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Statistics of Block Conductivity Through a Simple Bounded Stochastic Medium

GORDON A. FENTON

Department of Applied Mathematics, Technical University of Nova Scotia, Halifax, Canada

D. V. GRIFFITHS

Department of Engineering, University of Manchester, Manchester, England

A Monte Carlo approach is employed to estimate the distribution of an equivalent conductivity measure, the block conductivity, which characterizes the total flow rate through a two-dimensional bounded domain and which is itself a random variable. Chi-square goodness-of-fit tests indicate that the lognormal distribution is an appropriate choice for the block conductivity distribution. For square domains, the mean and variance of the block conductivity are seen to be closely approximated using the statistics of local averages of log conductivity.

1. INTRODUCTION

In this study seepage through a two-dimensional soil model with spatially random conductivity is considered via simulation. The quantities of interest are the total steady state flow rate through the medium and a block conductivity measure which characterizes this flow rate. For a two-dimensional isotropic heterogeneous medium the equation of steady groundwater flow followed is Laplace's equation,

$$\nabla \cdot [K \nabla \phi] = 0 \tag{1}$$

where K is the hydraulic conductivity and ϕ is the hydraulic head. No internal sources or sinks are considered. The site model considered, as illustrated in Figure 1, has impervious upper and lower boundaries and constant head applied to the right edge so that the mean flow is unidirectional. At this time the scope of the study is restricted to the two-dimensional case with these simple boundary conditions.

In that the interest is to predict flow rates through a bounded site having spatially random conductivity, block conductivity will be defined here on the basis of total flow rates. Specifically, for a particular realization of the spatially random conductivity, $K(\mathbf{x})$, on a given boundary value problem, the block conductivity, $\bar{K}$, is defined as

$$\bar{K} = \mu_k \left(\frac{Q}{Q_{\mu_k}} \right) \tag{2}$$

where $\mu_k = E[K]$ is the expected value of $K(\mathbf{x})$, Q is the total flow rate through the spatially random conductivity field, and Q_{μ_k} is the deterministic total flow rate through the mean conductivity field (having constant conductivity μ_k throughout the domain). For the simple boundary value problem under consideration, (2) reduces to

$$\bar{K} = \left(\frac{X_L}{Y_L} \right) \left(\frac{Q}{H} \right) \tag{3}$$

where H is the (deterministic) head difference between upstream and downstream faces. Since Q is dependent on $K(\mathbf{x})$, both Q and $\bar{K}$ are random variables, and it is the distribution of $\bar{K}$ that is of interest in this study. The definition of block conductivity used here essentially follows that of *Rubin and Gómez-Hernández* [1990] for a single block. Once the distribution of $\bar{K}$ is known, (3) is easily inverted to solve for the distribution of Q.

In the case of unbounded domains, considerable work has been done in the past few years to quantify a deterministic effective conductivity measure K_{eff} as a function of the mean and variance of ln K at a point. In one dimension, the effective conductivity is the harmonic mean (flow through a "series" of "resistors") while in two dimensions the effective conductivity is the geometric mean [*Matheron*, 1967]. For three dimensions *Gutjahr et al.* [1978] and *Gelhar and Axness* [1983] used a small-perturbation method valid for small variances in an unbounded domain. Specifically, for n dimensions,

$$K_{\text{eff}} = [\exp(\mu_{\ln K})] \left(1 - \frac{\sigma^2_{\ln K}}{2} \right) \qquad n = 1 \tag{4a}$$

$$K_{\text{eff}} = \exp(\mu_{\ln K}) \qquad n = 2 \tag{4b}$$

$$K_{\text{eff}} \simeq [\exp(\mu_{\ln K})] \left(1 + \frac{\sigma^2_{\ln K}}{6} \right) \qquad n = 3 \tag{4c}$$

where $\mu_{\ln K}$ and $\sigma^2_{\ln K}$ are the mean and variance of ln K respectively. Concerning higher-order moments, *Dagan* [1979] used a self-consistent model to estimate head and specific discharge variance for one-, two-, and three-dimensional flow in an infinite domain. *Smith and Freeze* [1979] investigated head variability in a finite two-dimensional domain using Monte Carlo simulation.

Dykaar and Kitanidis [1992*a*, *b*] present a method for finding K_{eff} in a bounded domain using a spectral decomposition approach. The variance of block conductivity is considered only briefly, through the use of simulations produced using fast Fourier transforms (FFT), to establish estimates of the averaging volume needed to reduce the variance to a negligible amount. No attempt was made to quantify the

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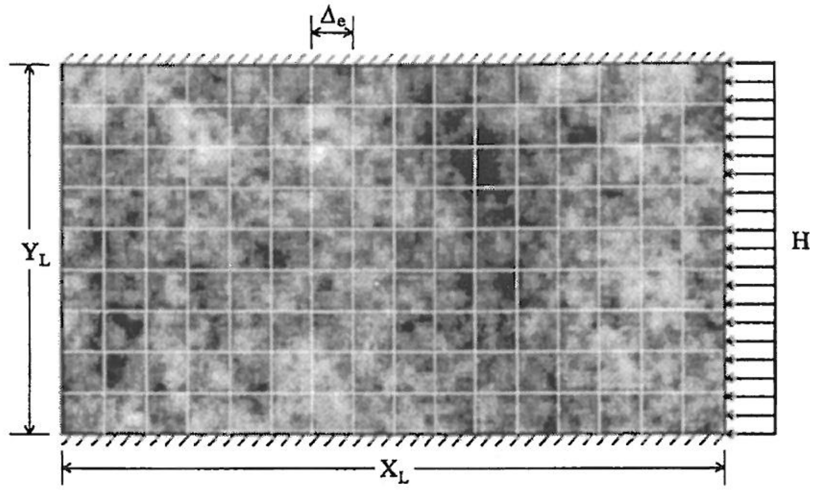

Fig. 1. Two-dimensional finite element model of soil mass having spatially random conductivity. Top and bottom surfaces are assumed impervious, and a constant head is applied to the right face.

variance of block conductivity. In perhaps the most pertinent work to this study, *Rubin and Gómez-Hernández* [1990] obtained analytical expressions for the mean and variance of block conductivity using perturbative expansions valid for small conductivity variance and based on some infinite-domain results. A first-order expansion was used to determine the block conductivity covariance function.

In agreement with previous studies by *Journel* [1980], *Freeze* [1975], *Smith and Freeze* [1979], *Rubin and Gómez-Hernández* [1990], *Dagan* [1979, 1981, 1986], it is assumed here that $Y = \ln K$ is an isotropic stationary Gaussian random field fully characterized by its mean $\mu_{\ln K}$, variance $\sigma^2_{\ln K}$ and correlation function $\rho_Y(\tau)$. This assumption is basically predicated on the observation that field measurements of conductivity are approximately lognormally distributed as shown by *Hoeksema and Kitanidis* [1985] and *Sudicky* [1986].

To solve (1) for the boundary value problem of Figure 1, the domain is discretized into elements of dimension $\Delta_1 \times \Delta_2$ (where $\Delta_1 = \Delta_2 = \Delta_e$ herein) and analyzed using the finite element method [*Smith and Griffiths*, 1988]. A realization of the random field $Y(\mathbf{x})$ is then generated using the local average subdivision method [*Fenton*, 1990; *Fenton and Vanmarcke*, 1990] and conductivities are assigned to individual elements using $K = e^Y$ (the conductivity within each element is assumed constant). The total flow rate computed for this field can be used in (3) to yield a realization of the block conductivity. Histograms of the block conductivities are constructed by carrying out a large number of realizations for each case considered.

2. Parameters and Finite Element Model

To investigate the effect of the form of the correlation function on the statistics of $\bar{K}$, three correlation functions were employed, all having exponential forms:

$$\rho^a_Y(\tau) = \exp\left\{-\frac{2}{\theta}(\tau_1^2 + \tau_2^2)^{1/2}\right\} \tag{5a}$$

$$\rho^b_Y(\tau) = \exp\left\{-\frac{\pi}{\theta^2}(\tau_1^2 + \tau_2^2)\right\} \tag{5b}$$

$$\rho^c_Y(\tau) = \exp\left\{-\frac{2}{\theta}(|\tau_1| + |\tau_2|)\right\} \tag{5c}$$

The first form is based on the findings of *Hoeksema and Kitanidis* [1985] but without the nugget effect which *Dagan* [1986] judges to have only a minor contribution when local averaging is involved. Notice that the second and third forms are separable and that the third form is not strictly isotropic. Each is characterized by a scale of fluctuation θ defined by *Vanmarcke* [1984] for an isotropic process to be

$$\theta = \int_{-\infty}^{\infty} \rho(\tau)\, d\tau = 2\int_0^{\infty} \rho(\tau)\, d\tau \tag{6}$$

where $\tau = |\boldsymbol{\tau}|$ in (5*a*) and (5*b*). In (5*c*), θ is taken as a directional scale of fluctuation so that, making use of separability,

$$\theta = 2\int_0^{\infty} \exp\left\{-\frac{2}{\theta}|\tau|\right\} d\tau. \tag{7}$$

The scale of fluctuation is generally interpreted as the separation distance beyond which points in the field become effectively uncorrelated.

As an alternative to the correlation function, the variance function, $\gamma(\Delta_1, \Delta_2)$, is defined by *Vanmarcke* [1984] to be

$$\gamma(\Delta_1, \Delta_2) = \frac{4}{(\Delta_1\Delta_2)^2}\int_0^{\Delta_1}\int_0^{\Delta_2} (\Delta_1 - \tau_1)(\Delta_2 - \tau_2)\rho_Y(\tau_1, \tau_2)\, d\tau_1\, d\tau_2 \tag{8}$$

The variance function reflects the reduction in variance which occurs when a random field is averaged over some rectangular domain, $\Delta_1 \times \Delta_2$. The variance functions corresponding to ρ_Y^a, ρ_Y^b, and ρ_Y^c are given by γ^a, γ^b, and γ^c, respectively, in the appendix.

It is well known that the block conductivity ranges from the harmonic mean in the limit as the aspect ratio X_L/Y_L of the site tends to infinity to the arithmetic mean as the aspect ratio reduces to zero. To investigate how the statistics of $\bar{K}$ change with practical aspect ratios, the study was conducted for ratios $X_L/Y_L \in \{1/9, 1, 9\}$. For an effective site dimension $D = (X_L Y_L)^{1/2}$, the ratio θ/D was varied over the interval [0.008, 4]. Four different coefficients of variation were considered; $\sigma_k/\mu_k \in \{0.5, 1.0, 2.0, 4.0\}$ corresponding to $\sigma^2_{\ln K} \in \{0.22, 0.69, 1.61, 2.83\}$. It was felt that this represented enough of a range to establish trends without greatly compromising the accuracy of statistical estimates (as $\sigma^2_{\ln k}$ increases, more realizations would be required to attain a constant level of accuracy).

As mentioned, individual realizations were analyzed using the finite element method (with four-node quadrilateral elements) to obtain the total flow rate through the domain. For each set of parameters mentioned above, 2000 realizations were generated and analyzed. No explicit attempt was made to track matrix condition numbers, but all critical calculations were performed in double precision and round-off errors were considered to be negligible.

3. Discussion of Results

The first task undertaken was to establish the form of the distribution of block conductivity $\bar{K}$. Histograms were plotted for each combination of parameters discussed in the previous section, and some typical examples are shown in Figure 2. To form the histograms, the conductivity axis was divided into 50 equal intervals or "buckets." Computed block conductivity values (equation (3)) were normalized with respect to μ_k, and the frequency of occurrence within each bucket was counted and then normalized with respect to the total number of realizations (2000) so that the area under the histogram becomes unity. A straight line was then drawn between the normalized frequency values centered on each bucket. Also shown on the plots are lognormal distributions fitted by estimating their parameters directly from the simulated data. A chi-square goodness-of-fit test indicates that the lognormal distribution was acceptable 93% of the time at the 5% significance level and 98% of the cases were acceptable at the 1% significance level (the significance level is the probability of mistakenly rejecting the lognormal hypothesis). Of those few cases rejected at the 1% significance level, no particular bias was observed, indicating that these were merely a result of the random nature of the analysis. The lowermost plot in Figure 2 illustrates one of the poorest fits which would be rejected at a significance level of 0.001%. Nevertheless, at least visually, the fit appears to be acceptable, demonstrating that the chi-square test can be quite sensitive.

Upon accepting the lognormal model, the two parameters $m_{\ln \bar{K}}$ and $s^2_{\ln \bar{K}}$, representing the estimated mean and variance of ln $(\bar{K})$, can be plotted as a function of the statistics of ln K and the geometry of the domain. Figures 3 and 4 illustrate the results obtained for the three correlation functions considered in (5*a*), (5*b*), and (5*c*). One can see that for square domains, where $X_L/Y_L = 1/1$, the statistics of $\bar{K}$ are closely approximated by

$$\mu_{\ln \bar{K}} \simeq \mu_{\ln K} \tag{9}$$

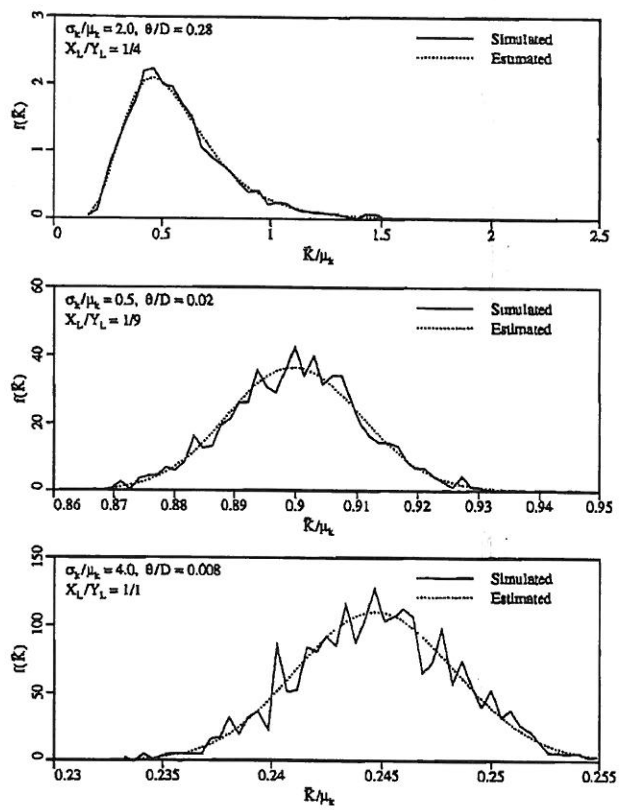

Fig. 2. Typical histograms of block conductivity for various block geometries and conductivity statistics. The estimated distribution is lognormal with parameters derived from the simulated data. Note that the scales change considerably from plot to plot.

$$\sigma_{\ln \bar{K}} \simeq \sigma_{\ln K}\sqrt{\gamma_D} \tag{10}$$

where $\mu_{\ln K} = \ln \mu_k - \frac{1}{2}\sigma^2_{\ln K}$ and $\gamma_D = \gamma(D, D)$ (see the appendix). Note that these are just the statistics one would obtain by averaging $Y(\mathbf{x}) = \ln K(\mathbf{x})$ over the block. Assuming the equality, the corresponding results in conductivity space are

$$\mu_{\bar{K}} = \mu_k \exp\{-\tfrac{1}{2}\sigma^2_{\ln K}(1-\gamma_D)\} \tag{11}$$

$$\sigma^2_{\bar{K}} = \mu_k^2 \exp\{-\sigma^2_{\ln K}(1-\gamma_D)\}[\exp(\sigma^2_{\ln K}\gamma_D) - 1] \tag{12}$$

If these expressions are extended beyond the range over which the simulations were carried out, then in the limit as $D \to 0$ they yield

$$\mu_{\bar{K}} \to \mu_k \tag{13a}$$

$$\sigma^2_{\bar{K}} \to \sigma^2_k \tag{13b}$$

since $\gamma_D \to 1$. This means that as the block size decreases, the statistics of the block conductivity approach those of the point conductivity, as expected. In the limit as $D \to \infty$, $\mu_{\bar{K}}$ approaches the geometric mean and $\sigma^2_{\bar{K}}$ approaches 0, which is to say that the block conductivity approaches the effective conductivity, again as expected.

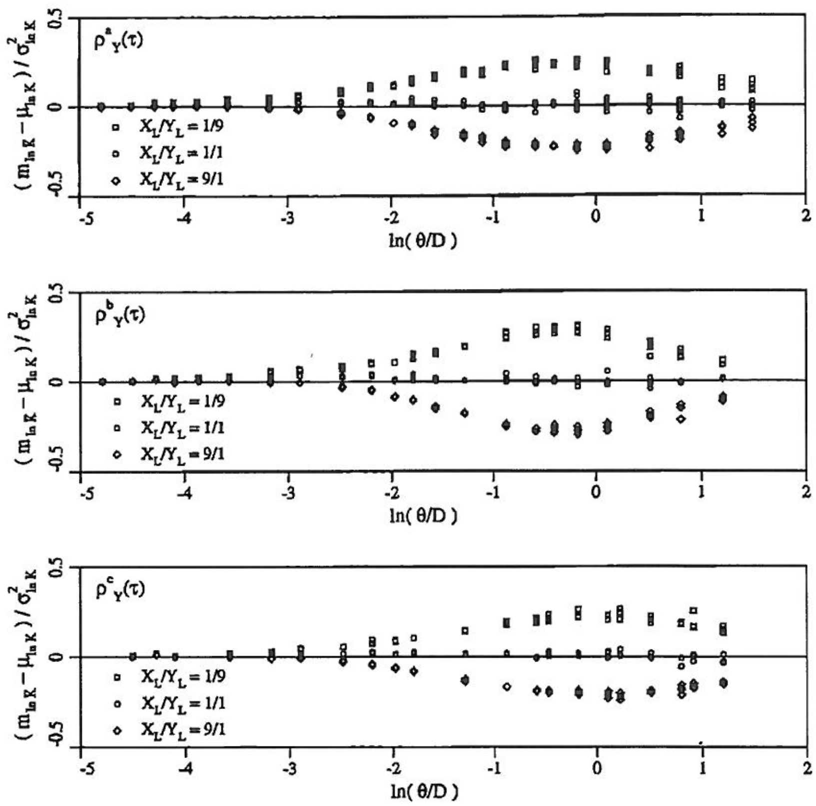

Fig. 3. Estimated mean log block conductivity $(m_{\ln \bar{K}} - \mu_{\ln K})/\sigma^2_{\ln K}$.

If both γ_D and the product $\sigma^2_{\ln K}\gamma_D$ are small, then first-order approximations to (11) and (12) are

$$\mu_{\bar{K}} = \mu_k \exp\{-\tfrac{1}{2}\sigma^2_{\ln K}\} \tag{14}$$

$$\sigma^2_{\bar{K}} = \mu_k^2 \exp\{-\sigma^2_{\ln K}\}(\sigma^2_{\ln K}\gamma_D) \tag{15}$$

Rubin and Gómez-Hernández [1990] obtain (14) if only the first term in their expression for the mean is considered. In the limit as $D \to 0$, additional terms in their expression yield the result $\mu_{\bar{K}} \to \mu_k$ in agreement with the result given by (13*a*). With respect to the variance, *Rubin and Gómez-Hernández* [1990] generalize (15) using a first-order expansion to give the covariance between two equal-sized square blocks separated by a distance **h** as a function of the covariance between local averages of ln K,

$$\mathrm{Cov}\,[\bar{K}(\mathbf{x}),\ \bar{K}(\mathbf{x}+\mathbf{h})] = \mu_k^2 \exp\{-\sigma^2_{\ln K}\}\ \mathrm{Cov}\,[Y_D(\mathbf{x}),\ Y_D(\mathbf{x}+\mathbf{h})] \tag{16}$$

where $Y_D(\mathbf{x})$ is the local average of Y over the block centered at $\mathbf{x}$. Equation (16) reduces to (15) in the event $\mathbf{h} = 0$ since Var $[Y_D(\mathbf{x})] = \sigma^2_{\ln K}\gamma_D$.

In many practical situations, neither γ_D nor $\sigma^2_{\ln K}\gamma_D$ are small, so that the approximations given by (14), (15), and (16) can be greatly in error. To illustrate this, consider a hypothetical example in which $\mu_k = 1$ and $\sigma^2_k = 16$ (so that $\sigma^2_{\ln K} = 2.83$). It is expected that for a very small block, the variance of the block conductivity should be close to σ^2_k, namely $\sigma^2_{\bar{K}} \simeq 16$ as predicted by (13*b*). However in this case, $\gamma \simeq 1$, and (15) yields a predicted variance of $\sigma^2_{\bar{K}} = 0.17$, roughly 100 times smaller than expected. Recall that (15) was derived on the basis of a first-order expansion and so is strictly only valid for $\sigma^2_{\ln K} \ll 1$.

For aspect ratios other than 1/1, Figures 3 and 4 show clear trends in the mean and variance of ln $\bar{K}$. At small aspect ratios in which the block conductivity tends toward the arithmetic mean, $m_{\ln \bar{K}}$ is larger than $\mu_{\ln K}$, reaching a peak at around $\theta = D$. At large aspect ratios where the block conductivity tends toward the harmonic mean, $m_{\ln \bar{K}}$ is smaller than $\mu_{\ln K}$, again reaching a minimum around $\theta = D$. Since the arithmetic and harmonic means bound the geometric mean above and below, respectively, the general form of the estimated results is as expected. While it appears that in the limit as $\theta \to 0$, both the small and large aspect ratio mean results tend toward the geometric mean, this is actually due to the fact that the effective size of the domain D/θ is tending to infinity so that the unbounded results of (4) apply. For such a situation, the small variances seen in Figure 4 are as expected. At the other extreme, as $\theta \to \infty$, there appears again to be convergence to the geometric mean for all three aspect ratios considered. In this case, the field becomes perfectly correlated, so that all points have the same permeability and $\mu_{\ln \bar{K}} = \mu_{\ln K}$ and $\sigma_{\ln \bar{K}} = \sigma_{\ln K}$ for any aspect ratio.

Appendix

The variance functions corresponding to the correlation functions (5) may be obtained through the use of (8). They are

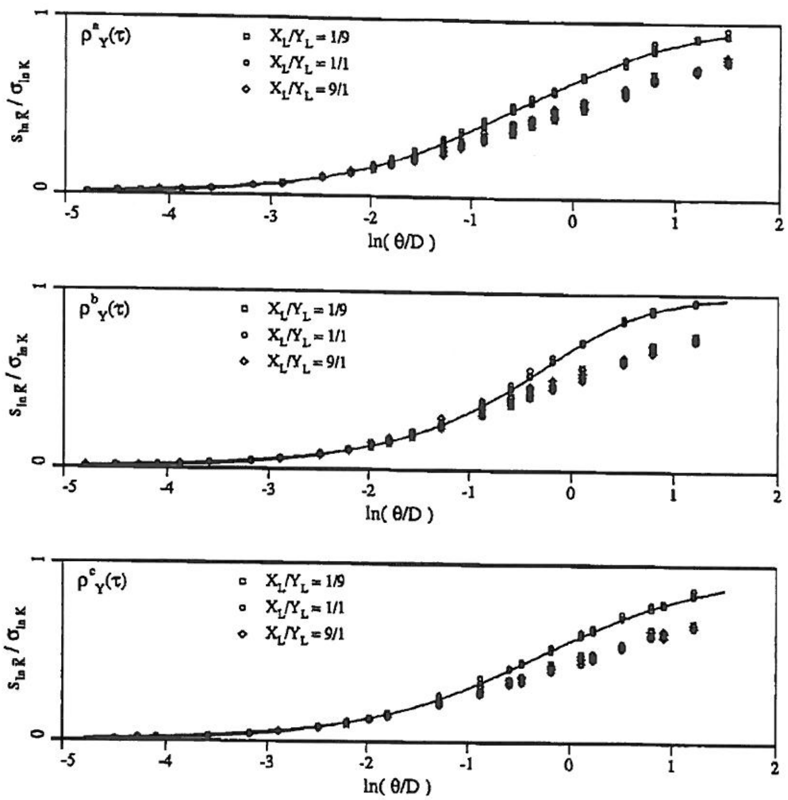

Fig. 4. Estimated standard deviation of log block conductivities, $s_{\ln \bar{K}}/\sigma_{\ln K}$. Solid line corresponds to $s_{\ln \bar{K}}/\sigma_{\ln K} = \gamma(D, D)^{1/2}$.

$$\gamma^a(\Delta_1, \Delta_2) = \tfrac{1}{2}[\gamma^a(\Delta_1)\gamma^a(\Delta_2|\Delta_1) + \gamma^a(\Delta_2)\gamma^a(\Delta_1|\Delta_2)] \quad (17a)$$

$$\gamma^b(\Delta_1, \Delta_2) = \gamma^b(\Delta_1)\gamma^b(\Delta_2) \quad (17b)$$

$$\gamma^c(\Delta_1, \Delta_2) = \gamma^c(\Delta_1)\gamma^c(\Delta_2) \quad (17c)$$

where,

$$\gamma^a(\Delta_i) = \left[1 + \left(\frac{\Delta_i}{\theta_i}\right)^{3/2}\right]^{-2/3},$$

$$\gamma^a(\Delta_i|\Delta_j) = \left[1 + \left(\frac{\Delta_i}{\theta^i_j}\right)^{3/2}\right]^{-2/3},$$

$$\theta^i_j = \theta_i\left[\frac{\pi}{2} + \left(1 - \frac{\pi}{2}\right)\exp\left\{-\left(\frac{2\Delta_j}{\pi\theta_j}\right)^2\right\}\right],$$

$$\gamma^b(\Delta_i) = \frac{\pi\Delta_i^2}{\theta_i^2}\left[\frac{\pi|\Delta_i|}{\theta_i}\operatorname{erf}\left\{\frac{\theta_i}{\sqrt{\pi}\Delta_i}\right\} - \exp\left\{-\frac{\theta_i^2}{\pi\Delta_i^2}\right\} - 1\right],$$

$$\gamma^c(\Delta_i) = \frac{\theta_i^2}{2\Delta_i^2}\left[\frac{2|\Delta_i|}{\theta_i} + \exp\left\{-\frac{2|\Delta_i|}{\theta_i}\right\} - 1\right]$$

in which θ_i is the directional scale of fluctuation (in this study, $\theta_1 = \theta_2 = \theta$). Note that since no closed form solution to the integral (8) exists for ρ^a_Y, (17a) is an approximation developed on the basis of numerical results due to *Vanmarcke* [1984].

NOTATION

Δ_e element side dimension.
γ variance function.
θ scale of fluctuation.
μ_k mean of hydraulic conductivity.
$\mu_{\bar{K}}$ mean of block conductivity.
$\mu_{\ln K}$ mean of log conductivity.
$\mu_{\ln \bar{K}}$ mean of log block conductivity.
ρ correlation function.
σ_k^2 variance of hydraulic conductivity.
$\sigma_{\bar{K}}^2$ variance of block conductivity.
$\sigma_{\ln K}^2$ variance of log conductivity.
$\sigma_{\ln \bar{K}}^2$ variance of log block conductivity.
τ physical lag vector.
ϕ hydraulic head.
D effective block dimension.
f frequency distribution function.
H head difference between upstream and downstream domain boundaries.
$\mathbf{h}$ interelement or interblock distance vector.
K hydraulic conductivity field.
$\bar{K}$ block conductivity.
K_{eff} effective conductivity.
$m_{\ln \bar{K}}$ estimated mean log block conductivity.
Q total flow rate through domain.
Q_{μ_k} total flow rate through domain having constant conductivity μ_k.
$s_{\ln \bar{K}}^2$ estimated variance of log block conductivity.
X_L dimension of domain in the x direction.

Y_L dimension of domain in the y direction.
Y log conductivity field, equal to ln K.
Y_D local average of log conductivity field over a block.

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G. A. Fenton, Department of Applied Mathematics, Technical University of Nova Scotia, Halifax, Nova Scotia, Canada B3J 2X4.
D. V. Griffiths, Department of Engineering, University of Manchester, Manchester M13 9PL, England.

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