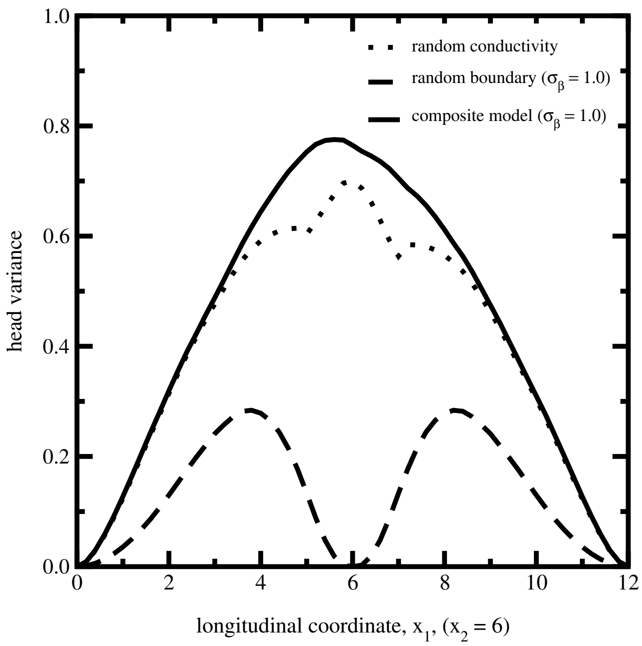

Figure 12. Head variance distributions for our composite media model and for two statistically homogeneous models with deterministic trends.

6. Summary

[31] When porous media are composed of diverse materials, statistical analysis of flow dynamics requires a systematic approach to nonstationarity. The composite medium model of *Winter and Tartakovsky* [2000, 2002] is a straightforward representation of the kinds of nonstationarity usually encountered in groundwater hydrology. It is based on two scales of heterogeneity: The large-scale distribution of units of uniform materials is represented by an arrangement of random volumes ("blocks") of different materials. Each block is composed of a single material; blocks do not overlap. Local variability within a block is represented by statistically homogeneous distributions of parameters, especially conductivity, specific to the block's material type.

[32] We used a very large number of Monte Carlo simulations to examine several aspects of the theory of composite media that are not easily investigated analytically. We investigated the properties of the composite medium model in the setting of Figure 1, which corresponds to an impermeable lens embedded in a permeable medium. The significance of this relatively simple setting is twofold. It allowed us to demonstrate the practical applicability of the composite media approach developed by *Winter and Tartakovsky* [2000, 2002]. Moreover, in numerical models of flow and transport, complex geological structures are commonly represented in numerical models of flow and transport as a collection of rectangular blocks with homogeneous hydraulic properties.

[33] First, we evaluated the accuracy of the low-order perturbation expansions that are the motivation for much of the theory. In principle, the composite medium theory allows expansions in small parameters $\sigma_{Y_M}^2$, instead of in σ_Y^2, the total variance across all materials of log conductivity. The variances $\sigma_{Y_M}^2$ are specific to each material, M, and are much smaller than σ_Y^2. We compared the small variance expansions of the first two moments of head in *Winter and Tartakovsky* [2000, 2002] to Monte Carlo simulations. The agreement is excellent in all cases, suggesting that first-order in $\sigma_{Y_M}^2$ expansions lead to reliable approximations of the first two moments.

[34] Second, we compared the relative importance of large-scale and local variability in the composite medium model. Our preliminary results make it clear that large-scale block variability can have a significant effect on the moments of head.

[35] Third, we compared the complete composite medium model to linear trend approximations that represent heterogeneity as a deterministic trend in log conductivity. Models that represent nonstationarity as a deterministic trend in mean conductivity underestimate the state of uncertainty because they do not account for uncertainty in the block geometry. They indicate an unwarranted certainty about the spatial distribution of mean head and they usually underestimate head variance.

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