Groundwater flow in heterogeneous composite aquifers

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[1] We introduce a stochastic model of flow through highly heterogeneous, composite porous media that greatly improves estimates of pressure head statistics. Composite porous media consist of disjoint blocks of permeable materials, each block comprising a single material type. Within a composite medium, hydraulic conductivity can be represented through a pair of random processes: (1) a boundary process that determines block arrangement and extent and (2) a stationary process that defines conductivity within a given block. We obtain second-order statistics for hydraulic conductivity in the composite model and then contrast them with statistics obtained from a standard univariate model that ignores the boundary process and treats a composite medium as if it were statistically homogeneous. Next, we develop perturbation expansions for the first two moments of head and contrast them with expansions based on the homogeneous approximation. In most cases the bivariate model leads to much sharper perturbation approximations than does the usual model of flow through an undifferentiated material when both are applied to highly heterogeneous media. We make this statement precise. We illustrate the composite model with examples of one-dimensional flows which are interesting in their own right and which allow us to compare the accuracy of perturbation approximations of head statistics to exact analytical solutions. We also show the boundary process of our bivariate model is equivalent to the indicator functions often used to represent composite media in Monte Carlo simulations. *INDEX TERMS:* 1869 Hydrology: Stochastic processes; 1829 Hydrology: Groundwater hydrology; 1832 Hydrology: Groundwater transport; 3210 Mathematical Geophysics: Modeling; *KEYWORDS:* random, stochastic, nonstationary, effective, upscaled, decomposition

1. Introduction

[2] It has become common to quantify uncertainty in groundwater flow models by treating hydraulic conductivity, K, and derived quantities like hydraulic head, h, as random fields. For steady state flows the statistics of h can be obtained from the stochastic flow equation

$$\nabla \cdot [K(\mathbf{x})\nabla h(\mathbf{x})] + f(\mathbf{x}) = 0 \qquad (1)$$

when boundary conditions are given and the statistics of K and the (random) source function $f(\mathbf{x})$ are known. Usually boundary and initial conditions are also uncertain, but their effects are additive, so we limit our attention here to the effects of highly variable conductivity.

[3] Following *Winter and Tartakovsky* [2000], we concentrate in this paper on flow through composite porous media. A composite medium consists of disjoint facies, or blocks of internally homogeneous materials. An obvious example is a stratified porous medium in which the individual layers correspond to different materials, for instance sandstones and limestones. *Winter and Tartakovsky* [2000] models composite media as a bivariate stochastic process that depends on (1) the random geometry of the blocks, primarily the locations of their boundaries, and (2) on the random spatial distribution of hydraulic conductivity within a block.

[4] We use the Reynolds decomposition $\mathcal{A}(\mathbf{x}) = \overline{\mathcal{A}}(\mathbf{x}) + \mathcal{A}'(\mathbf{x})$ to represent a random field $\mathcal{A}$ as the sum of a mean, $\overline{\mathcal{A}}(\mathbf{x})$, and a zero-mean random deviation, $\mathcal{A}'(\mathbf{x})$, with variance $\sigma^2_{\mathcal{A}}(\mathbf{x})$. The average steady state flow equation becomes

$$\nabla \cdot \left[\overline{K}(\mathbf{x})\nabla \overline{h}(\mathbf{x})\right] - \nabla \cdot \overline{\mathbf{r}}(\mathbf{x}) + \overline{f}(\mathbf{x}) = 0 \qquad (2)$$

which consists of a deterministic mean part, $\overline{K}\nabla\overline{h}$, and a deterministic residual flux, $\overline{\mathbf{r}} = -\overline{K'\nabla h'}$.

[5] Solutions of (2) require the mean conductivity, $\overline{K}(\mathbf{x})$, and in most cases, a method for closing an expansion of $\overline{\mathbf{r}}(\mathbf{x})$. Usually $\overline{\mathbf{r}}(\mathbf{x})$ is approximated through perturbation expansions based on σ^2_Y, the variance of $Y = \ln K$, the logarithm of conductivity. This approach works well so long as σ^2_Y is small. Suppose that the usual assumptions of stochastic hydrology hold: (1) The statistics of conductivity within individual blocks of material are known, (2) the conductivity of each material is statistically homogeneous, and (3) the variance of conductivity within a material is small, along with (4) the statistics of the block geometry are known and (5) the scale used to measure conductivity is much smaller than the scale of the blocks. Then our composite medium model can be applied and solutions for

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$\overline{h}(\mathbf{x})$ can be sharpened by developing expressions for $\overline{K}(\mathbf{x})$ and $\overline{\mathbf{r}}(\mathbf{x})$ that reflect heterogeneity at the larger, across-block scale. Additionally, we can approximate $\sigma_h^2(\mathbf{x})$ and thus obtain reasonably tight bounds on $\overline{h}(\mathbf{x})$.

[6] A considerable literature has grown up that analyzes Darcy flows in statistically homogeneous media [*Shvidler*, 1964; *Dagan*, 1989; *Gelhar*, 1993; *Dagan and Neuman*, 1997]. It has wide utility because many applications of Darcy's Law deal with horizontal flow in a single layer of a stratified medium and there it is reasonable to assume that σ_Y^2 is small. The case is different at larger scales where conductivity statistics are affected by variations among blocks of various materials. In particular, *McMillan and Gutjahr* [1986] and *Desbarats and Bachu* [1994] found that vertical correlation scales of hydraulic conductivity are meaningless for many stratified aquifers, while *Gómez-Hernández and Wen* [1998] questioned the multi-Gaussian nature of conductivity fields in fractured geologic environments.

[7] One approach for dealing with composite media is to superimpose a deterministic trend on a homogeneous random field of (log) hydraulic conductivity [*Neuman and Jacobsen*, 1984; *Rajaram and McLaughlin*, 1990; *Indelman and Rubin*, 1995]. While this approach incorporates some information about the geological structure of a medium, it has important disadvantages. First, it assumes a homogeneous correlation structure throughout a composite medium. Consequently, it becomes necessary to assume that the conductivity variances in different geological blocks are the same (a dubious assumption) and correlations between points in one block are the same as correlations between points in different blocks (a very dubious assumption). Secondly, this approach does not provide a means for quantifying structural uncertainty of the medium.

[8] Another approach to describing hydraulic conductivity in composite media is to represent conductivity as a multi-component random field, but without regard to the material membership of specific points. *Rubin and Journel* [1991] used indicator functions to simulate multi-modal distributions of random conductivity fields. *Desbarats* [1987, 1990] numerically analyzed flow and transport in log conductivity fields with bimodal distributions. *Rubin* [1995] derived an analytical expression for the effective conductivity of bimodal formations. Although superficially similar to the model proposed by *Winter and Tartakovsky* [2000] and analyzed here, multi-modal models differ from the composite model in several important respects. In particular, they do not use geometrical information about the arrangement of blocks. Instead, these models lump observations of conductivity together and then estimate statistics as if the medium were homogeneous. In most cases such an approach leads to very coarse estimates of $\overline{K}(\mathbf{x})$, values of σ_Y^2 that are large, and hence expansions for $\overline{\mathbf{r}}(\mathbf{x})$ that are inaccurate. Since they result in constant mean conductivity and variance, we refer to such models as homogeneous approximations.

[9] *Winter and Tartakovsky* [2000] discusses mean flow in composite porous media. We extend that analysis in several directions. In section 2 we derive second order statistics and densities for $K(\mathbf{x})$ in composite media. Then we are in a position to compare the homogeneous approximation to the composite medium model in section 3. *Winter and Tartakovsky* [2000] points out that the homogeneous approximation can lead to artificially high variances of log conductivity. We derive the results on which that conclusion is based and also give precise criteria for when one model is to be preferred to another. We develop perturbation approximations in section 4 and are able thereby to justify the claim of *Winter and Tartakovsky* [2000] that the composite medium model leads to sharper perturbation expansions than other models, specifically the homogeneous approximation. Equally important, we also determine the variance of h in section 4. We illustrate the composite medium model with a one-dimensional example in section 5. Since we can obtain an analytic solution in this case, we can evaluate the accuracy of perturbation approximations. *Winter et al.* [2002] give numerous examples of flows through higher dimensional composite media. We examine the relationship between the random boundary representation and indicator probabilities in Appendix A. Since our Green's Function solutions for the first two moment of h require integration over the random boundary process which much of our theory is based on, it is important to see their equivalence.

2. Statistics of Composite Media

[10] In general, a porous medium contains units of many types of material. In the composite model, units are disjoint blocks and each unit is itself a statistically homogeneous medium of specific material type M_i. We follow *Winter and Tartakovsky* [2000] and consider porous media composed of only two types of material (M_1 and M_2) for the moment. Extensions to multiple materials are obvious, and we give them at the end of this section. A point, $\mathbf{x}$, of the medium lies in M_1 with probability $P[\mathbf{x} \in M_1] = P_1(\mathbf{x})$ and in material M_2 with probability $P[\mathbf{x} \in M_2] = 1 - P[\mathbf{x} \in M_1] = P_2(\mathbf{x})$. As noted, *Winter and Tartakovsky* [2000] supposes that the random field K has homogeneous densities $p_i(k(\mathbf{x}))$, $p_i(k(\mathbf{x}), k(\mathbf{y}))$,... within the units $i = 1, 2$. Usually, but not necessarily, $p_i(k)$ is log-normal. The discussion in this section does not require small $\sigma_{Y_i}^2$, although perturbation approximations of heads will be much more robust when the $\sigma_{Y_i}^2$ are small.

[11] Since the conductivity density, $p(k)$, is the marginal over M of $p(k, M) = p(k|M)P_M(\mathbf{x}) = p_M(k)P[\mathbf{x} \in M]$, *Winter and Tartakovsky* [2000] easily shows that for any point $\mathbf{x}$,

$$p(k) = P_1(\mathbf{x})p_1(k) + P_2(\mathbf{x})p_2(k) \tag{3}$$

is the location-dependent mixture of the within-unit densities, p_1 and p_2, where the weighting function is the probability of block membership. When the point $\mathbf{x}$ is deep within block i (far from the corresponding boundaries), $P_i \approx 1$ and $p(k) \approx p_i(k)$. As $\mathbf{x}$ approaches a boundary between the materials, $p(k)$ approaches the average of p_1 and p_2.

[12] The joint distribution $p(k(\mathbf{x}), k(\mathbf{y})) \equiv p(k_x, k_y)$ is also easy to derive. Using $P_{ij}(\mathbf{x}, \mathbf{y}) = P[\mathbf{x} \in M_i, \mathbf{y} \in M_j]$ and $p_{ij}(k_x, k_y) = p(k_x, k_y|\mathbf{x} \in M_i, \mathbf{y} \in M_j)$ to simplify the notation,

$$\begin{aligned} p(k(\mathbf{x}), k(\mathbf{y})) = {} & P_{11}(\mathbf{x},\mathbf{y})p_{11}(k_x,k_y) + P_{12}(\mathbf{x},\mathbf{y})p_1(k_x)p_2(k_y) \\ & + P_{21}(\mathbf{x},\mathbf{y})p_2(k_x)p_1(k_y) + P_{22}(\mathbf{x},\mathbf{y})p_{22}(k_x,k_y) \end{aligned} \tag{4}$$

if we make the reasonable physical assumption that $K(\mathbf{x})$ and $K(\mathbf{y})$ are independent when $\mathbf{x}$ and $\mathbf{y}$ are in different materials, i.e., $p_{ij}(k_x, k_y) = p_i(k_x)p_j(k_y)$. Higher order densities can be similarly derived, but are not needed in the remainder of our discussion.

[13] Let the constants, $\overline{K}_j$ and σ_j, be the mean and standard deviation respectively of conductivity in material j. It follows from (3) and elementary properties of mixtures that the ensemble average of $K(\mathbf{x})$ is a weighted sum of means in the two material types [*Winter and Tartakovsky*, 2000],

$$\overline{K}(\mathbf{x}) = P_1(\mathbf{x})\overline{K}_1 + P_2(\mathbf{x})\overline{K}_2. \tag{5}$$

Since the weights depend on the location, $\mathbf{x}$, it is clear that $\overline{K}$ is not constant. Of course, $\overline{K}(\mathbf{x}) \approx \overline{K}_i$ when $\mathbf{x}$ is deep in M_i.

[14] The ensemble variance,

$$\sigma_K^2(\mathbf{x}) = P_1(\mathbf{x})\sigma_1^2 + P_2(\mathbf{x})\sigma_2^2 + P_1(\mathbf{x})P_2(\mathbf{x})\left(\overline{K}_1 - \overline{K}_2\right)^2, \tag{6}$$

is small far from a boundary (where either $P_1 \approx 1$ or $P_2 \approx 1$) so long as $\sigma_{max} = \max(\sigma_1, \sigma_2)$ is small; but its magnitude near a boundary depends on $(\overline{K}_1 - \overline{K}_2)^2$ and can become quite large.

[15] Given conductivity covariance $C_i(\rho)$ within the material M_i, it is easy to show that the covariance of conductivities $K(\mathbf{x})$ and $K(\mathbf{y})$ separated by a distance $\rho = \|\mathbf{x} - \mathbf{y}\|$ is

$$\begin{aligned} C_K(\mathbf{x},\mathbf{y}) = {} & P_{11}(\mathbf{x},\mathbf{y})C_1(\rho) + P_{22}(\mathbf{x},\mathbf{y})C_2(\rho) + \big[P_{11}(\mathbf{x},\mathbf{y}) \\ & - P_1(\mathbf{x})P_1(\mathbf{y})\big]\overline{K}_1^2 + [P_{22}(\mathbf{x},\mathbf{y}) - P_2(\mathbf{x})P_2(\mathbf{y})]\overline{K}_2^2 \\ & + \big[P_{12}(\mathbf{x},\mathbf{y}) + P_{21}(\mathbf{x},\mathbf{y}) - P_1(\mathbf{x})P_2(\mathbf{y}) \\ & - P_2(\mathbf{x})P_1(\mathbf{y})\big]\overline{K}_1\overline{K}_2. \end{aligned} \tag{7}$$

Clearly (7) reduces to $\sigma_K^2(\mathbf{x})$ when $\mathbf{x} = \mathbf{y}$. Also, $C_K(\mathbf{x}, \mathbf{y}) = 0$ when $\|\mathbf{x} - \mathbf{y}\|$ is large enough that $K(\mathbf{x})$ and $K(\mathbf{y})$ are effectively independent.

[16] Formulae for geological formations consisting of multiple facies, $M = 1, \ldots, n$ are analogous,

$$p(k) = \sum_{i=1}^{n} p_i(k)\,P_i(\mathbf{x}), \tag{8}$$

$$\overline{K}(\mathbf{x}) = \sum_{i=1}^{n} P_i(\mathbf{x})\,\overline{K}_i, \tag{9}$$

$$\sigma_K^2(\mathbf{x}) = \sum_{i=1}^{n} P_i(\mathbf{x})\sigma_i^2 + \sum_{i=1}^{n}\sum_{j>i}^{n} P_i(\mathbf{x})\,P_j(\mathbf{x})\left(\overline{K}_i - \overline{K}_j\right)^2, \tag{10}$$

and

$$\begin{aligned} C_K(\mathbf{x},\mathbf{y}) = {} & \sum_{i=1}^{n} P_{ii}(\mathbf{x},\mathbf{y})C_i(\rho) + \sum_{i=1}^{n}[P_{ii}(\mathbf{x},\mathbf{y}) - P_i(\mathbf{x})P_i(\mathbf{y})]\overline{K}_i^2 \\ & + \sum_{i=1}^{n}\sum_{j>i}^{n}\big[P_{ij}(\mathbf{x},\mathbf{y}) + P_{ji}(\mathbf{x},\mathbf{y}) - P_i(\mathbf{x})P_j(\mathbf{y}) \\ & - P_j(\mathbf{x})P_i(\mathbf{y})\big]\overline{K}_i\overline{K}_j. \end{aligned} \tag{11}$$

Formulae for log hydraulic conductivity can be obtained by substituting Y for K in (3)–(11).

3. Homogeneous Approximation

[17] We compare our inhomogeneous model to models in which an inherently inhomogeneous composite medium, Ω, is treated as a homogeneous random field. We examine the case of two blocks, M_1 and M_2, since extensions to multiple blocks are obvious. The homogeneous approximation arises when we take a random sample from Ω of measurements of K without regard to their membership in material M_1 or M_2. The constant probability, Q_i, that a point drawn without knowledge of the medium's structure lies in M_i is obviously

$$Q_i = \frac{V_i}{V} \approx \frac{\int_\Omega P[\mathbf{x} \in M_i]\,d\mathbf{x}}{\int_\Omega d\mathbf{x}}, \tag{12}$$

where V is the total volume of Ω and V_i is the volume occupied by material M_i. Since the homogeneous model ignores facts about the spatial distribution of the two materials, $p(k) = Q_1p_1(k) + Q_2p_2(k)$.

[18] For a sample of size n the expected value of the sample mean, $\hat{Y}$, is

$$\overline{Y}_{hom} \equiv E\big[\hat{Y}\big] = \frac{1}{n}\sum_{j=1}^{n} E\big[Y_j\big] = \frac{1}{n}\sum_{j=1}^{n}[Q_1\overline{Y}_1 + Q_2\overline{Y}_2] = Q_1\overline{Y}_1 + Q_2\overline{Y}_2. \tag{13}$$

The maximum error, $\mathcal{E}(\mathbf{x}) = |Q_1 - P_1(\mathbf{x})|\overline{Y}_1 + |Q_2 - P_2(\mathbf{x})|\overline{Y}_2$, in the homogeneous approximation of the mean is zero only at points where $Q_i = P_i(\mathbf{x})$.

[19] More importantly, *Rubin* [1995] and *Winter and Tartakovsky* [2000] show that the expected value of the sample variance, s^2, is

$$\sigma^2_{Y_{hom}} \equiv E\big[s^2\big] = Q_1\sigma^2_{Y_1} + Q_2\sigma^2_{Y_2} + Q_1Q_2\left(\overline{Y}_1 - \overline{Y}_2\right)^2. \tag{14}$$

Here we discuss the implications of this fact. In most cases $(\overline{Y}_1 - \overline{Y}_2)^2 \gg 1$ so $\sigma^2_{Y_{hom}} > 1$. In fact, for small variances $\sigma^2_{Y_i}, \sigma^2_{Y_{hom}}$ will only be small when (1) either $Q_1 \approx 0$ or $Q_2 \approx 0$, or (2) $\overline{Y}_1 \approx \overline{Y}_2$. In each of those cases a homogeneous model is obviously a good approximation. In other cases the homogeneous model yields large σ_Y^2 and thus will lead to incorrect perturbation approximations for $\bar{\mathbf{r}}(\mathbf{x})$.

[20] To make this precise, we examine the variance $\sigma^2_{Y_{hom}}(\mathbf{Q})$ as a function of $\mathbf{Q} = (Q_1, Q_2)^T$. Its maximum for $Q_1 \in [0, 1]$,

$$\sigma^2_{max} = \frac{\sigma^2_{Y_1} + \sigma^2_{Y_2}}{2} + \frac{\left[\sigma^2_{Y_1} - \sigma^2_{Y_2}\right]^2}{4\left[\overline{Y}_1 - \overline{Y}_2\right]^2} + \frac{\left[\overline{Y}_1 - \overline{Y}_2\right]^2}{4} \tag{15}$$

occurs at

$$Q_1^{max} = \frac{1}{2} + \frac{\sigma^2_{Y_1} - \sigma^2_{Y_2}}{2\left[\overline{Y}_1 - \overline{Y}_2\right]^2} \tag{16}$$

so long as $|\sigma^2_{Y_1} - \sigma^2_{Y_2}| < \left[\overline{Y}_1 - \overline{Y}_2\right]^2$; otherwise it occurs at the end-points where $\sigma^2_{max} = \sigma^2_{Y_1}\left(= \sigma^2_{Y_2}\right)$ when $Q_1{}^{max} = 1$ $(= 0)$.

[21] When $\sigma^2_{Y_1} > \sigma^2_{Y_2}\left(\sigma^2_{Y_1} < \sigma^2_{Y_2}\right)$ there will be values of Q_1 for which $\sigma^2_{Y_1} > \sigma^2_{Y_{hom}}\left(\sigma^2_{Y_2} > \sigma^2_{Y_{hom}}\right)$. Hence there will be cases in which the homogeneous approximation leads to tighter perturbation expansions than the heterogeneous model. This obviously occurs when $Q_1^{max} = 1$ $(Q_1^{max} = 0)$. Otherwise,

$\sigma^2_{Y_1} > \sigma^2_{Y_{hom}}$ $(\sigma^2_{Y_2} > \sigma^2_{Y_{hom}})$ when $Q_1 < Q_1^0 = [\sigma^2_{Y_1} - \sigma^2_{Y_2}]/[\overline{Y}_1 - \overline{Y}_2]^2$ $(Q_2 < Q_2^0 = [\sigma^2_{Y_2} - \sigma^2_{Y_1}]/[\overline{Y}_1 - \overline{Y}_2]^2)$. It is worth noting that $Q_1^{max} - Q_1^0 = Q_2^{max}$. When $Q_1 \approx 1$, a homogeneous model based on material 1 is obviously called for, and a homogeneous model in material 2 is probably appropriate when $0 < Q_1 < Q_1^0$. When $Q_1^0 < Q_1$, a heterogeneous model is in order.

4. Statistics for Flow in Composite Media

[22] Once $\overline{K}(\mathbf{x})$ has been found, the flow problem reduces to finding $\bar{\mathbf{r}}(\mathbf{x}) = -\overline{K'(\mathbf{x})\nabla h'(\mathbf{x})}$ for given $P[\mathbf{x} \in M_i]$ or, equivalently for given boundary process $p(\beta)$. The residual fluxes within a unit, $\bar{\mathbf{r}}_i(\mathbf{x})$, can be obtained in a variety of ways. In this paper we use an approach based on random Green's functions [cf. *Neuman and Orr*, 1993; and *Tartakovsky and Neuman*, 1998].

[23] We consider flow in a domain, $\Omega = \Omega_1 \cup \Omega_2$, composed of two disjoint units Ω_1 and Ω_2, with an uncertain boundary, $\Gamma_{12}(\mathbf{x})$, between them. More complicated cases are easy to derive from this one, and in fact, most problems collapse to this one anyway since the influence of boundary uncertainty is usually restricted to boundaries between two units.

[24] In this case, the random hydraulic conductivity $K(\mathbf{x})$ belongs to either of the distinct populations

$$K(\mathbf{x}) = \begin{cases} K_1(\mathbf{x}) & \mathbf{x} \in \Omega_1 \\ K_2(\mathbf{x}) & \mathbf{x} \in \Omega_2, \end{cases} \tag{17}$$

and the steady state flow problem (1) can be rewritten as

$$\nabla \cdot [K_i(\mathbf{x})\nabla h_i(\mathbf{x})] + f(\mathbf{x}) = 0 \quad \mathbf{x} \in \Omega_i \tag{18}$$

subject to the boundary

$$h_i(\mathbf{x}) = H(\mathbf{x}) \quad \mathbf{x} \in \Gamma_D = \Gamma_{D_1} \cup \Gamma_{D_2} \tag{19}$$

$$K_i(\mathbf{x})\nabla h_i(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) = Q(\mathbf{x}) \quad \mathbf{x} \in \Gamma_N = \Gamma_{N_1} \cup \Gamma_{N_2} \tag{20}$$

and the contact surface, $\Gamma_{12} = \Omega_1 \cap \Omega_2$, conditions

$$h_1(\mathbf{x}) = h_2(\mathbf{x}) \quad \mathbf{x} \in \Gamma_{12} \tag{21}$$

$$K_1(\mathbf{x})\nabla h_1(\mathbf{x}) \cdot \mathbf{n}_1 = K_2(\mathbf{x})\nabla h_2(\mathbf{x}) \cdot \mathbf{n}_2. \tag{22}$$

Of course, the head distribution in (1) now takes the form $h(\mathbf{x}) \equiv h_i(\mathbf{x})$ for $\mathbf{x} \in \Omega_i$.

[25] We compute the ensemble statistics in two steps. First, we condition our calculations on known location of the boundary. The corresponding conditional mean of a random field $\mathcal{A}(\mathbf{x})$ is denoted in the sequel by $\hat{\mathcal{A}}(\mathbf{x}) \equiv \overline{\mathcal{A}(\mathbf{x}|\Gamma_{12})}$. Second, we average over the ensemble of Γ_{12}.

[26] Taking the conditional (for fixed Γ_{12}) mean of (18)–(22) yields

$$\nabla \cdot \left[\overline{K}_i \nabla \hat{h}_i - \hat{\mathbf{r}}_i\right] + \overline{f} = 0 \quad \mathbf{x} \in \Omega_i \tag{23}$$

subject to the boundary

$$\hat{h}_i = \overline{H} \quad \mathbf{x} \in \Gamma_D \tag{24}$$

$$\left[\overline{K}_i \nabla \hat{h}_i - \hat{\mathbf{r}}_i\right] \cdot \mathbf{n} = \overline{Q} \quad \mathbf{x} \in \Gamma_N \tag{25}$$

and the contact surface conditions (where, of course, $\mathbf{n}_1 = -\mathbf{n}_2 \equiv \mathbf{n}$)

$$\hat{h}_1 = \hat{h}_2 \quad \mathbf{x} \in \Gamma_{12} \tag{26}$$

$$\left[\overline{K}_1 \nabla \hat{h}_1 - \hat{\mathbf{r}}_1\right] \cdot \mathbf{n} = -\left[\overline{K}_2 \nabla \hat{h}_2 - \hat{\mathbf{r}}_2\right] \cdot \mathbf{n} \quad \mathbf{x} \in \Gamma_{12}. \tag{27}$$

Assuming that the driving forces f', H' and Q' are statistically independent from K_j', we show in Appendix B that the conditional residual fluxes $\hat{\mathbf{r}}_j(\mathbf{x})$ are given exactly by

$$\hat{\mathbf{r}}_j(\mathbf{x}) = \sum_{i=1}^{2} \int_{\Omega_i} \mathbf{a}_{ij}(\mathbf{x}, \mathbf{y}) \nabla_\mathbf{y} \hat{h}_i(\mathbf{y}) d\mathbf{y} + \sum_{i=1}^{2} \int_{\Omega_i} \mathbf{b}_j(\mathbf{x}, \mathbf{y}) \hat{\mathbf{r}}_i(\mathbf{y}) d\mathbf{y} \tag{28}$$

where the second-rank tensors $\mathbf{a}_{ij}$ and $\mathbf{b}_j$ are the mixed conditional statistical moments,

$$\begin{aligned} \mathbf{a}_{ij}(\mathbf{x}, \mathbf{y}) &= \left\langle K_j'(\mathbf{x}) K_i'(\mathbf{y}) \nabla_\mathbf{y} \nabla_\mathbf{x}^T \mathcal{G}(\mathbf{y}, \mathbf{x}) \right\rangle \\ \mathbf{b}_j(\mathbf{x}, \mathbf{y}) &= \left\langle K_j'(\mathbf{x}) \nabla_\mathbf{y} \nabla_\mathbf{x}^T \mathcal{G}(\mathbf{y}, \mathbf{x}) \right\rangle. \end{aligned} \tag{29}$$

Here the angle brackets are equivalent to placing a "hat" over the entire expression. The random Green's function $\mathcal{G}$ is defined, for each realization of Γ_{12}, as the solution of (18)–(22) with $f(\mathbf{x}) = \delta(\mathbf{x} - \mathbf{y})$, the Dirac delta function, and the homogeneous boundary conditions.

[27] Evaluating these moments requires some kind of approximation. This problem is known as a problem of closure, and it is traditionally solved by perturbation analyses in a small parameter σ_Y^2, the variance of (natural) log hydraulic conductivity, $Y(\mathbf{x}) = \ln K(\mathbf{x})$ [*Dagan*, 1989; *Neuman and Orr*, 1993; *Tartakovsky and Neuman*, 1998]. It is at this step where the advantages of our approach become apparent. Since the kernels $\mathbf{a}_{ij}$ and $\mathbf{b}_j$ are defined for each of the geological facies separately, we can use the standard perturbation expansions in the variances, $\sigma^2_{Y_j}$, which, as discussed in the previous sections, are relatively small compared with the total variance σ_Y^2. The first-order (in $\sigma^2_{Y_j}$) approximation of the residual flux is given by

$$\hat{\mathbf{r}}_j^{(1)}(\mathbf{x}) = K_{G_j}(\mathbf{x}) \sum_{i=1}^{2} \int_{\Omega_i} K_{G_i}(\mathbf{y}) C_{Y_{ij}}(\mathbf{x}, \mathbf{y}) \nabla_\mathbf{y} \nabla_\mathbf{x}^T G(\mathbf{y}, \mathbf{x}) \, \nabla_\mathbf{y} \hat{h}^{(0)}(\mathbf{y}) \, d\mathbf{y} \tag{30}$$

where $K_{G_j} = \exp(\overline{Y}_j)$ is the geometric mean of K_j, $C_{Y_{ij}}(\mathbf{x}, \mathbf{y}) = \overline{Y_i'(\mathbf{x}) Y_j'(\mathbf{y})}$ is the correlation function, and $G(\mathbf{y}, \mathbf{x}) = \hat{\mathcal{G}}^{(0)}(\mathbf{y}, \mathbf{x})$ is the zeroth-order approximation of the conditional mean Green's function. If hydraulic conductivities of the blocks Ω_1 and Ω_2 are uncorrelated, one has

$$\hat{\mathbf{r}}_j^{(1)}(\mathbf{x}) = K_{G_j}(\mathbf{x}) \int_{\Omega_j} K_{G_j}(\mathbf{y}) C_{Y_{jj}}(\mathbf{x}, \mathbf{y}) \nabla_\mathbf{y} \nabla_\mathbf{x}^T G(\mathbf{y}, \mathbf{x}) \nabla_\mathbf{y} \hat{h}^{(0)}(\mathbf{y}) d\mathbf{y}. \tag{31}$$

[28] Now the first two terms in the perturbation expansion, $\hat{h}(\mathbf{x}) = \hat{h}^{(0)}(\mathbf{x}) + \hat{h}^{(1)}(\mathbf{x}) + \ldots$ are easily found as (Appendix B)

$$\begin{aligned} \hat{h}^{(0)}(\mathbf{x}) = &\sum_{i=1}^{2} \int_{\Omega_i} \overline{f}(\mathbf{y}) G(\mathbf{y}, \mathbf{x}) d\mathbf{y} - \sum_{i=1}^{2} \int_{\Gamma_{D_i}} \overline{H}_i(\mathbf{y}) K_{G_i}(\mathbf{y}) \mathbf{n} \\ &\cdot \nabla_\mathbf{y} G(\mathbf{y}, \mathbf{x}) d\mathbf{y} + \sum_{i=1}^{2} \int_{\Gamma_{N_i}} \overline{Q}_i(\mathbf{y}) G(\mathbf{y}, \mathbf{x}) d\mathbf{y}. \end{aligned} \tag{32}$$

and

$$\hat{h}^{(1)}(\mathbf{x}) = -\sum_{i=1}^{2} \int_{\Omega_i} \left[K_{G_i} \frac{\sigma_{Y_i}^2}{2} \nabla \hat{h}^{(0)}(\mathbf{x}) - \hat{\mathbf{r}}_i^{(1)}(\mathbf{x}) \right] \cdot \nabla G(\mathbf{y}, \mathbf{x})\, d\mathbf{y}\,. \tag{33}$$

[29] We now recall that the first-order approximation of the solution to the mean flow equations (23)–(27), $\hat{h}^{[1]} \equiv \hat{h}^{(0)} + \hat{h}^{(1)}$, was obtained by fixing the boundary Γ_{12} between the two geological facies Ω_1 and Ω_2. It now remains to average this solution over all possible realizations of Γ_{12}, i.e., to evaluate the integral

$$\overline{h}^{[1]}(\mathbf{x}) = \int \hat{h}^{[1]}(\mathbf{x})\, p(\Gamma_{12})\, d\Gamma_{12}\,. \tag{34}$$

[30] The uncertainty associated with our head estimator, $\overline{h}^{[1]}$, can be characterized by head variance $\sigma_h^2(\mathbf{x}) = \overline{h'(\mathbf{x})h'(\mathbf{x})}$. We show in Appendix B that for any given boundary configuration Γ_{12}, the first-order approximation of the conditional head variance can be found as

$$\left[\hat{\sigma}_h^2(\mathbf{x})\right]^{(1)} = -\sum_{i=1}^{2} \int_{\Omega_i} \hat{C}_{K_i h}^{(1)}(\mathbf{y}, \mathbf{x}) \nabla_{\mathbf{y}} \hat{h}^{(0)}(\mathbf{y}) \cdot \nabla_{\mathbf{y}} G(\mathbf{y}, \mathbf{x}) d\mathbf{y} \tag{35}$$

where the first-order approximation of the conditional cross-covariance $\hat{C}_{k_i h}(\mathbf{y}, \mathbf{x}) = \widehat{K_i'(\mathbf{y}) h'(\mathbf{x})}$ is given by

$$\hat{C}_{K_i h}^{(1)}(\mathbf{y}, \mathbf{x}) = -K_{G_i}(\mathbf{y}) \sum_{j=1}^{2} \int_{\Omega_j} K_{G_j}(\mathbf{z})\, C_{Y_{ij}}(\mathbf{y}, \mathbf{z})\, \nabla_{\mathbf{z}} \hat{h}^{(0)}(\mathbf{z}) \cdot \nabla_{\mathbf{z}} G(\mathbf{z}, \mathbf{x})\, d\mathbf{z}. \tag{36}$$

In deriving (35) we assumed that the driving forces, f, h, and Q, are deterministic. Extensions to the case of random driving forces are relatively straightforward [*Tartakovsky and Neuman*, 1999].

[31] Assuming, as before, that hydraulic conductivities of different geological facies are statistically independent, (36) reduces to

$$\hat{C}_{K_i h}^{(1)}(\mathbf{y}, \mathbf{x}) = -K_{G_i}(\mathbf{y}) \int_{\Omega_i} K_{G_i}(\mathbf{z}) C_{Y_{ii}}(\mathbf{y}, \mathbf{z}) \nabla_{\mathbf{z}} \hat{h}^{(0)}(\mathbf{z}) \cdot \nabla_{\mathbf{z}} G(\mathbf{z}, \mathbf{x}) d\mathbf{z}. \tag{37}$$

In analogy to (34),

$$\left[\sigma_h^2(\mathbf{x})\right]^{(1)} = \int \left[\hat{\sigma}_h^2(\mathbf{x})\right]^{(1)} p(\Gamma_{12})\, d\Gamma_{12}\,. \tag{38}$$

5. Example: One-Dimensional Flow

[32] We illustrate our approach with examples of one-dimensional flows. Since we can obtain the exact solution to (23)–(27) in this case, we can compare the accuracy of perturbation expansions. Furthermore, many porous media problems consist of vertical flows in heterogeneous media, so this problem is also important in its own right.

[33] Consider steady state one-dimensional flow,

$$\frac{d}{dx}\left[K(x)\frac{dh(x)}{dx}\right] = 0 \quad x \in (0, 1) \tag{39}$$

subject to the boundary conditions

$$K(x)\frac{dh(x)}{dx} = -q \quad x = 0 \tag{40}$$

$$h(x) = 0 \quad x = 1. \tag{41}$$

The porous medium consists of two materials (say, sand and clay) with random hydraulic conductivities $K_1(x)$ and $K_2(x)$ connected together at the point β, so that now $\Omega_1 = (0, \beta)$, $\Omega_2 = (\beta, 1)$,

$$K(x) = \begin{cases} K_1(x) & 0 < x < \beta \\ K_2(x) & \beta < x < 1 \end{cases} \tag{42}$$

and

$$h(\beta^-) = h(\beta^+) \tag{43}$$

$$K_1(\beta^-)\frac{dh(x=\beta^-)}{dx} = K_2(\beta^+)\frac{dh(x=\beta^+)}{dx}\,. \tag{44}$$

Here β^+ and β^- indicate the limit as $x \to \beta$ from the left and the right, respectively. The exact position of the point of contact is not known precisely. Instead, it is assumed that β is a normally distributed random variable with known mean $\overline{\beta}$ and variance σ_β^2. Hydraulic conductivities $K_1(x)$ and $K_2(x)$ are treated as log normal (multivariate) statistically homogeneous random fields.

[34] For any given β, the zeroth-order approximation of the Green's function for this problem, $G(y, x)$ satisfies (39)–(44) with $K_i(x)$ replaced by their constant geometric means K_{G_i}, the source function replaced by the delta function, and with homogeneous boundary conditions. Following *Stakgold* [1998, p. 91], one can easily show that, for $0 < x < \beta$,

$$G(y,x) = \begin{cases} \frac{x-y}{K_{G_1}}\mathcal{H}(y-x) + \frac{\beta-x}{K_{G_1}} + \frac{1-\beta}{K_{G_2}} & 0 < y < \beta \\ \frac{1-y}{K_{G_2}} & \beta < y < 1 \end{cases} \tag{45}$$

and, for $\beta < x < 1$,

$$G(y,x) = \begin{cases} \frac{1-x}{K_{G_2}} & 0 < y < \beta \\ \frac{x-y}{K_{G_2}}\mathcal{H}(y-x) + \frac{1-x}{K_{G_2}} & \beta < y < 1 \end{cases} \tag{46}$$

where the Heaviside function $\mathcal{H}$ is the one-dimensional equivalent of the indicator functions used in the previous sections.

[35] For the problem under consideration, it is easy to show that one-dimensional versions of (32), (31), and (33) give rise to the conditional mean,

$$\hat{h}^{(0)}(x) = \overline{q}\begin{cases} \frac{\beta-x}{K_{G_1}} + \frac{1-\beta}{K_{G_2}} & 0 < x < \beta \\ \frac{1-x}{K_{G_2}} & \beta < x < 1 \end{cases} \tag{47}$$

$$\hat{r}_1^{(1)}(x) = -\overline{q}\,\sigma_{Y_1}^2 \tag{48}$$

$$\hat{r}_2^{(1)}(x) = -\overline{q}\,\sigma_{Y_2}^2 \tag{49}$$

and

$$\hat{h}^{(1)}(x) = \overline{q}\begin{cases} \frac{\sigma_{Y_1}^2}{2}\frac{\beta-x}{K_{G_1}} + \frac{\sigma_{Y_2}^2}{2}\frac{1-\beta}{K_{G_2}} & 0 < x < \beta \\ \frac{\sigma_{Y_2}^2}{2}\frac{1-x}{K_{G_2}} & \beta < x < 1. \end{cases} \tag{50}$$

Hence

$$\hat{h}^{[1]}(x) = \overline{q}\begin{cases} \left(1 + \frac{\sigma_{Y_1}^2}{2}\right)\frac{\beta-x}{K_{G_1}} + \left(1 + \frac{\sigma_{Y_2}^2}{2}\right)\frac{1-\beta}{K_{G_2}} & 0 < x < \beta \\ \left(1 + \frac{\sigma_{Y_2}^2}{2}\right)\frac{1-x}{K_{G_2}} & \beta < x < 1. \end{cases} \tag{51}$$

Determining the mean head distribution, $\overline{h}^{[1]}(x)$, requires evaluating the integral (34). Before doing that, we investigate the accuracy of the first-order approximation by comparing it with the exact solution of (39)–(44).

[36] Direct integration of (39)–(44) leads to

$$h(x) = q\mathcal{H}(\beta - x)\left[\int_x^\beta \frac{ds}{K_1(s)} + \int_\beta^1 \frac{ds}{K_2(s)}\right] + q\mathcal{H}(x-\beta)\int_x^1 \frac{ds}{K_2(s)}. \tag{52}$$

Assuming that $K_i(x)$ are log-normal statistically homogeneous fields gives, for any realization of β,

$$\hat{h}(x) = \overline{q}\begin{cases} \frac{\beta-x}{K_{H_1}} + \frac{1-\beta}{K_{H_2}} & 0 < x < \beta \\ \frac{1-x}{K_{H_2}} & \beta < x < 1. \end{cases} \tag{53}$$

where $K_{H_i} = K_{G_i}\exp\left(-\sigma_{Y_i}^2/2\right)$ are the harmonic means of $K_i(x)$.

[37] Comparing the approximate solution (51) with the exact solution (53) shows that our perturbative solution is a good approximation of the exact one so long as $\exp(\sigma_{Y_i}/2) \approx 1 + \sigma_{Y_i}/2$ is a good approximation. The latter is strictly valid for $\sigma_{Y_i} < 2$, which seems reasonable for most materials consisting of a single geological unit. (As was discussed above, fractured segments of a geological unit can be modeled as a separate unit with its own hydraulic conductivity.) By contrast, modeling Ω as a statistically uniform medium would result in effective conductivity $K_H = K_G \exp(-\sigma_Y^2/2)$ whose perturbative solution contains an approximation $\exp(\sigma_Y/2) \approx 1 + \sigma_Y/2$. Since for composite materials σ_Y might be much larger that 2, the standard perturbation analysis might not work.

[38] We now proceed to average our solutions (51) or (53) over all possible realizations of β. For truncated normally distributed β, the probability density function $p(\beta)$ has the form

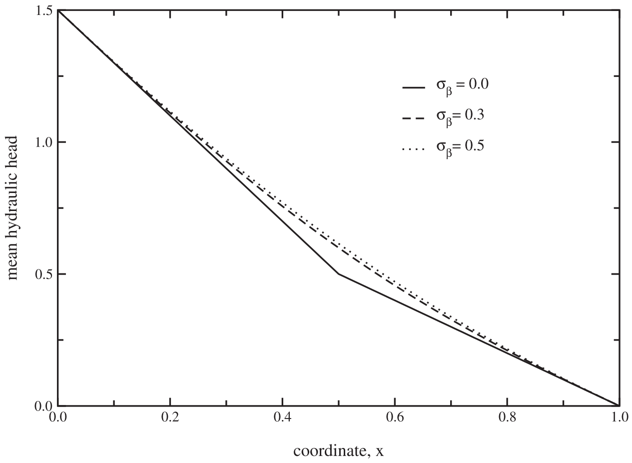

Figure 1. Mean hydraulic head distribution for $\overline{q}/K_{H_1} = 2$, $\overline{q}/K_{H_2} = 1$ and several values of the standard deviation σ_β.

$$\begin{aligned} p(\beta) &= \frac{1}{W}\exp\left[-\frac{1}{2}\left(\frac{\beta-\overline{\beta}}{\sigma_\beta}\right)^2\right] \\ W(\overline{\beta}, \sigma_\beta) &= \int_0^1 \exp\left[-\frac{1}{2}\left(\frac{\beta-\overline{\beta}}{\sigma_\beta}\right)^2\right]d\beta. \end{aligned} \tag{54}$$

Substituting (53) and (54) into (34) yields the mean hydraulic head. Mean head profiles for $\overline{q}/K_{H_1} = 2$ and $\overline{q}/K_{H_2} = 1$ are shown in Figure 1. Uncertainty in the location of the contact affects both mean head, $\overline{h}(x)$, and its derivative. The magnitude of σ_β, the standard deviation of β, is a measure of location uncertainty. Supposing that $\overline{\beta} = 1/2$ and considering $\overline{h}(x)$ first, we see that large σ_β leads to an almost linear trend from one boundary value to the other (Figure 1). This is to be expected, since in this case we are basically not sure whether there is one material or two; hence $P(x \in M_1) \approx P(x \in M_2)$. In the deterministic case ($\sigma_\beta = 0$ and $\overline{\beta} = \beta$), mean head $\overline{h}(x)$ exhibits typical behavior: linear trends in each material and continuity at the boundary, but with a change in slope,

$$\overline{h}(x) = \overline{q}\begin{cases} \frac{\beta-x}{K_{H_1}} + \frac{1-\beta}{K_{H_2}} & 0 < x < \beta \\ \frac{1-x}{K_{H_2}} & \beta < x < 1. \end{cases} \tag{55}$$

Other values of σ_β induce intermediate behavior with the greatest effect near the location of the expected contact. Mean hydraulic gradient, the reciprocal of effective conductivity, is similarly affected (Figure 2).

[39] In the deterministic boundary case ($\sigma_\beta = 0$) there is a jump at the boundary, just as there should be. The conductivity random fields are known to be different on each side of the known boundary. Large σ_β, on the other hand, shows an influence of location uncertainty throughout the domain with a nearly linear trend in the gradient between the fixed boundary points. Of course, intermediate values of σ_β cause mean head gradients to fall between these two extremes.

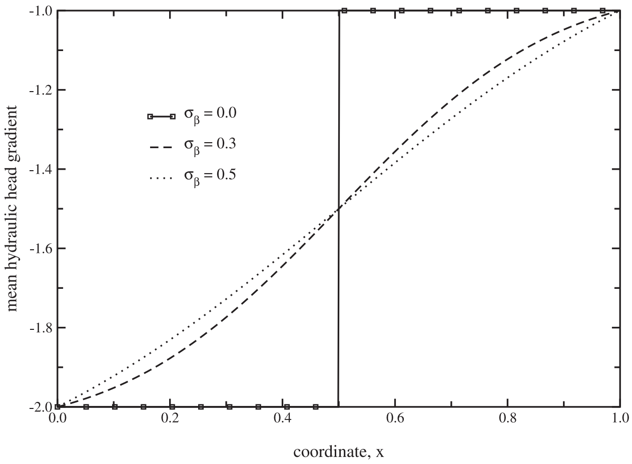

Figure 2. Mean head gradient distribution for $\overline{q}/K_{H_1} = 2$, $\overline{q}/K_{H_2} = 1$ and several values of the standard deviation σ_β.

[40] If the medium consists of a single material, (55) reduces to a well known relation [*Dagan*, 1989; and *Gelhar*, 1993]

$$\overline{h}(x) = \frac{\overline{q}}{K_H}(1 - x) \tag{56}$$

where $K_{H_1} = K_{H_2} \equiv K_H$

[41] By way of example, Figure 3 presents the one-dimensional version of (38) based on exponential covariance functions, $C_{Y_i}(x, y) = \sigma^2_{Y_i}\exp(-|x - y|/l_{Y_i})$ with the correlation length l_{Y_i} in the *i*th material. The boundary conditions dictate that variance is high on the constant flow boundary at $x = 0$ and is zero on the boundary at $x = 1$ where head is constant (Figure 3). This is the case even when there is no uncertainty about the position of the interface between materials ($\sigma^2_\beta = 0$). In Figure 3 the expected interface between the two different materials is at $x = 0.5$, so there is a clear distinction in head variance between the two materials when the location of the interface is certain. Figure 3 makes it clear that uncertainty about the location of the interface is an additional source of variability in our estimates of mean head. Interface uncertainty increases the head variance at every point in the interval (0, 1) relative to the fixed interface ($\sigma^2_\beta = 0$). The greater is our uncertainty about the location of β, the greater is the head variance. Of course head variance decreases no matter how large our uncertainty in the location of β as we approach the fixed head boundary at $x = 1$.

6. Summary

[42] We have analyzed flow in highly heterogeneous aquifers composed of distinct geological facies, or blocks. Our approach consists of representing such media as a doubly stochastic process that depends on (1) the random locations of block boundaries and (2) the random spatial distribution of hydraulic conductivity within a block. Hence the model explicitly includes uncertainty about the large-scale structure of heterogeneous media which is a source of variation that is usually excluded from analysis. This leads to statistically inhomogeneous random conductivity fields. Although more general formulations of inhomogeneous fields are possible, our model covers many cases of practical interest in groundwater hydrology. To illustrate our approach we derived an analytical solution for one-dimensional flow in a medium composed of two distinct blocks whose conductivities and contact point, i.e., boundary location, are random.

[43] Our approach provides a natural framework for incorporating the results of aquifer characterization in stochastic models. First, the method includes the kinds of spatially distributed material heterogeneities, especially uncertain block boundaries, that are found in most characterization studies. Second, error models for characterization techniques can be explicitly included in models of random block boundaries. And third, the outputs of different statistical characterizations can be combined probabilistically.

[44] The main technical contribution of our model is that it increases the range of applicability of perturbation expansions used in stochastic hydrogeology. These expansions are usually carried out in the variance of log-conductivity, which is therefore assumed to be small. However, the assumption of small variance becomes questionable in aquifers composed of many facies. In our approach, the perturbation parameters are the within-block conductivity variances which are much smaller than their homogeneous counterpart.

[45] We conclude by mentioning three outstanding issues we are currently investigating. First, we are evaluating the relative importance of the two types of uncertainty in different groundwater flow systems. It is obvious that in some flow systems structural uncertainty due to between-block boundaries dominates. For instance, the locations of pinchouts and high conductivity zones seem to be the main factors in determining flow in layered fractured media [*Gómez-Hernández and Wen*, 1998]. On the other hand, highly uniform media are most likely dominated by within-block variation. The analytical solution presented in Figure 3 suggests a method for comparing the possible behavior of flows in the more general, multidimensional media described by equation (38). Second, our model should allow us to investigate the relation between measurement volume

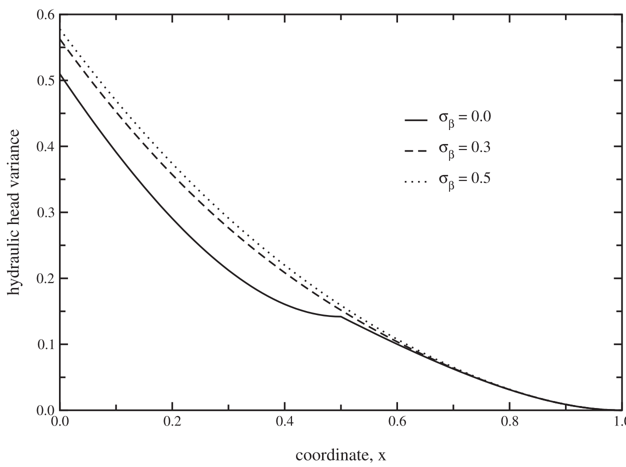

Figure 3. Hydraulic head variance for $\overline{q}^2\sigma^2_{Y_1}/K_{H_1} = 2$, $\overline{q}^2\sigma^2_{Y_2}/K_{H_2} = 1, l_{Y_1} = 0.5, l_{Y_2} = 0.25$ and several values of the standard deviation σ_β.

and scale of cross-block inhomogeneities. Since our model incorporates multiple spatial scales, it may provide a theoretical basis for the experimental results of *Tidwell and Wilson* [1999] who have found that hydraulic conductivity increases with support volume in some cases while in others it decreases. Third, we are currently extending our one-dimensional applications to more general examples through numerical simulations in multiple dimensions. The approach, which depends on Monte Carlo simulation of the integrals in (34) and (38), relies on the nonlocal finite element analysis introduced by *Guadagnini and Neuman* [1999].

Appendix A: Label and Boundary Processes

[46] A composite porous medium is made up of disjoint blocks of internally (statistically) uniform materials. We assume that sufficient geophysical data are available to characterize the boundary process. The boundary process is a probability measure on the set of possible boundaries, $\{\beta\} = \{\beta_1,\ldots, \beta_n\}$, between $n + 1$ blocks. Each β_i is a (possibly closed) surface in the aquifer Ω. When data is not available to characterize the material membership process, $P[\mathbf{x} \in M]$, the question arises how to obtain the membership process from the boundaries.

[47] Our model requires a given point, $\mathbf{x}$, to have only one label, i.e., $\Sigma_{i=1}^{n_M} P_i(\mathbf{x}) = 1$ where we suppose the medium is composed of n_M materials. This is different from dual-continuum models [e.g., *Gerke and van Genuchten*, 1993] in which points, corresponding to small volumes, may include several different types of material. We suppose that the space of membership functions is measurable with measure $P(M)$ so that

$$P[\mathbf{x}_1 \in M_1,\ldots,\mathbf{x}_m \in M_m] = \int_{\{M|(\mathbf{x}_1\in M_1,\ldots,\mathbf{x}_m\in M_m)\}} dP(M). \quad \text{(A1)}$$

Below we write $p(M)dM = dP(M)$ for convenience. Suppose a boundary is specified by a family of random set functions, β, with a joint measure $p(\beta)d\beta = dP(\beta)$. Obviously

$$P[\mathbf{x} \in M] = \int_{\{\beta|\mathbf{x}\in M\}} p(\beta)d\beta. \quad \text{(A2)}$$

Since (A2) is too abstract to be of much use, we examine two important special cases in the remainder of this section: stratified media and media with lense-like inclusions.

[48] In what follows, $\mathbf{x}$ may be a point in a one-dimensional ($\mathbf{x} = x$), two-dimensional ($\mathbf{x} = (x, z)^T$) and three dimensional ($(x, y, z)^T$) porous media, respectively; We suppose z is the vertical coordinate.

A1. Stratified Media

[49] Consider first, a perfectly stratified medium in which boundaries between material types are horizontal and the only uncertainty is the location of the boundary in the vertical direction. Suppose the medium has n_M parallel layers arranged vertically from the first at the bottom to the n_Mth at the top. This case is equivalent to a one-dimensional problem in which the boundaries, β_i, are points on the z-axis. The boundary process is defined by $p(\beta_1,\ldots, \beta_{n_M-1})$ the probability density that the ith boundary is located at β_i. Since there are $n_M - 1$ boundary points,

$$\begin{aligned} P_i(z) &= \frac{1}{N}P\left[\beta_1 < \ldots \beta_{i-1} < z < \beta_i < \ldots < \beta_{n_M-1}\right] \\ &= \frac{1}{N}\int_{-\infty}^{z} d\beta_1 \ldots \int_{\beta_{i-2}}^{z} d\beta_{i-1} \int_{z}^{\infty} d\beta_{n_M-1} \ldots \\ &\quad \int_{z}^{\beta_{i+1}} p\left(\beta_1,\ldots,\beta_{i-1},\beta_i,\ldots,\beta_{n_M-1}\right)d\beta_i. \end{aligned} \quad \text{(A3)}$$

The constraint that $\beta_i < \beta_{i+n}$ follows from the vertical ordering of the materials which restricts the portion of $\beta_1 \times \ldots \times \beta_{n_M-1}$ that is sampled. The normalizing constant,

$$\begin{aligned} N &= \int_{-\infty}^{\infty} d\beta_{n_M-1} \int_{-\infty}^{\beta_{n_M-1}} d\beta_{n_M-2} \ldots \int_{-\infty}^{\beta_2} p\left(\beta_1,\ldots,\beta_{n_M-1}\right)d\beta_1 \\ &= P\left[\beta_1 < \ldots < \beta_{n_M-1}\right], \end{aligned} \quad \text{(A4)}$$

reflects the ordering constraint. (A3) includes media with finite, but uncertain, upper and lower bounds, β_1 and β_{n_M-1}, since in that case it is actually possible that $\mathbf{x}$ lies outside (above or below) the medium entirely.

[50] In many cases, we can make the reasonable physical assumption that the boundaries are pair-wise independent, $p_{ij}(\beta_i, \beta_j) = p_i(\beta_i)p_j(\beta_j)$, because the location of a boundary in a stratified medium is essentially a result of (1) the times when the deposition process started and stopped and (2) the extent of erosion; and those events are all approximately independent. Then

$$\begin{aligned} P_i(z) &= \frac{1}{N}\int_{-\infty}^{z} p_1(\beta_1)d\beta_1 \ldots \int_{\beta_{i-2}}^{z} p_{i-1}d\beta_{i-1} \\ &\quad \int_{z}^{\infty} p_{n_M-1}d\beta_{n_M-1} \ldots \int_{z}^{\beta_{i+1}} p_i(\beta_i)d\beta_i. \end{aligned} \quad \text{(A5)}$$

This is, of course, a much more convenient form than (A3), and is one that will appear in many applications because the independence assumption is so often physically plausible.

[51] It is worth pointing out that (A3) actually defines a probability, since it is obvious that (1) $0 \le P_i \le 1$; (2) $P[\mathbf{x} \in M_i \cap \mathbf{x} \in M_j] = 0$ for $i \ne j$; and (3) it is tedious, but not too hard to show that $\Sigma_{i=1}^{M} P_i(\mathbf{x}) = 1$.

[52] The simplest case, a stratified medium composed of two materials with fixed (deterministic) upper (B_U) and lower (B_L) boundaries, and random interface, β, between the materials is often useful in applications. Here $P_1(\mathbf{x}) = P[z < \beta] = \int_z^{B_u} p(\beta)d\beta$ and $P_2(\mathbf{x}) = P[\beta < z] = \int_{B_L}^{z} p(\beta)d\beta$. Of course, it may be that $B_U \to \infty$ and $B_L \to -\infty$. When that is so and $\beta \sim N[\bar{\beta}, \sigma_\beta^2]$ is a normal random variate with mean $\bar{\beta}$ and variance σ_β^2, we have $P_1 = \frac{1}{2}\mathrm{erfc}\left(\frac{z-\bar{\beta}}{\sqrt{2}\sigma_\beta}\right)$.

[53] The case where the boundary process of a stratified medium is a random field, $\beta_i = \beta_i(\mathbf{u})$ ($\mathbf{u}$ being u_x or $(u_x, u_y)^T$ in two or three dimensions, respectively), is similar. To restrict discussion to stratified media, we require that $P[\beta_i(\mathbf{u}) \cap \beta_j(\mathbf{u})] = 0$ for all $i \ne j$ and at any $\mathbf{u}$. Porous media in which layers intersect should be modeled as lense-structured media. Geostatistics based on aquifer characterization studies can generally be used to parameterize $\beta_i = \beta_i(\mathbf{u}; W(\mathbf{u}))$, especially to derive means, $\bar{\beta}_i(\mathbf{u}; W(\mathbf{u}))$ and variances, $\sigma_{\beta_i}^2(\mathbf{u}; W(\mathbf{u}))$. In many cases, parameterization W

is either $W(\mathbf{u}) = W$, a constant set of parameters, or at least $\overline{W}(\mathbf{u}) = W$; also $\sigma^2_{\beta_i}(\mathbf{u}) = \sigma^2_{\beta_i}$, another constant, in many cases. Usually polynomials or trigonometric series will suffice to represent $\beta_i(\mathbf{u}; W)$. This requires that the distance between strata is large compared to our uncertainty about boundary locations, $\overline{\| \beta_i - \beta_j \|^2} \gg \max\left(\sigma^2_{\beta_i}, \sigma^2_{\beta_j}\right)$. As before

$$P_i(z) = P\left[\beta_1(\mathbf{u}; w_1) < \ldots < \beta_{i-1}(\mathbf{u}; w_{i-1}) < z < \beta_i(\mathbf{u}; w_i) < \ldots < \beta_{n_M-1}(\mathbf{u}; w_{n_M-1})\right] \tag{A6}$$

which is the analog of (A3) except now the boundary value depends on $\mathbf{u}$ explicitly.

[54] A particularly important example is a two-dimensional medium composed of two semi-infinite layers separated by a boundary, $\beta(x; W) = \overline{\beta}(x) + \epsilon$, that is the sum of a mean function, $\overline{\beta}(x)$, and a zero-mean constant-variance normal variate, $\epsilon \sim N\ [0, \sigma^2_\beta]$. Then $P[\mathbf{x} \in M_1] = P[z < \beta(x)] = \frac{1}{2}\mathrm{erfc}\left(\frac{z-\overline{\beta}}{\sqrt{2}\sigma_\beta}\right)$ is the probability that the point $\mathbf{x}$ is in material M_1, the lower layer.

A2. Lense-Structured Media

[55] In these models n discrete lenses, L_i ($i = 1, \ldots, n$), of one type of material (M_1) are embedded in another material (M_2). Each lens has a volume, V_i ($i = 1, \ldots, n$), within which $p_1(k_1, \ldots, k_m)$ is the finite-dimensional density for M_1 of conductivity at points $\mathbf{x}_1, \ldots, \mathbf{x}_m$ in L_i. The probability that a given point $\mathbf{x}$ is in the ith lense is $P[L_i] \equiv P[\mathbf{x} \in L_i]$, that $\mathbf{x}$ is both in the ith and the jth lenses is $P[L_iL_j]$, and so on. The total (random) volume occupied by M_1 is $V_1 = \cup_{i=1}^{n} V_i$. Extensions to systems composed of lenses of more than one type of material are obvious.

[56] For given n,

$$P_1(\mathbf{x}) = P[\mathbf{x} \in L_1 \cup \ldots \cup \mathbf{x} \in L_n] = \sum_{j=1}^{n} P\left[L_j\right] - \sum_{j}^{n} \sum_{i<j}^{n} P\left[L_iL_j\right] + \sum \sum_{i<j<k} \sum P\left[L_iL_jL_k\right] - \ldots + (-1)^n P[L_1L_2 \ldots L_n]. \tag{A7}$$

If the n lenses are pair-wise disjoint, (A7) reduces to

$$P_1(\mathbf{x}) = \sum_{j=1}^{n} P\left[L_j\right]. \tag{A8}$$

If, on the other hand, lense locations are pair-wise independent,

$$P_1(\mathbf{x}) = \sum_{j=1}^{n} P\left[L_j\right] - \sum_{i<j} \sum P[L_i]P\left[L_j\right] - \ldots + (-1)^n P[L_1]P[L_2] \ldots P[L_n]. \tag{A9}$$

In either case, $P_1(\mathbf{x})$ depends on just $P[L_j]$.

[57] In many applications, lenses can be modeled as random convex surfaces characterized by a random center of mass, $\mathbf{c}$, and the random distance, $D_\beta(\mathbf{c}, \Theta)$, from the center to a point β on the boundary. This distance depends on the angle Θ – in two dimensions $\Theta = \theta$ and in three dimensions $\Theta = (\theta, \phi)$ – between the center and the given boundary point. Spherical lenses do not depend on Θ.

[58] A point lies in a convex lense L_i with probability

$$P[\mathbf{x} \in L_i] = \int p_i(\mathbf{c})\mathcal{I}_i(\mathbf{c})d\mathbf{c} \qquad \mathcal{I}_i(\mathbf{c}) = \int_{\|\mathbf{x}-\mathbf{c}\|}^{\infty} p_i\left(D_\beta(\mathbf{c}, \Theta_\mathbf{x})|\mathbf{c}\right)dD_\beta. \tag{A10}$$

The inner integral $\mathcal{I}_i(\mathbf{c}) = P[\|\mathbf{x} - \mathbf{c}\| < D_\beta(\mathbf{c}, \Theta_\mathbf{x})|\mathbf{c}]$ probabilistically determines the shape of L_i, and is basically the same as the ones we dealt with in (A5) and (A6) except for the change to spherical coordinates and the dependence on (1) $\mathbf{c}$ and (2) the direction from $\mathbf{c}$ to $\mathbf{x}$ as measured by $\Theta_\mathbf{x}$.

[59] In some cases, more complex material boundaries can be satisfactorily approximated by sets of intersecting convex subblocks. Then (A8) does not apply, but the probability model can still be kept fairly simple if the (possibly) intersecting subblocks can be considered independent as in (A9). When block boundaries are too irregular to represent with intersecting subblocks, calculating $P[L_j]$ can be prohibitively complicated and may not be justified even if n is known. A homogeneous mixture model based on Q_i in (12) is probably suitable.

Appendix B: Derivation of Mean Flow Equations

[60] To derive $\hat{\mathbf{r}}_i(\mathbf{x})$, the residual flux conditioned on block membership, we begin by subtracting (23)–(27) from (18)–(22). This yields the boundary-value problem for head perturbations $h'(\mathbf{x})$,

$$\nabla \cdot \left[K_i \nabla h'_i + K'_i \nabla \hat{h}_i + \hat{\mathbf{r}}_i\right] + f' = 0 \qquad \mathbf{x} \in \Omega_i \tag{B1}$$

subject to the boundary

$$h'_i = H' \qquad \mathbf{x} \in \Gamma_D \tag{B2}$$

$$\left[K_i \nabla h'_i + K'_i \nabla \hat{h}_i + \hat{\mathbf{r}}_i\right] \cdot \mathbf{n} = Q' \qquad \mathbf{x} \in \Gamma_N \tag{B3}$$

and contact surface, Γ_{12}, conditions

$$h'_1 = h'_2 \qquad \mathbf{x} \in \Gamma_{12} \tag{B4}$$

$$\left[K_1 \nabla h'_1 + K'_1 \nabla \hat{h}_1 + \hat{\mathbf{r}}_1\right] \cdot \mathbf{n}_1 = \left[K_2 \nabla h'_2 + K'_2 \nabla \hat{h}_2 + \hat{\mathbf{r}}_2\right] \cdot \mathbf{n}_2 \qquad \mathbf{x} \in \Gamma_{12} \tag{B5}$$

We rewrite (B1) for the whole domain Ω

$$\nabla \cdot \left[K \nabla h' + K' \nabla \hat{h} + \hat{\mathbf{r}}\right] + f' = 0 \qquad \mathbf{x} \in \Omega \tag{B6}$$

where K and $\hat{\mathbf{r}}$ take the values of K_i and $\hat{\mathbf{r}}_i$ when $\mathbf{x} \in \Omega_i$. Then, multiplying (B6) by the Green's function $\mathcal{G}(\mathbf{y}, \mathbf{x})$ defined after (29) and integrating over Ω yields

$$\sum_{i=1}^{2} \int_{\Omega_i} \nabla_\mathbf{y} \cdot \left[K_i(\mathbf{y}) \nabla_\mathbf{y} h'(\mathbf{y})\right] \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} + \sum_{i=1}^{2} \int_{\Omega_i} \nabla_\mathbf{y} \cdot \left[K'_i(\mathbf{y}) \nabla_\mathbf{y} \hat{h}(\mathbf{y})\right] \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} + \sum_{i=1}^{2} \int_{\Omega_i} \nabla_\mathbf{y} \cdot \hat{\mathbf{r}}_i(\mathbf{y}) \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} + \int_{\Omega} f'(\mathbf{x}) \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} = 0. \tag{B7}$$

Applying Green's formula to the first integral, applying Green's identity to the remaining divergence integral, and recalling (B2), (B3), and the definition of $\mathcal{G}(\mathbf{y}, \mathbf{x})$ yields, for $\mathbf{x} \in \Omega_j$ ($j = 1, 2$),

$$
\begin{aligned}
h'(\mathbf{x}) = &- \sum_{i=1}^{2} \int_{\Omega_i} K_i'(\mathbf{y}) \nabla_{\mathbf{y}} \hat{h}(\mathbf{y}) \cdot \nabla_{\mathbf{y}} \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} \\
&- \sum_{i=1}^{2} \int_{\Omega_i} \hat{\mathbf{r}}_i(\mathbf{y}) \cdot \nabla_{\mathbf{y}} \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} \\
&- \sum_{i=1}^{2} \int_{\Gamma_{D_i}} H'(\mathbf{y}) K_i(\mathbf{y}) \mathbf{n}_i \cdot \nabla_{\mathbf{y}} \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} \\
&+ \sum_{i=1}^{2} \int_{\Gamma_{N_i}} Q_i'(\mathbf{y}) \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} + \int_{\Omega} f'(\mathbf{y}) \, \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} \\
&+ \int_{\Gamma_{12}^-} \mathbf{n}_1 \cdot \Big[K_1(\mathbf{y}) \nabla_{\mathbf{y}} h'(\mathbf{y}) + K_1'(\mathbf{y}) \nabla_{\mathbf{y}} \hat{h}(\mathbf{y}) \\
&+ \hat{\mathbf{r}}_1(\mathbf{y}) \Big] \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} \\
&+ \int_{\Gamma_{12}^+} \mathbf{n}_2 \cdot \Big[K_2(\mathbf{y}) \nabla_{\mathbf{y}} h'(\mathbf{y}) + K_2'(\mathbf{y}) \nabla_{\mathbf{y}} \hat{h}(\mathbf{y}) \\
&+ \hat{\mathbf{r}}_2(\mathbf{y}) \Big] \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} \\
&- \int_{\Gamma_{12}^-} \mathbf{n}_1 \cdot K_1(\mathbf{y}) \nabla_{\mathbf{y}} \mathcal{G}(\mathbf{y}, \mathbf{x}) h'(\mathbf{y}) d\mathbf{y} \\
&- \int_{\Gamma_{12}^+} \mathbf{n}_2 \cdot K_2(\mathbf{y}) \nabla_{\mathbf{y}} \mathcal{G}(\mathbf{y}, \mathbf{x}) h'(\mathbf{y}) d\mathbf{y}. \qquad \text{(B8)}
\end{aligned}
$$

Along Γ_{12}, $\mathbf{n}_1 = -\mathbf{n}_2$, and continuity conditions (B4)–(B5) and analogous conditions for $\mathcal{G}$ hold so that

$$
\begin{aligned}
h'(\mathbf{x}) = &- \sum_{i=1}^{2} \int_{\Omega_i} K_i'(\mathbf{y}) \nabla_{\mathbf{y}} \hat{h}(\mathbf{y}) \cdot \nabla_{\mathbf{y}} \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} \\
&- \sum_{i=1}^{2} \int_{\Omega_i} \hat{\mathbf{r}}_i(\mathbf{y}) \cdot \nabla_{\mathbf{y}} \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} \\
&- \sum_{i=1}^{2} \int_{\Gamma_{D_i}} H'(\mathbf{y}) K_i(\mathbf{y}) \mathbf{n}_i \cdot \nabla_{\mathbf{y}} \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} \\
&+ \sum_{i=1}^{2} \int_{\Gamma_{N_i}} Q_i'(\mathbf{y}) \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} \\
&+ \int_{\Omega} f'(\mathbf{y}) \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y}. \qquad \text{(B9)}
\end{aligned}
$$

Assuming that the driving forces f', H' and Q' are statistically independent from K_j', operating with $K_j'(\mathbf{x}) \nabla_{\mathbf{x}}$ and taking the ensemble mean leads directly to (28).

[61] Multiplying (B9) by $h'(\mathbf{y})$ and taking the ensemble mean, while retaining the first-order terms, give rise to (35). Multiplying (B9) by $K_i'(\mathbf{y})$ and following the analogous procedure yields to (36).

[62] Expanding the conditional mean flow equations (23)–(27) into powers of $\sigma_{Y_i}^2$ and collecting the terms of the same order leads to the following recursive set of boundary-value problems (for $n = 0, 1$),

$$\nabla \cdot \left[K_{G_i} \nabla \hat{h}_i^{(n)} \right] + \mathcal{F}_i^{(n)} = 0 \qquad \mathbf{x} \in \Omega_i \qquad \text{(B10)}$$

subject to the boundary,

$$\hat{h}_i^{(n)} = \mathcal{H}^{(n)} \qquad \mathbf{x} \in \Gamma_D \qquad \text{(B11)}$$

$$K_{G_i} \nabla \hat{h}^{(n)} \cdot \mathbf{n} = \mathcal{Q}^{(n)} \qquad \mathbf{x} \in \Gamma_N, \qquad \text{(B12)}$$

and contact surface conditions ($\mathbf{x} \in \Gamma_{12}$)

$$\hat{h}_1^{(n)} = \hat{h}_2^{(n)} \qquad \text{(B13)}$$

$$K_{G_1} \nabla \hat{h}_1^{(n)} \cdot \mathbf{n}_1 + \mathcal{S}_1^{(n)} = K_{G_2} \nabla \hat{h}_2^{(n)} \cdot \mathbf{n}_2 + \mathcal{S}_2^{(n)} \qquad \text{(B14)}$$

where

$$\mathcal{F}_i^{(0)}(\mathbf{x}) = \bar{f}(\mathbf{x})$$

$$\mathcal{F}_i^{(1)}(\mathbf{x}) = \nabla \cdot \mathbf{F}_i(\mathbf{x})$$

$$\mathbf{F}_i(\mathbf{x}) = K_{G_i} \frac{\sigma_{Y_i}^2}{2} \nabla \hat{h}_i^{(0)}(\mathbf{x}) - \hat{\mathbf{r}}_i^{(1)}(\mathbf{x}) \qquad \text{(B15)}$$

$$\mathcal{H}_i^{(0)}(\mathbf{x}) = \overline{H}(\mathbf{x}) \qquad \mathcal{H}_i^{(1)}(\mathbf{x}) = 0 \qquad \text{(B16)}$$

$$\mathcal{Q}_i^{(0)}(\mathbf{x}) = \overline{Q}(\mathbf{x}) \qquad \mathcal{Q}_i^{(1)}(\mathbf{x}) = -\mathbf{n} \cdot \mathbf{F}_i(\mathbf{x}) \qquad \text{(B17)}$$

and

$$\mathcal{S}_i^{(0)}(\mathbf{x}) = 0 \qquad \mathcal{S}_i^{(1)}(\mathbf{x}) = \mathbf{n} \cdot \mathbf{F}_i(\mathbf{x}). \qquad \text{(B18)}$$

[63] One can solve the above boundary-value problems by a variety of methods. Since $G(\mathbf{y}, \mathbf{x})$ is already known, we write the solutions as (32) and (33).

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