

Mean Flow in Composite Porous Media

C. L. Winter and Daniel M. Tartakovsky

Computer Research and Applications Group (CIC-3) and Center for Nonlinear Studies, Los Alamos National Laboratory

Abstract. We develop probabilities and statistics for the parameters of Darcy flows through saturated porous media composed of units of different materials. Our probability model has two levels. On the local level, a porous medium is composed of disjoint, statistically homogeneous volumes (or blocks) each of which consists of a single type of material. On a larger scale, a porous medium is an arrangement of blocks whose extent and location are uncertain. Using this two-scaled model, we derive general formulae for the probability distribution of hydraulic conductivity and its mean; then we develop general perturbation expansions for mean head. We express distributions and parameters in terms of mixtures of locally homogeneous block densities weighted by large-scale block membership probabilities.

1. Introduction

Hydrogeologists use Darcy's Law to model the flow of water through saturated porous media. In a steady-state regime without sources or sinks, Darcy's Law coupled with conservation of mass yields the flow equation (FE), $\nabla \cdot [K(\mathbf{x})\nabla h(\mathbf{x})] = 0$. If hydraulic conductivity K be known at every point \mathbf{x} , FE (supplemented with appropriate boundary conditions) provides the hydraulic head distribution, $h(\mathbf{x})$. However, groundwater applications of FE are often complicated by a high degree of spatial variability in K combined with limited sampling. This leads to uncertainty in the values of $K(\mathbf{x})$ and thus, of $h(\mathbf{x})$. It has become common [Dagan, 1989; Gelhar, 1993; Dagan and Neuman, 1997] in groundwater models to quantify this uncertainty by treating K and h as random fields. Since this renders FE stochastic, the problem of solving it becomes the problem of determining the probability density function (*pdf*) of h or its ensemble moments. In this paper we concentrate on estimating the first such moment, mean head $\bar{h}(\mathbf{x})$.

In most studies, $K(\mathbf{x}) = \bar{K}(\mathbf{x}) + K'(\mathbf{x})$ is represented as the sum of a mean, $\bar{K}(\mathbf{x})$, and a zero-mean random deviation, $K'(\mathbf{x})$. The overbar, indicates the operation of taking the expected value, or ensemble mean. Similarly, $h(\mathbf{x}) = \bar{h}(\mathbf{x}) + h'(\mathbf{x})$. Hence, taking the ensemble mean of FE gives

$$\nabla \cdot [\bar{K}(\mathbf{x}) \nabla \bar{h}(\mathbf{x})] + \nabla \cdot \overline{K'(\mathbf{x}) \nabla h'(\mathbf{x})} = 0. \quad (1)$$

Solving for $\bar{h}(\mathbf{x})$ requires estimating the mean hydraulic conductivity, $\bar{K}(\mathbf{x})$, and evaluating the residual flux, $\bar{\mathbf{r}}(\mathbf{x}) = -\overline{K'(\mathbf{x}) \nabla h'(\mathbf{x})}$. While different approximations of the residual flux $\bar{\mathbf{r}}$ have been proposed all of them employ perturbation expansions based on the variance σ_Y^2 of log con-

ductivity, $Y(\mathbf{x}) = \ln K(\mathbf{x})$. This approach works well so long as σ_Y^2 is small, *i.e.* the geological formation is "mildly" heterogeneous.

The assumption of mild heterogeneity is reasonable for aquifers composed of a single geological unit, where it seems plausible that the values of $Y(\mathbf{x})$ will fall within a narrow range. This is frequently used to justify the further assumption that the permeability field is weakly homogeneous, *i.e.* that \bar{K} and σ_Y^2 are constants. A considerable literature has grown up that treats Darcy flows in statistically homogeneous media.

This traditional approach might fail when different geologic facies are present. At larger scales conductivity statistics may be affected by differences among various geological units. Deriving constant mean conductivity \bar{K} from available hard data (measurements of K at points \mathbf{x}_i within different geological facies) can result in large variance σ_Y^2 . This, in turn, makes applicability of the usual perturbation approximations questionable.

We present a composite medium model for dealing with such geological formations. The advantages of our model over the homogeneous approach are twofold: Technically, the model allows sharper closures for perturbation expansions within statistically homogeneous blocks. Physically, we can use the composite model to evaluate the effects of structural heterogeneity on differential flow paths. This is impossible with the homogeneous model which washes out structural variability. Equally important, our composite model provides an explicit expression for uncertainty near boundaries.

The essence of our paper is that we can reduce errors in our estimates of $\bar{K}(\mathbf{x})$ and $\bar{\mathbf{r}}(\mathbf{x})$ by accounting for the (uncertain) geometry of various geological units. Our approach is applicable to a large class of highly heterogeneous, composite porous media: those that consist of disjoint geological facies. The proposed model is based on two random processes, (*i*) a large-scale process defining the spatial distribution of geological units, and (*ii*) a within-unit process specifying $K(\mathbf{x})$ for each material. The spatial distribution of facies is defined by $P[\mathbf{x}_1 \in M_1, \dots, \mathbf{x}_n \in M_n]$, the probability that the points $\mathbf{x}_1, \dots, \mathbf{x}_n$ are labeled by material types M_1, \dots, M_n or, equivalently, by $P[\beta_{ij}(\mathbf{x})]$, the probability that the boundary between materials M_i and M_j is the surface $\beta_{ij}(\mathbf{x})$. Within a block of given material type M , the homogeneous *pdf*, $p_M(k_1, \dots, k_n)$, specifies the likelihood that K takes values k_1, \dots, k_n at points $\mathbf{x}_1, \dots, \mathbf{x}_n$. We suppose the usual assumptions of stochastic hydrogeology hold: The statistics of the block geometry (for instance, the stratigraphy) are known, as are the homogeneous densities, p_M , for material types, and $\sigma_{Y_M}^2$ is small within materials.

We demonstrate that $\bar{K}(\mathbf{x})$ and $\bar{\mathbf{r}}(\mathbf{x})$ can be approximated by weighting within-block statistics or *pdfs*, p_M , with

the spatial distribution process, P . By doing so, we can calculate our statistics in two stages, first by conditioning on material type and then by calculating a marginal over all types. The first stage allows us to use traditional approaches and results based on small perturbations (e.g., Tartakovsky and Neuman, 1998) since boundaries are fixed at this stage. Moreover, our approach enables us to use relatively small within-block values of $\sigma_{Y_M}^2$ to expand $\bar{\mathbf{F}}(\mathbf{x})$ which greatly extends the range of applicability of perturbation expansions.

The composite medium model provides a natural framework for incorporating the results of aquifer characterization (soft data) in stochastic models since the method includes the kinds of spatially distributed material heterogeneities that are found in most characterization studies. Error models from characterization techniques can be explicitly included in P or, equivalently, in models of random block boundaries. Additionally, the outputs of different characterizations can be combined using standard techniques like Bayesian updating since the block-averaging model is probabilistic.

Our statistically heterogeneous model differs from the models of *Rajaram and McLaughlin* [1990] and *Indelman and Rubin* [1995], who superimposed deterministic trends on homogeneous random fields. Since our model allows for various correlation structures in different geological facies, it accommodates the geophysical phenomena that produce statistically distinct facies. Moreover, our model incorporates uncertainty in the facies geometry which can be important for proper estimation of system states. Our approach 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.

2. Conductivity Statistics

In general, geological formations consist of various facies, each facies having its own (multivariate) random permeability field determined by a probability density. Here we consider formations composed of only two types of material for simplicity, since extensions to multiple materials are obvious. A point, \mathbf{x} , of the medium lies in material M_1 with probability $P_1(\mathbf{x}) = P[\mathbf{x} \in M_1]$ and in material M_2 with probability $P_2(\mathbf{x}) = P[\mathbf{x} \in M_2] = 1 - P_1(\mathbf{x})$. Following the classical homogeneous approach in stochastic hydrogeology, we suppose that within each facies, M_i ($i = 1, 2$), distributions $p_i(k) = p_{M_i}(k(\mathbf{x}))$ are homogeneous. To simplify the notation, we drop the dependence of k on location below except where it is needed for clarity.

The conductivity *pdf* for the entire medium, $p(k)$, is the marginal of $p(k, M) = p(k|M)P[M]$. Since the conditional probability fixes the labeling, $p(k|M) = I_1(\mathbf{x}; M)p_1(k) + I_2(\mathbf{x}; M)p_2(k)$ where the indicator function $I_i(\mathbf{x}; M) = 1$ if $\mathbf{x} \in M_i$ and is 0 otherwise. Thus, $p(k) = p_1(k)P_1(\mathbf{x}) + p_2(k)P_2(\mathbf{x})$ is the location-dependent mixture of the within-unit densities, p_1 and p_2 , where the weighting function is the probability, P_i , of block membership. Note that $p(k)$ is valid for multiple dimensions. When the point \mathbf{x} is deep within block M_i , $P_i \cong 1$ and $p(k) \cong p_i(k)$. As \mathbf{x} approaches a boundary between the materials, $p(k)$ approaches the average of p_1 and p_2 . It follows from elementary properties of mixtures that the ensemble average of $K(\mathbf{x})$ must be a weighted sum of the (constant) means, \bar{K}_j , in the two ma-

terial types,

$$\bar{K}(\mathbf{x}) = \bar{K}_1 P_1(\mathbf{x}) + \bar{K}_2 P_2(\mathbf{x}). \quad (2)$$

Since the weights depend on the location, \mathbf{x} , it is clear that $\bar{K}(\mathbf{x})$ is not constant. We have also derived space-dependent variance and two-point correlation functions.

It is worthwhile to mention here that applications of the indicator functions for describing flow and transport in composite materials is not new [*Rubin*, 1995]. The novelty of our approach consists of (i) establishing the equivalency between the indicator functions and boundary processes and (ii) using the latter to derive in the following sections the closed-form moments equations for the system states.

3. Residual Flux

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 surface, $\beta(\mathbf{x})$, between them. More complicated cases are easy to derive from this one. Then the labeling process is fully defined by the boundary process so that density, $p(k)$, becomes the marginal of $p(k, \beta) = p(k|\beta)p(\beta)$. Suppose for the moment that $\beta(\mathbf{x})$ is fixed, so we know the volumes, Ω_1 and Ω_2 , occupied by M_1 and M_2 , respectively. Accounting for continuity of heads and fluxes along the boundary $\beta(\mathbf{x})$, and assuming for the sake of simplicity that hydraulic properties of the two materials are uncorrelated, we derive (following *Tartakovsky and Neuman* [1998]) an approximation of the residual flux conditioned on β ,

$$\frac{\bar{\mathbf{r}}_i^{(1)}(\mathbf{x}|\beta)}{K_{G_i}^2} = \int_{\Omega_i} C_{Y_i}(\mathbf{x}, \mathbf{y}) \nabla_{\mathbf{y}} \nabla_{\mathbf{x}}^T G(\mathbf{y}, \mathbf{x}) \mathbf{J}(\mathbf{y}) d\mathbf{y}. \quad (3)$$

Here K_{G_i} is the geometric mean of K_i ; $C_{Y_i}(\mathbf{x}, \mathbf{y})$ denotes the two-point covariance function; the Green's function $G(\mathbf{y}, \mathbf{x})$ satisfies FE with $K(\mathbf{x})$ replaced by K_{G_1} for $\mathbf{x} \in \Omega_1$ and K_{G_2} for $\mathbf{x} \in \Omega_2$; and $\mathbf{J}(\mathbf{x})$ is the hydraulic head gradient resulting from such substitution.

The approximation of the residual flux (3) is based on an asymptotic expansion in powers of $\sigma_{Y_i}^2$. The superscript of $\bar{\mathbf{r}}_j^{(1)}$ indicating the first term in this expansion. The perturbation expansion does not affect the operation of taking the expected value of $\bar{\mathbf{F}}(\mathbf{x}|\beta)$ with respect to β , so the residual flux in (1) has the form

$$\bar{\mathbf{F}}(\mathbf{x}) \cong \int \left[\bar{\mathbf{r}}_1^{(1)}(\mathbf{x}|\beta) + \bar{\mathbf{r}}_2^{(1)}(\mathbf{x}|\beta) \right] p(\beta) d\beta. \quad (4)$$

This integral can be evaluated either analytically, or numerically by Monte Carlo simulations. The former is feasible when we can obtain explicit expressions for $\bar{\mathbf{r}}_i$ in terms of β , as is the case in our 1-D example. In the latter approach, the surface $\beta(\mathbf{x})$ can be represented by polynomials or trigonometric series with random coefficients. In particular, useful case occurs when $\beta(\mathbf{x}) = \bar{\beta}(\mathbf{x}) + \epsilon$ is the sum of a deterministic mean, $\bar{\beta}(\mathbf{x})$, and a normal variate $\epsilon \in N[0, \sigma_\epsilon^2]$.

The advantage of breaking $\bar{\mathbf{F}}(\mathbf{x}|\beta)$ into $\bar{\mathbf{r}}_1$ and $\bar{\mathbf{r}}_2$ is that perturbation expansions can be taken separately for each in terms of $\sigma_{Y_1}^2$ and $\sigma_{Y_2}^2$ which are usually much smaller than σ_Y^2 .

4. Homogeneous Approximation

The homogeneous approximation arises when we take a random sample from Ω of measurements of K without regard

to their membership in a material M_i . The homogeneous approximation of the residual flux $\bar{\mathbf{f}}(\mathbf{x})$ is based on perturbation in the total variance of log-conductivity Y [Tartakovsky and Neuman, 1998]. The latter is given by

$$\sigma_Y^2 = Q\sigma_{Y_1}^2 + (1-Q)\sigma_{Y_2}^2 + Q(1-Q)(\bar{Y}_1 - \bar{Y}_2)^2 \tag{5}$$

where Q is the probability that a point is of type M_1 regardless of its location. It is clear that Q does not depend on location, so that σ_Y^2 is uniform throughout the whole flow domain Ω in the homogeneous approximation. Furthermore, σ_Y^2 will usually be large even if each material is mildly heterogeneous ($\sigma_{Y_i}^2 < 1, i = 1, 2$) since \bar{Y}_1 and \bar{Y}_2 are quite different due to differences between the two materials (e.g. sand and clay). An equation analogous to (5) was derived in [Rubin, 1995] for conductivity fields with bi-modal distributions.

5. Computational Examples

We illustrate advantages of the proposed approach by consider two examples which deal with one- and two-dimensional steady-state flows in composite media. The one-dimensional example serves to demonstrate explicitly the increased robustness of the proposed perturbation expansions, while the two-dimensional example demonstrates how our approach can be realized numerically.

5.1 One-dimensional flow

Consider a medium consisting of two materials with random hydraulic conductivities $K_1(x)$ and $K_2(x)$ connected at a random point β . Since the one-dimensional medium is bounded, we may as well suppose it is $[0, 1]$. Let β be a normally distributed random variable with mean $\bar{\beta}$ and variance σ_β^2 that has been truncated to fit on $[0, 1]$. Constant flux q_0 is prescribed at the boundary $x = 0$, and zero hydraulic head is maintained at the boundary $x = 1$.

Under these conditions, (1) can be solved exactly and also by the perturbation analysis described in the previous sections. The exact solution leads to the effective conductivities

given by harmonic means, $K_{H_i} = K_{G_i} \exp(-\sigma_{Y_i}^2/2)$, for each material ($i = 1, 2$); while the perturbation solution gives rise to the following approximations, $K_{H_i} \approx K_{G_i}(1 - \sigma_{Y_i}^2/2)$. On the other hand, a homogeneous description of the porous medium results in the global effective conductivity given by the harmonic mean, $K_H = K_G \exp(-\sigma_Y^2/2)$, and the corresponding perturbation expansion of the exponent in variance σ_Y^2 which is given by (5). Clearly, such perturbation solutions would work as long as $\sigma_{Y_i}^2, \sigma_Y^2 \ll 2$. As was demonstrated above, while the condition $\sigma_{Y_i}^2 \ll 2$ is reasonable for most geological settings, the condition $\sigma_Y^2 \ll 2$ is not.

5.2 Two-dimensional flow

For most multi-dimensional flow problems exact closed-form analytical solutions are not available, and one has to solve the perturbation equations numerically. We do so below for steady-state flow through the domain composed of an inner square with random hydraulic conductivity K_2 embedded in an outer square with random conductivity K_1 ($K_2 \ll K_1$). Constant heads are imposed on the vertical sides of the outer square, while the other two sides are impermeable. (We plan to investigate more complex geometries in the future.) The half-length of the outer square is taken to be $a = 6$, while the half-length of the inner square b is taken to be a log-normally distributed random variable with mean $\bar{b} = 1.2$ and variance σ_b^2 that has been truncated to fit on $[0, 6]$.

Details of the numerical evaluation of (3) and (4) in multiple dimensions will be presented elsewhere (Guadagnini, Tartakovsky and Winter, in preparation). Here we provide a brief overview of the numerical procedure: (i) the flow domain is discretized so that the mean boundary of the inner square ($\bar{b} = 1.2$) fits the numerical mesh; (ii) a number of realizations of b are generated using a re-normalized distribution in order to evaluate the random integral (4). This re-normalization is performed to insure that all realizations of b conform to the grid; (iii) for all realizations of b the corresponding Green's functions, G , and conditional residual fluxes (3) are calculated following Guadagnini and Neuman [1999]; (iv) the conditional residual flux is averaged over all realizations of b to obtain (4); and, finally, (v) the mean flow equation (1) is solved to provide the mean pressure distribution, $\bar{h}(x_1, x_2)$. The latter is found to be in perfect agreement with Monte Carlo simulations.

An example of such calculations is given in Figure 1 which shows the mean head distributions in the longitudinal cross-sections ($x_2 = 6$) of the flow domain. Uncertainty about the size of the inner square clearly affects mean head, \bar{h} . The magnitude of σ_β , the standard deviation of $\beta = \ln b$, is a measure of size uncertainty. Large σ_β leads to an almost linear trend in the longitudinal cross-section of mean head 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, $P[x \in M_1] \approx P[x \in M_2]$.

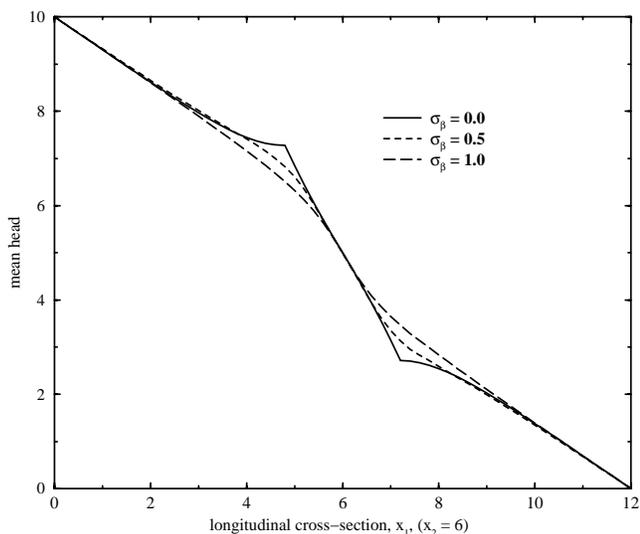


Figure 1. Mean hydraulic head distribution in the longitudinal cross-section ($x_2 = 6$) of the flow domain for several values of the standard deviation σ_β .

Acknowledgments. We are grateful to Len Margolin for initial discussions. This work was supported by Los Alamos National Laboratory under LDRD 98604.

The Editor and the authors would like to thank the reviewers of this manuscript.

References

- Dagan, G. *Flow and Transport in Porous Formations*, 465 pp., Springer-Verlag, New York.
- Dagan, G. and S.P. Neuman (editors), *Subsurface Flow and Transport: the Stochastic Approach*, Proc. 2nd Kovacs Colloquium, Intern. Hydrological Programme of UNESCO, Paris, France, January 26-28, 1997.
- Deutsch, C.V. and A.G. Journel. *Geostatistical Software Library and User's Guide*, 340 pp., Oxford University Press, New York, 1992.
- Gelhar, L.W. *Stochastic Subsurface Hydrology*, 390 pp., Prentice-Hall, New Jersey, 1993.
- Guadagnini, A. and S.P. Neuman, Nonlocal and localized analyses of conditional mean steady-state flow in bounded, randomly nonuniform domains, 1. Theory and computational approach. *Water Resour. Res.*, 35, 2999-3018, 1999.
- Indelman, P. and Y. Rubin, Flow in heterogeneous media displaying linear trend in the log conductivity. *Water Resour. Res.*, 31, 1257-1265, 1995.
- Rajaram, H. and D. McLaughlin, Identification of large-scale spatial trends in hydrologic data. *Water Resour. Res.*, 26, 2411-2423, 1990.
- Rubin, Y., Flow and transport in bimodal heterogeneous formations, *Water Resour. Res.*, 31, 2461-2468, 1995.
- Tartakovsky, D.M., and S.P. Neuman, Transient flow in bounded randomly heterogeneous domains: 1. Exact conditional moment equations and recursive approximations. *Water Resour. Res.*, 34, 1-12, 1998.

D. M. Tartakovsky and C. L. Winter, Computer Research and Applications Group (CIC-3), MS B256, Los Alamos National Laboratory, Los Alamos, NM 87545. (e-mail:dmt@lanl.gov; winter@lanl.gov)

(Received September 7, 1999; revised January 18, 2000; accepted April 14, 2000.)