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Earth Sciences Division

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A Semianalytical Approach to Spatial Averaging of Hydraulic Conductivity in Heterogeneous Aquifers

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Abstract.

Numerical models of groundwater flow require hydraulic conductivity values to be assigned to the grid blocks covering the flow domain. However, field-measured conductivities tend to be measured at a different scale (usually smaller) than that of the grid blocks. The present paper describes a novel approach for upscaling field values to block-scale, which combines the rigorous result of small-value perturbation analysis with a plausible generalization of the first-order results to large variance. Also the correlation lengths are assumed to be comparable to block size. Steady-state flow through a block of stochastically heterogeneous medium with constant hydraulic head values at the two opposite sides is analyzed. An upscaling rule and relationship is obtained between the local-scale hydraulic conductivity and the expected mean and variance of block-scale conductivity, where the block size is comparable with the correlation scale of the local conductivity field. The rather simple expressions obtained are validated using data from numerical experiments. Furthermore, a generalized spatial power-averaging method to calculate the block-scale conductivity from values of local-scale conductivity is developed, in which the exponent value is given as a function of the ratios of flow domain dimensions to the respective correlation lengths.

1. Introduction

The theory of fluid flow in statistically heterogeneous aquifers is well developed. The starting point for this theory is usually the flow resistance as a local spatial function of the geological media, i.e., the local hydraulic conductivity. Typically, the spatial variation of the local hydraulic conductivity is described as a random process with a given statistical distribution and covariation function. For numerical modeling of groundwater flow, one needs to assign hydraulic conductivities to grid blocks that cover the flow domain. For porous flow, the law of spatial averaging of hydraulic conductivity is often quite different from a simple arithmetic averaging of local-scale conductivity values. One needs to know which upscaling rule to apply from local-scale conductivity to conductivity averaged over large blocks (i.e., the block-scale conductivity) to properly simulate flow through heterogeneous aquifiers. On the other hand, to investigate practical environmental problems such as groundwater contamination and the design of underground waste disposal sites, one also needs to estimate the information loss on spatial variation of flow velocities due to the generally large griding used in the numerical models. Taking into account these losses, it is possible to define effective grid macrodispersion parameters to describe solute advective dispersion in aquifers.

The goal of the present paper is to find the upscaling rule and relationship between the local-scale hydraulic conductivity and the expected mean and variance of block-scale conductivity, where the block size is comparable with the correlation scale of the local conductivity field.

In recent years different approaches to this problem have been published. *Rubin and Gomez-Hernandez* [1990] developed a first-order approximation for the expected mean and variance of the effective block transmissivity of a heterogeneous aquifer, and investigated by numerical simulation the variations of these parameters. *Ababou and Gelhar* [1990] obtained particular solutions for effective conductivity of finite one-dimensional flow domains using the local mean and the local mean slope of log conductivity. *Durloevsky* [1991] numerically examined the effective block transmissivity for the special case of periodic structure of the local hydraulic conductivity field. *Desbarats* [1992a, 1994] developed a geostatistical model for the block conductivity. In his model, conductivity at the block scale is obtained empirically as a spatial power averaging of local-scale values. *Dukaar and Kitanidis* [1993] determined the effective block transmissivity using a numerical method based on the Taylor-Aris moment analysis. In the works of *Indelman and Dagan* [1993] and *Indelman* [1993], the general approach for upscaling local hydraulic conductivity to the global block value was given for isotropic and locally anisotropic media and some closed expressions were obtained by small-value perturbation analysis. *Neuman et al.* [1992] and *Neuman and Orr* [1993] developed an exact expression for the mean Darcy flux within bounded domain by using a residual flux. The residual flux depends on domain size, and the general form of the integral equation for which it was obtained. *Paleologos et al.* [1996] derived a first-order approximation for effective conductivity by using this exact expression and generalized the first-order result to strongly heterogeneous media.

All these publications mentioned above do not contain exact equations for the mean and variance of block-scale conductivity of strongly heterogeneous medium for a general three-dimensional flow with arbitrary block sizes.

The present paper describes an approach for problem of block-scale, which combines the rigorous result of small-value perturbation analysis with a plausible generalization of this first-order product to large variance. The rather simple expressions thus obtained are validated using data from numerical experiments. The approach described below also allows us to re-examine the spatial power averaging method for local data. *Landau and Lifshitz* [1960] conjectured that for three-dimensional dielectric conductivity of a medium an appropriate additive quantity is the cubic root of the conductivity values. Much later, *Desbarats* [1992b], and *Debarats and Bachu* [1994] developed a power averaging method for flow in heterogeneous aquifers by using numerical modeling. In present paper a general case is studied in which a new expression for the averaging exponent is derived.

2. Spatial averaging of conductivity

This section presents a semianalytical method for averaging local-scale hydraulic conductivities of a statistically heterogeneous aquifer to obtain block-scale conductivities. The method is based on an extrapolation of results obtained by the small-value perturbation technique. This development follows the hypothesis used by *Gelhar and Axness* [1983], *Gelhar* [1993], *Paleologos et al.* [1996] for the generalization of first-order results to estimate an effective conductivity of strongly heterogeneous media.

2.1 Definition of the problem

Consider a heterogeneous aquifer with a scalar point, local-scale hydraulic conductivity field that can be modeled as a random function $K(\mathbf{x})$ over spatial coordinates $\mathbf{x}=\{x_1,x_2,x_3\}$. The conductivity is often observed to be asymmetrically distributed, and in standard practice, a lognormal distribution is found to be a good approximation of empirical conductivity data. Following *Dagan* [1989], *Gelhar* [1993], and others, let us assume the random function $Y(\mathbf{x})=\ln K(\mathbf{x})$ to be stationary, ergodic, and Gaussian. Then we define the two first moments of $Y(\mathbf{x})$ as:

$$E[Y(\mathbf{x})] = \mu\,, \tag{1a}$$

$$Var[Y(\mathbf{x})] = \sigma^2\,, \tag{1b}$$

$$Cov[Y(\mathbf{x}), Y(\mathbf{x}+\mathbf{u})] = \sigma^2\rho(u)\,, \tag{1c}$$

where the autocorrelation function $\rho(u)$ has an isotropic structure with the same correlation scale λ in all principal directions of the Cartesian coordinate system $\mathbf{x}=\{x_1,x_2,x_3\}$.

Next, consider the flow domain with spatial dimension $\mathbf{L} = \{L_1,L_2,L_3\}$. Let us use a ratio of L_i to the correlation scale λ as an indicator of the physical spatial dimension of flow. If all the ratios L_i/λ are non-zero, it indicates that flow is three-dimensional in space. If one of the ratios tends to zero, the flow is two-dimensional. For the case when two ratios are zero, the flow has a one-dimensional structure. Following the finite differential method for numerical modeling of flow, we cover the flow domain by a grid of blocks with the length of each side given by b_i ($b_i \leq L_i$) for each direction of the coordinate

system. We intend to assign to each block a value of hydraulic conductivity k_b appropriately averaged over the block volume. For the widely used case of planar flow, where $b_3 = L_3$, we can define the transmissivity of block T_b as $T_b = b_3 \cdot k_b$.

The following problem should be investigated. Because a block value is defined as an average of the random function $K(\mathbf{x})$, we consider the block-scale value to be a realization of random function $K_b(\mathbf{x})$. Thus, the goal of this paper is to find the upscaling rule, or the relationship between two first spatial moments of $K_b(\mathbf{x})$ and the moments of $K(\mathbf{x})$ or its transformation $Y(\mathbf{x})$.

2.2 Bounding values for block conductivity moments and proposed upscaling equations

The block-scale conductivity can be obtained by averaging the hydraulic gradient and the hydraulic conductivity over a block with a volume V. *Rubin and Gomez-Hernandez* [1990] gave the following expression for the k_b value for an isotropic porous medium:

$$k_b = V^{-1} \int_V \mathbf{q}(\mathbf{x}) dx (V^{-1} \int_V \mathbf{J}(\mathbf{x}) dx)^{-1}; \quad \mathbf{q}(\mathbf{x}) = -k(\mathbf{x}) \nabla h; \quad \mathbf{J}(\mathbf{x}) = \nabla h, \tag{2}$$

where h is the hydraulic head.

Note that in this expression, the block-scale value depends not only on the local conductivity, but also on the flow gradient. The most significant form of the flow gradient on the hydraulic spatial averaging (as it was shown by *Shvidler* [1986], *Dagan* [1989], *Desbarats* [1992a, 1994], *Indelman et al.* [1996]) is the strongly divergent/convergent flow, i.e., the local part of flow domain surrounding a pumping or injection well.

Generally, however, for the other largest part of the flow domain, the hydraulic head changes gradually in space. The quasi-parallel flow in one direction should be considered as a more common model of groundwater flow.

For quasi-parallel flow, the limits of a block volume tending to zero or infinity provide the bounds for the expected mean $k_b = E[K_b]$ of block-scale conductivity, which can be written in the form:

$$k_a \geq k_b \geq k_{ef}; \quad k_a = k_g \exp(\frac{1}{2}\sigma^2), \tag{3a}$$

where k_a is the arithmetic mean of $K(\mathbf{x})$, $k_g = \exp(\mu)$ the geometric mean, and k_{ef} the value of effective conductivity for uniform flow in an infinite medium. Correspondingly, the bounds for the variance are:

$$0 \leq Var[K_b(\mathbf{x})] \leq Var[K(\mathbf{x})]. \tag{3b}$$

A number of theoretical works seeking the effective conductivity of an infinite heterogeneous medium was published, including *Shvidler* [1964, 1986], *Matheron* [1967], *Gelhar and Axness* [1983], and *Dagan* [1989, 1993]. The main result of these investigations is that an equation for the effective conductivity has the following form for the case of lognormal local hydraulic conductivity distribution with isotropic autocovariance [*Gelhar*, 1993] :

$$k_{ef} = k_g \exp\left[\sigma^2(\frac{1}{2} - g_{11})\right]; \quad g_{11} = n^{-1}, \tag{4}$$

where n (n = 1,2,3) is the spatial dimension of the flow.

Note that eq. (4) is rigorous only for the one- and two-dimensional flow cases. It has not yet been proven rigorously for three-dimensional flow, and the equation is obtained by a generalization of the first-order result using perturbation techniques, and by regarding it as a truncation of the Taylor series expansion for the exponential function [*Gelhar*, 1993]. Theoretical contribution in support of eq. (4) was obtained by *Dagan* [1993] who showed it to be valid for the second-order approximation in σ^2. Unfortunately, there is still no theoretical proof of convergence of the perturbation series for any given σ^2. Numerical Monte Carlo simulations for the determination of effective conductivity for three-dimensional flow by *Neuman and al.* [1992], and *Dukaar and Kitanidis* [1993] show very good agreement between predictions by eq.(4) and numerical results for the range of variance values between one and seven. Thus, practically speaking, one can say that eq. (4) is valid for effective conductivity for all these flow-spatial dimensions.

Let us propose that an equation for the expected mean of the block-scale conductivity has the same structure as eq. (4):

$$k_b = k_g \exp\left[\sigma^2(\frac{1}{2} - g_{scale})\right], \tag{5}$$

where g_{scale}, which we call the upscaling function, depends on the ratio of block sizes to the correlation scale of local hydraulic conductivity for a given autocorrelation function $\rho(u)$. It is clear that to satisfy the upper boundary value of eq. (3a), the upscaling function should tend to 0 for the very small block size. For the lower boundary, it tends to g_{11} when the block size tends to infinity. Theoretical contributions in supports of eq. (5) were

obtained by *Paleologos et al.* [1996], that used development of *Neuman and Orr* [1993] for effective conductivity of bounded media.

Following *Desbarats* [1992b], assume that $Y_b(\mathbf{x}) = \ln K_b(\mathbf{x})$ is stationary and multivariate Gaussian, and also assume that

$$Var[Y_b(\mathbf{x})] = \sigma^2 \cdot \varsigma_{scale}, \tag{6a}$$

so that the coefficient of variance of the block-scale conductivity C_v is given by:

$$C_v = \frac{\sqrt{Var[K_b(\mathbf{x})]}}{k_b} = \frac{\sqrt{Var[\exp Y_b(\mathbf{x})]}}{k_b} = \sqrt{\exp(\sigma^2 \varsigma_{scale}) - 1}\ , \tag{6b}$$

where ς_{scale} is a variance upscaling function gradually changing from 1 to 0 for the block volume changing from 0 to infinity for any given autocorrelation $\rho(u)$.

2.3 Small perturbation and first-order approximation

In this section we outline the first-order results to find the particular structure of the upscaling function for quasi-parallel flow. For this, consider three-dimensional block-scale steady state flow in the x_1 direction with the following boundary conditions: constant non-random hydraulic head drop Δh_1 between the two opposite sides of the block along x_1; and closed boundary conditions on all other sides of the block. For a random local-scale conductivity, the total flux Q_b through the block is a random value for the given external gradient $J_1 = \Delta h_1/b_1$. Thus, the expected mean and variance of block-scale conductivity are:

$$k_b = J_1^{-1}\Omega^{-1}E[Q_b], \tag{7a}$$

$$Var[k_b] = J_1^{-2}\Omega^{-2}Var[Q_b], \tag{7b}$$

where $\Omega = b_2 b_3$ is a cross section of the block that is normal to flow. Using the standard practice of the small perturbation analysis [*Dagan*, 1989], and starting with the integral of Darcy's law $Q = -\int_{\Omega} k \nabla h dx_2 dx_3$, $k = \exp(\mu + Y')$, we formally expand $h = h^{(0)} + h^{(1)} + h^{(2)} + \cdots$ and $\exp(Y') = 1 + Y' + 0.5Y'^2 + \cdots$ to obtain:

$$Q = Q^{(0)} + Q^{(1)} + Q^{(2)} + \ldots \tag{8a}$$

where

$$Q^{(0)} = \Omega J_1 k_g ; Q^{(1)} = k_s b_1^{-1} \int_0^{b_1} \int_{\Omega} \left(J_1 Y' - \frac{\partial h^{(1)}}{\partial x_1} \right) dx_1 dx_2 dx_3 \tag{8b}$$

$$Q^{(2)} = k_g b_1^{-1} \int_0^{b_1} \int_{\Omega} \left(\frac{Y^2}{2} J_1 - Y' \frac{\partial h^{(1)}}{\partial x_1} \right) dx_1 dx_2 dx_3 \quad , \tag{8c}$$

where Y' is the centered random function, $Y' = Y - \mu$.

The first-order result is $E[Q_b] = Q^{(0)} - E[Q^{(2)}]$; and $Var[Q_b] = Var[Q^{(1)}]$. Taking into account the boundary conditions and the ensemble averaging eqs. (8a) and (8b), we obtain:

$$E[Q_b] = J_1 \Omega k_g \left[1 + \sigma^2 (\frac{1}{2} - g_3) \right]; \quad g_3 = \int_0^{b_1} \int_0^{b_2} \int_0^{b_3} \xi(x_1, x_2, x_2) dx_1 dx_2 dx_3 , \tag{9a}$$

$$Var(Q_b) = k_g^2 J_1^2 b_1^{-2} Var \left[\int_0^{x_1} \int_0^{x_2} \int_0^{x_3} Y'(\mathbf{x}) dx_1 dx_2 dx_3 \right], \tag{9b}$$

where ξ can be formally represented by a combination of the Green function for the Laplace equation and the autocorrelation function [*Shvidler*, 1986]:

$$\xi(x_1, x_2, x_3) = \int_0^{b_1} \int_0^{b_2} \int_0^{b_3} \nabla G_{x_1} \cdot \nabla \rho_{x'_1} dx_1 dx_2 dx_3 \tag{9c}$$

The hard work to analytically integrate (9c) for the finite-domain Green function was first made by *Shvidler* [1986], who applied the autocorrelation function of the symmetric-exponential structure:

$$\rho(u) = \prod_{i=1}^{n} \exp\left(-\frac{u_i}{\lambda}\right); \quad u_i = \left|x_i' - x_i'\right| \tag{10}$$

The resulting equation for g_3 for a block that has different lengths in all three directions has the form:

$$g_3 = \frac{1}{6}\left[1 - \varphi(\frac{b_1}{\lambda})\right]\left[2 + \varphi(\frac{b_2}{\lambda}) + \varphi(\frac{b_3}{\lambda}) + 2\varphi(\frac{b_2}{\lambda})\varphi(\frac{b_3}{\lambda})\right] \tag{11a}$$

where function φ is a "directional" dimensionless variance of the expected mean of random function along a given axis, i.e.,:

$$\varphi(u) = u^{-2}\int_0^u\int_0^u \exp(-\left|u - u'\right|)du du' = 2u^{-2}\left[\exp(-u) + u - 1\right] \tag{11b}$$

Combining eqs. (9a) and (11a) for eq. (7a) gives the first-order value for the expected mean of block-scale conductivity:

$$k_b = k_g\left[1 + \sigma^2(\frac{1}{2} - g_3)\right] \tag{12}$$

For the variance of block-scale conductivity, we easily find from eqs. (7b) and (9b) that

$$\begin{aligned} Var[k_b] &= k_g^2\sigma^2 V^{-2}\int_V\int_V \rho(\mathbf{x} - \mathbf{x}')d\mathbf{x}d\mathbf{x}' = k_g^2\sigma^2\varsigma_3; \\ \varsigma_n &= \prod_{i=1}^{n} u_i^{-2}\int_0^{u_i}\int_0^{u_i} \exp\left(-\left|u_i - u_i'\right|\right)du du' = \prod_{i=1}^{n}\varphi(\frac{b_i}{\lambda})_i. \end{aligned} \tag{13}$$

The equations for g and ς can be applied for any flow spatial dimension. By letting b_3 equal to zero, we obtain the equations for g_2 and ς_2 for flow in two dimensions, and by

additionally letting b_2 equal to zero, we obtain the equations for g_1 and ς_1 for one dimensional flow. Note that for a block with equal lengths in all n spatial dimensions, $g_n = (1-\varsigma_n)/n$.

Formally we could also use small perturbation analysis by expanding the local conductivity around its arithmetic mean, i.e., $K = k_a + k'$. Taking into account that for the lognormal distribution and small values of the variance, $Var[K(\mathbf{x})]/k_a^2 \approx \sigma^2$ and autocorrelation of local conductivity, $\rho_k(u) \rightarrow \rho(u)$, and then using the same technique as above, we obtain a slightly different first-order result for the two first moments of block-scale conductivity. It can be written for the general n-dimensional case as:

$$k_b = k_g \exp\left(\frac{\sigma^2}{2}\right)(1-\sigma^2 g_n), \tag{14}$$

$$Var[k_b] = k_a^2 \sigma^2 \cdot \varsigma_n . \tag{15}$$

To generalize the first-order results, we adopt a conjecture used by *Gelhar and Axness* [1983], *Gelhar* [1993], and *Paleolougos et al.* [1996], which considers an expression like eq.(14) as the first two terms of a series. Thus we can consider eqs. (12) and (14) as the product of the Taylor series expansion of the proposed equation (eq. 5) for the expected mean of the block-scale conductivity. It yields the value of upscaling function g_{scale} in eq. (5) to be $g_{scale} = g_n$. By substituting in eq. (11a) the bounding values for the ratio of the block size to correlation scale, it is easy to find that for very large blocks $g_n = n^{-1}$, and for the small block sizes $g_n \rightarrow 0$. Thus, the bounding values for the upscaling function are satisfied.

For the variance of block-scale conductivity, we can replace the value of conductivity on the expected mean of block-scale conductivity k_b in eqs. (12) and (14) and extend it for large variance values using the *Desbarats* [1992b] assumption that $Y_b(\mathbf{x})$ has a lognormal distribution. This gives the value of upscaling function ς_{scale} in eq. (6) as $\varsigma_{scale} = \varsigma_n$.

Let us consider the equations for the upscaling function for two frequently used correlation functions: exponential

$$\rho(u) = \exp\left[-\sqrt{\sum_{i=1}^{n}\left(\frac{u_i}{\lambda}\right)^2}\right]; \quad u_i = \left|x_i' - x_i''\right|, \tag{16a}$$

and Gaussian

$$\rho(u) = \prod_{i=1}^{n}\exp-\left(\frac{u_i}{\lambda_o}\right)^2; \quad u_i = \left|x_i' - x_i''\right| \quad \lambda_0 = \frac{4}{\pi}\lambda \tag{16b}$$

It is impossible to directionally integrate the exponential correlation to obtain the close form integral even for the variance. We can geometrically relate the separation r used in eq. (16a) and the separation $r' = \sum_{i=1}^{n}\left|u_i' - u_i''\right|$ used in eq. (10) by the inequality:

$$\frac{r'}{\sqrt{n}} \le r \le r'. \tag{17}$$

Thus, the bounds for upscaling functions for the case of exponential correlation can be written in the following form

$$g_n(\frac{b_1}{\lambda\sqrt{n}},..,\frac{b_n}{\lambda\sqrt{n}}) \geq g_{scale} \geq g_n(\frac{b_i}{\lambda},..,\frac{b_n}{\lambda});$$
$$\varsigma_n(\frac{b_1}{\lambda\sqrt{n}},..,\frac{b_n}{\lambda\sqrt{n}}) \leq \varsigma_{scale} \leq \varsigma_n(\frac{b_1}{\lambda},..,\frac{b_n}{\lambda}) \tag{18}$$

Direct numerical calculation of the four- and six-times integral to obtain the ς_2 and ς_3 values for the exponential correlation can be compared with the analytical estimation by using eq. (13). The comparison shows that the analytical solution in eq. (13) for symmetric-exponential correlation is favorable for predicting the value of the exponential correlation with a maximum absolute error of less than 0.01 by replacing the correlation scale λ by the effective scale λ_e, where $\lambda_e = \alpha\lambda$. It was found that the value of the numerical constant α is 1.25 for the two-dimensional case and 1.5 for the three-dimensional one. Furthermore, for all calculations for the exponential correlation case, the equations should be used with the replacement of the actual correlation scale by the effective correlation scale.

For the Gaussian autocorrelation function, direct substitution in eqs. (9b) and (11b) gives the same form as eq. (13) but with different values of the multiplication product φ. Thus, in the equation for ς_{scale} we should replace $\varphi(\frac{b_i}{\lambda})$ by $\varphi'(\frac{b_i}{\lambda_0})$, where

$$\varphi'(u) = u^{-2}\int_0^u\int_0^u \exp\left[-(u-u')^2\right]du\,du' = u^{-2}(\sqrt{\pi}u\cdot erf(u) + \exp(-u^2) - 1). \tag{19}$$

Using the linear property for the first-order approximation we can find the equation for the autocorrelation function $Y_b(\mathbf{x})$ (Appendix A). The results given in Appendix A show that the correlation scale of block conductivity is equal to $b_i+\lambda$. It is

approximately equal to the scale of local conductivity for small block size and equal to block side length for a large b_i/λ ratio.

Unfortunately, we cannot evaluate g_n for any given dimension of flow and Gaussian autocorrelation. For a one-dimensional flow case, the equation for g_1 for this correlation has the same structure as that of the function for exponential correlation, but with $\varphi(\frac{b_1}{\lambda})$ replaced by $\varphi'(\frac{b_1}{\lambda_0})$. We will assume that such a substitution is also valid for two- and three-dimensional flow.

Thus, this subsection presents an analysis that allows us to find approximate upscaling functions for the expected mean and variance for block-scale conductivity. These functions depend on physical flow dimension, the type of autocorrelation of log local conductivity, and the ratios of block lengths in different directions to the correlation scale of the local conductivity.

2.4 Effective transmissivity of an uniform confined aquifer

For regional-scale modeling, a planar two-dimensional model of flow averaged over the vertical coordinate (i.e., over aquifer thickness) is often used. The transmissivity of aquifer T can be defined by using the Dupuit-Forscheimer-Boussiness assumption [*Bear*, 1979] as:

$$T(x,y) = \int_0^{L_3} k(\mathbf{x})dx_3 , \tag{20a}$$

where L_3 is the thickness of the aquifer.

Note, that according to this definition the transmissivity is a simple arithmetic average of conductivity, which is valid for the following very special cases: a) when there is a perfect layered aquifer with scalar local conductivity; and b) when the local hydraulic conductivity is a tensor with the vertical component tending to infinity. *Dagan* [1989], taking into account these limitation of arithmetic vertical averaging, suggested the following definition for the transmissivity of a heterogeneous aquifer:

$$T(x_1, x_2) = k_{\text{efu}} L_3 , \tag{20b}$$

where k_{efu} is the effective conductivity value.

It is physically clear that to estimate the effective transmissivity of a very thin aquifer, one should use the value of k_{efu} equal to the effective conductivity for two-dimensional flow. Now, to obtain the effective transmissivity for any aquifer thickness we can formally calculate the block-scale conductivity for the block size in each direction to be equal to the size of the flow domain in this direction ($b_i = L_i$). Consider the case of a two-dimensional planar uniform flow (L_1/λ and $L_2/\lambda \to \infty$). The calculation of g_{scale} for this case,:

$$g_{scale} = g_3(\infty, \infty, L_3 / \lambda) = \frac{1}{6}\left[2 + \varphi(\frac{L_3}{\lambda})\right], \tag{21a}$$

gives the value of effective transmissivity T_{ef} as:

$$T_{ef} = L_3 k_{efu} = L_3 k_g \exp\left[\frac{\sigma^2}{6}\left(1 - g_T(\frac{L_3}{\lambda})\right)\right], \tag{21b}$$

where $g_T(u) = \varphi(u)$ for the symmetric-exponential correlation of local-scale conductivity, $g_T(u) = \varphi(u/\alpha)$ for the exponential correlation, and $g_T(u) = \varphi'(u)$ for the Gaussian

correlation. From eqs. (21a) and (21b) one can see that to increase the value of the ratio of the aquifer thickness to the correlation scale, the effective conductivity k_{efu} must change from the effective conductivity of two-dimensional flow to the effective conductivity of three-dimensional flow. The other bounding case for the transmissivity value that should be considered is the one-dimensional flow, i.e., $L_1/\lambda \to \infty$ and $L_2/\lambda \to 0$, for which we obtain:

$$T_{ef} = L_3 k_{efu} = L_3 k_g \exp\left(-\frac{\sigma^2}{2} g_T(\frac{L_3}{\lambda})\right). \tag{22}$$

Now we try to expand the relationship (22) to obtain an approximate expression of the effective transmissivity for the case of anisotropic spatial correlation of local conductivity. Consider the anisotropic correlation of $Y(\mathbf{x})$ field with the horizontal scale λ_h ($\lambda_h = \lambda_1 = \lambda_2$) larger than the vertical scale λ_v ($\lambda_v = \lambda_3$). Under such conditions the effective horizontal conductivity of a uniform medium can also be calculated by using eq. (4) with the value of g_{11} in terms of the ratio of correlation scales $\varepsilon = \lambda_1/\lambda_3$ [*Gelhar, 1993, p.111*]:

$$g_{11} = \frac{1}{2}\frac{1}{\varepsilon^2 - 1}\left[\frac{\varepsilon^2}{\sqrt{\varepsilon^2 - 1}} arctg\sqrt{\varepsilon^2 - 1} - 1\right] \tag{23a}$$

Then, on the basis of eq. (21a), the expression for the g_{scale} function for anisotropic aquifer is proposed to have the following structure with numerical constants a, b:

$$g_{scale} = \frac{g_{11}}{a}\left[b + \varphi(\frac{L_3}{\lambda_3})\right]. \tag{23b}$$

To the obtain the unknown constants a and b, we take into account the physical bounds for the upscaling function, i.e., the value for the two-dimensional flow case ($L_3/\lambda_3 \rightarrow 0$, $g_{scale} \rightarrow 1/2$), and that for the three-dimensional case ($L_3/\lambda_3 \rightarrow \infty$, $g_{scale} \rightarrow g_{11}$). These considerations produce the following proposed expression for the effective transmissivity of an anisotropic aquifer:

$$T_{ef} = L_3 k_{efu} = L_3 k_g \exp\left[\sigma^2\left(\frac{1}{2}(1 - g_T(\frac{L_3}{\lambda_3})) - g_{11}(1 - g_T(\frac{L_3}{\lambda_3}))\right)\right]. \tag{23c}$$

Figure 1 shows the relationship between the effective transmissivity of an aquifer and the dimensionless aquifer thickness for the case of a Gaussian correlation of local-scale conductivity and for different ε values. All the curves were calculated for $\sigma^2 = 1$, and they were normalized by dividing the results by the effective transmissivity value for two-dimensional flow.

2.5 Power averaging of the local-scale conductivity data

In this subsection we outline an approach within the framework presented above to find the exponent of the power-averaging method that is used for spatial averaging local-scale conductivity data to obtain the block-scale conductivity. Following *Desbarats* [1992b], and *Desbarats and Bachu* [1994], we define the spatial average value $\hat{k}_b$ of the point random function $K(\mathbf{x})$ over the volume V as:

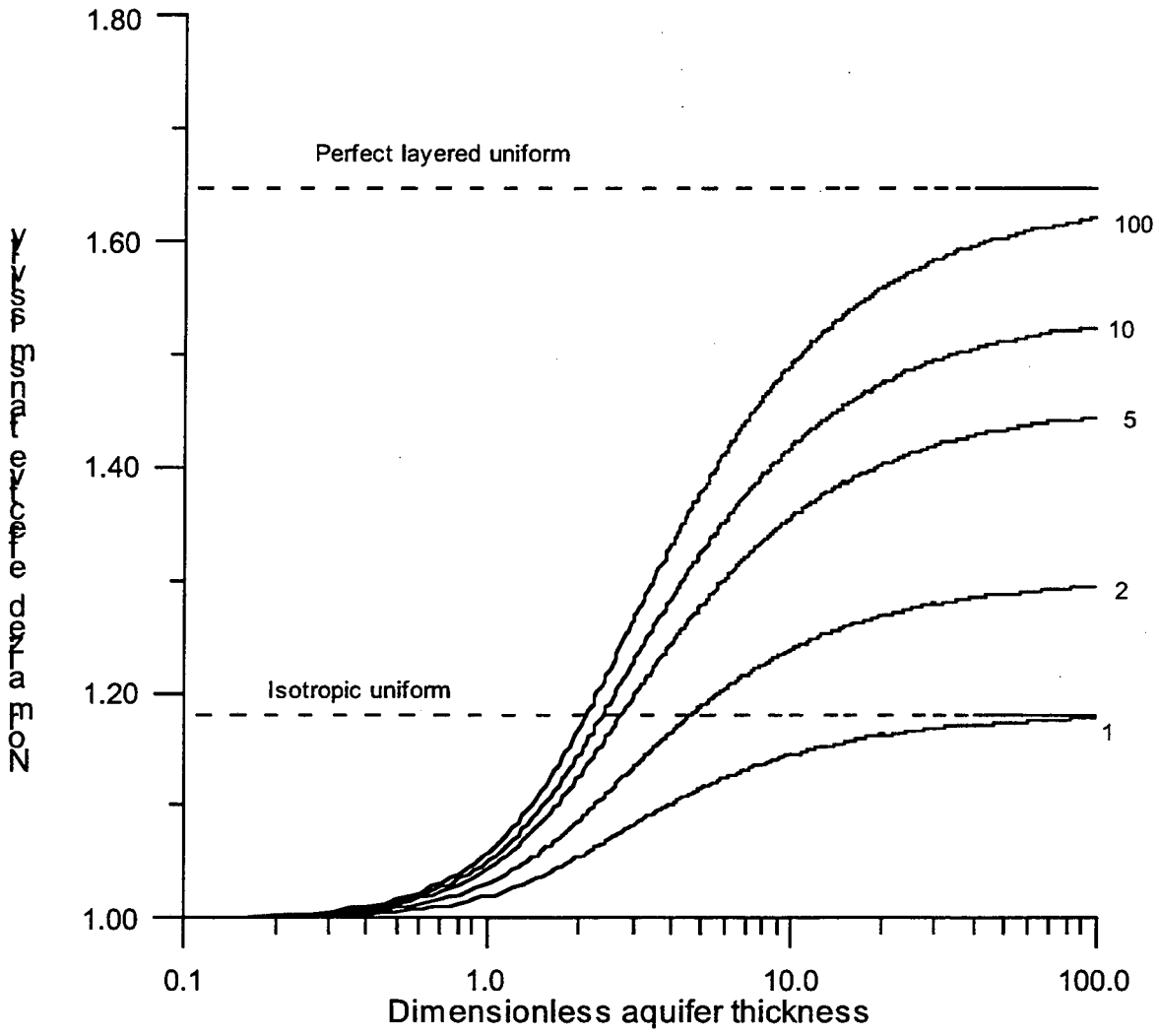

Figure 1. Gaussian correlation relationship between effective transmissivity and aquifer thickness (see text). Curves are labeled by the ratio of horizontal to vertical direction hydraulic conductivity correlation scale (ε).

$$\hat{k}_b = \left[V^{-1} \int_V K(\mathbf{x})^{\omega} dV \right]^{\frac{1}{\omega}}, \quad \omega \neq 0;$$
$$\hat{k}_b = \exp\left[V^{-1} \int_V \ln K(\mathbf{x}) dV \right], \ \omega = 0. \tag{24}$$

For $\omega = -1$, $\omega = 0$, and $\omega = 1$, eq. (24) yields harmonic, geometric, and arithmetic averaging, respectively. To evaluate the appropriate exponent value from the geometry of

flow domain, let us consider the following useful relationship from the properties of the ensemble "power" mean of lognormal distribution:

$$E\left[K(\mathbf{x})^{\omega}\right]^{\frac{1}{\omega}} = \exp\left[\mu + \omega\frac{\sigma^2}{2}\right] = k_g \exp\left(\omega\frac{\sigma^2}{2}\right). \tag{25}$$

To reach the expected mean of block-scale conductivity power-averaged over the block with volume V, let us consider the associated transformation for ln K_b. Starting from eq. (24) we obtain

$$\begin{aligned} E[\ln \hat{K}_b] &= \omega^{-1}E\left[\ln\left(V^{-1}\int_v \exp\left(\omega(\mu + Y')\right)dV\right)\right] \approx \\ &\mu + \omega^{-1}E\left[\ln\left(1 + V^{-1}\int_v\left(\omega Y' + \frac{\omega^2}{2}Y'^2 + \cdots\right)dV\right)\right], \end{aligned} \tag{26a}$$

$$Var[\ln \hat{K}_b] \approx \omega^{-2}E\left[\ln\left(1 + V^{-1}\int_v(\omega Y' + \cdots)dV\right)\right]^2, \tag{26b}$$

and taking into account that for a small x value of $\ln(1+x) \approx x - x^2/2$, after integration and averaging we have:

$$E[\ln K_v] \approx \mu + \frac{\omega}{2}\sigma^2(1-\varsigma_n), \tag{27a}$$

$$Var[\ln K_v] \approx \sigma^2\varsigma_n. \tag{27b}$$

Using the precondition that a distribution of ln K_v is a normal distribution, taking into account eq. (25), and using the power-averaging method of local data over the block, we finally have the expected mean $E[K_v]$ of block-scale conductivity,

$$E[K_v] = k_g \exp\left[\frac{\sigma^2}{2}(\omega(1-\varsigma_n) + \varsigma_n)\right]. \tag{28}$$

To estimate the value of exponent ω, we compare eq. (28) to the proposed upscaling equation (eq. 5) for the expected mean of the block-scale conductivity. This gives the relationship for ω,

$$\omega = 1 - \frac{2g_{scale}}{1-\varsigma_n}. \tag{29}$$

Using this exponential value for averaging, one can calculate the power-averaged values of k_v that has the same expected mean as the hydraulically averaged k_b values. Taking into account that for an n-dimensional block with equal side length $g_{scale} = (1-\varsigma_n)/n$; we obtain the known bound results [*Desbarats*, 1992b] for n-dimensional flow: $\omega = 1 - 2n^{-1}$. Thus, for the one-dimensional flow case, ω = -1; for the two-dimensional case, ω = 0; and for the three-dimensional case, ω = 1/3; note that these values do not depend on block size.

For horizontal flow in a confined aquifer that has a thickness comparable to the correlation scale of local conductivity and a horizontal grid block side length much greater than the correlation scale (i.e., $\varsigma_n \rightarrow 0$), according to eqs. (21a), (21b), and (29) the value of ω is

$$\omega = 1 - \frac{1}{3}\left[2 + g_T\left(\frac{L_3}{\lambda}\right)\right]. \tag{30a}$$

This value gradually increases from 0 to 1/3 with increasing aquifer thickness L_3 (Figure 2). For an anisotropic aquifer the value of exponent ω can also be predicted by using eqs. (23c) and (29):

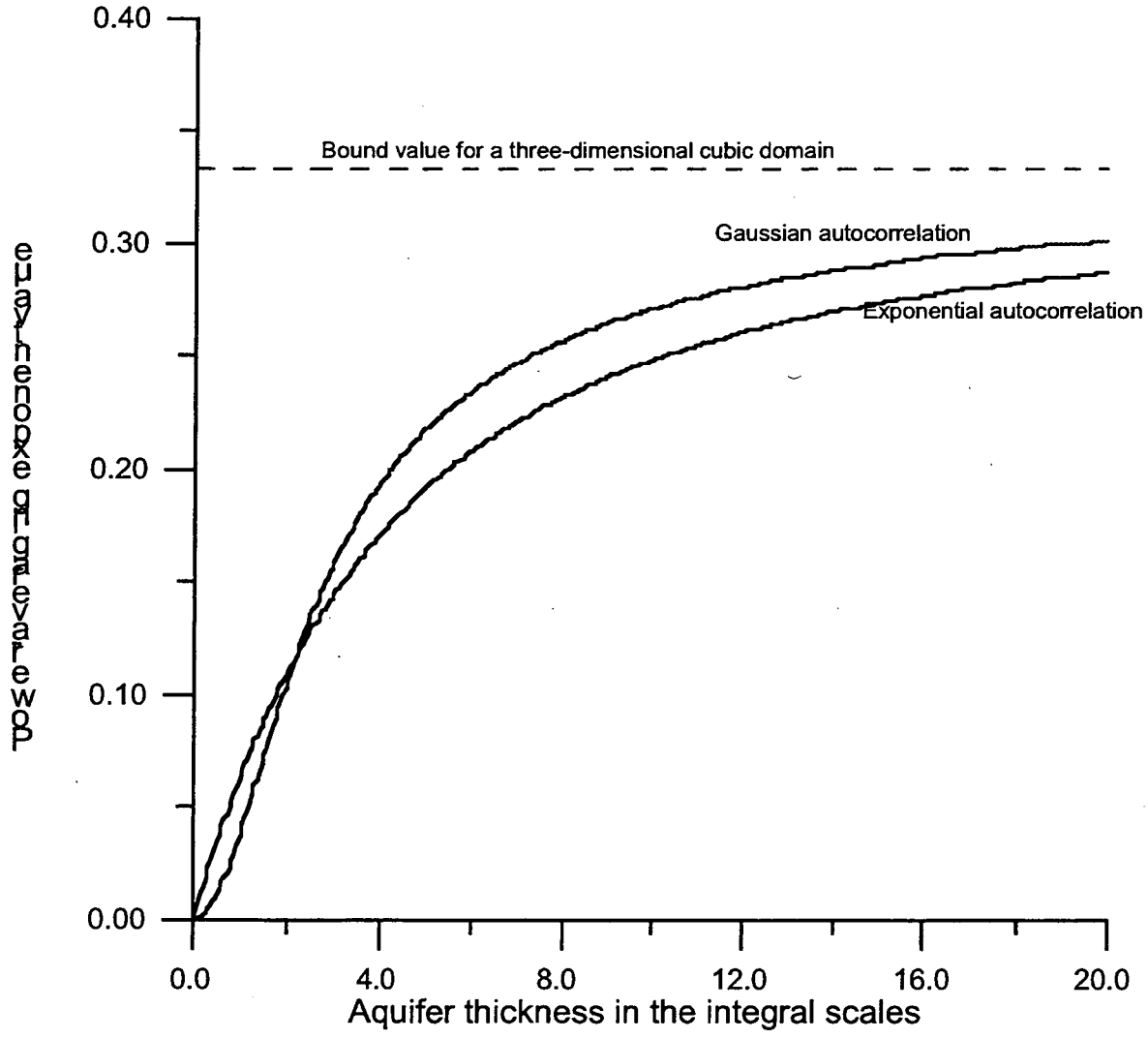

Figure 2. Relationship between the exponent ω value and the aquifer thickness.

$$\omega = \left[1 - g_T\left(\frac{L_3}{\lambda}\right)\right](1 - 2g_{11}). \tag{30b}$$

Note that here the value of ω changes from 0 to 1 and is different from the one proposed by *Desbarats and Bachu's* [1994] relationship for ω ($\omega = 1 - 2g_{11}$), which is valid only for a very thick aquifer where $L_3/\lambda_3 \rightarrow \infty$.

It is also interesting to note that if we want to calculate the effective conductivity of the flow domain **L** confined in all directions by using the power-averaging method, the

value of exponent ω depends on the ratio of domain side-length along the mean flow direction (L_1) to the domain side-lengths normal to it (L_2, L_3). This means that for a given aquifer thickness L_3 and $L_1 \neq L_2$, different values of ω are obtained for cases of the mean flow gradient applied along L_1 and L_2, respectively. Such an apparent aquifer anisotropy is due to the limitation of flow "freedom" in a heterogeneous confined flow domain.

Thus, results obtained in this subsection are a new addition to the *Desbarats'* [1992b] equation for power-averaging of local spatial data to simulate the hydraulic averaging of a heterogeneous medium. For equal block side lengths in all n dimensions of flow, the exponent value (ω) depends only on the physical dimension of the flow. However, for an arbitrary ratio of block side-lengths it also depends on these lengths, and can be calculated using eq. (29).

3. Verification against numerical results

A number of assumptions were made to determine the upscaling equations for the expected mean and variance of block-scale conductivity. In this section the semianalytical equations for the expected mean of block conductivity and its variances are verified against numerical results found in recent publications.

3.1 One-dimensional flow

In general, to obtain the expected mean and variance of block-scale conductivity for the one-dimensional flow case, one does not need detailed numerical flow modeling, because the value of block-scale conductivity for a grid block with size b_1 can be directly obtained by harmonic averaging the local data. In this subsection we would like to verify

two of the preconditions used: a) is spatially power-averaged block conductivity distribution a lognormal-like distribution? b) can upscaling eqs. (5) and (6b) predict the expected mean and the coefficient of variance of one-dimensional block-scale conductivity for large σ^2 values? One particular problem results from these two preconditions. In Appendix B one can find that for a lognormal distributed local conductivity field with the exponential structure of correlation, the correlation scale of conductivity is essentially less than the scale of log conductivity for large variance σ^2 values. Thus, in this subsection we will also examine what is the effective correlation scale of local conductivity.

For purposes previously mentioned, the exponential correlated one-dimensional process was precisely simulated on a fine grid with the ratio of spacing to correlation scale equals to 0.05 and different values of σ^2. The total length L_1 of each realization was 250 times the correlation scale. For each realization, the numerical one-dimensional analog of eq. (24) with the exponent value $\omega = -1$ was used to calculate the conductivity averaged over the blocks of length b_1. Figure 3 shows the empirical cumulative probabilities of the logarithm of block-scale conductivity for one-dimensional flow obtained by power-averaging local conductivities with $\sigma^2 = 3$. One can see from this figure that distributions of averaged conductivity appear lognormal for the wide range of cumulative probability values. This supports the precondition of lognormal distribution of block-scale values of conductivity.

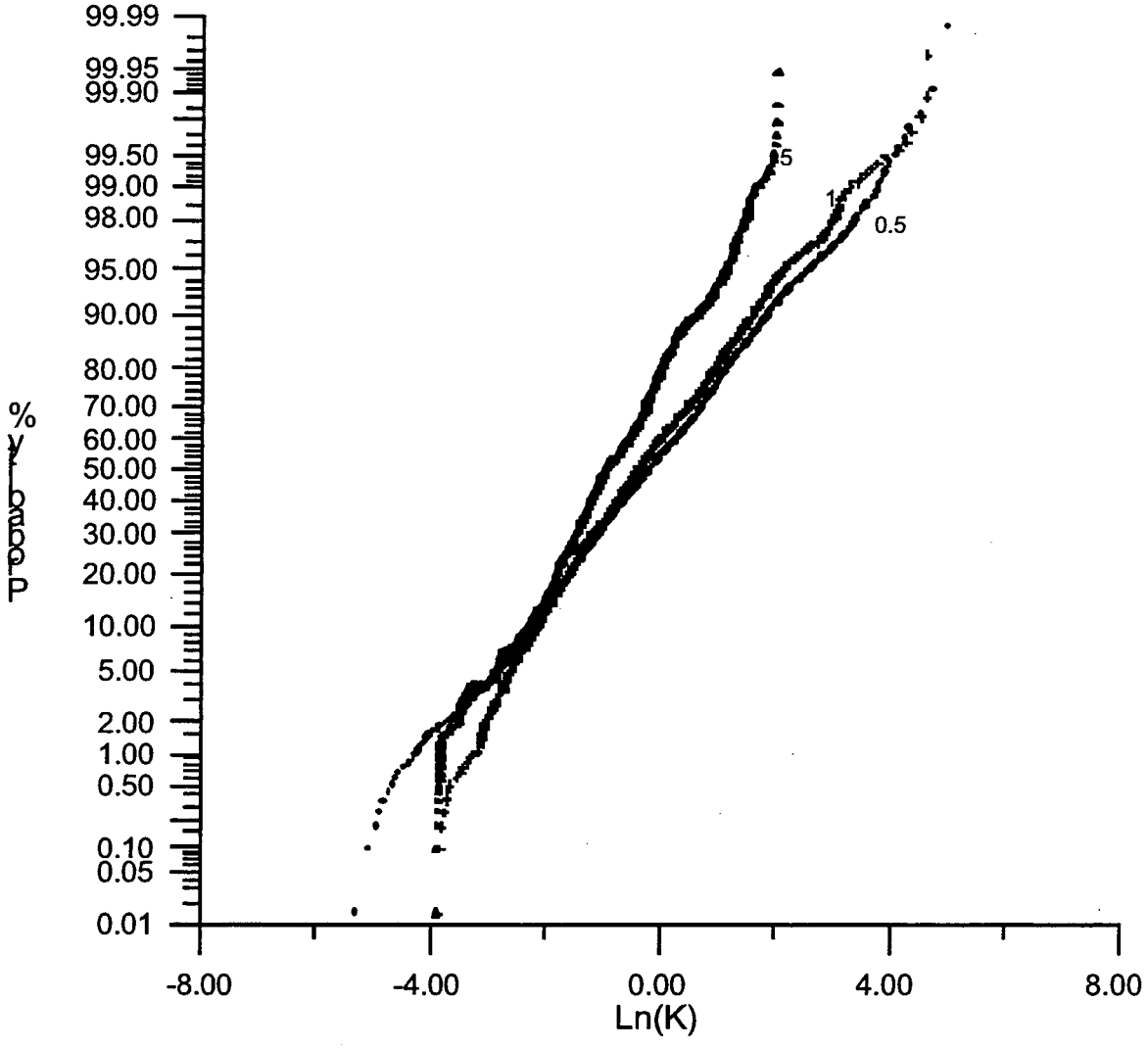

Figure 3. The empirical cumulative probabilities of the log of block-scale conductivity for one-dimensional flow. Curves are labeled by the ratio of the block-side length to the correlation scale (see text).

In Figures 4 and 5 one can see the analytical and numerical calculations of the expected mean and the coefficient of variance of block-scale conductivity for the one-dimensional case. Numerical results were obtained by power-averaging with the exponential value $\omega = -1$ over the blocks of the exponential correlated one-dimensional

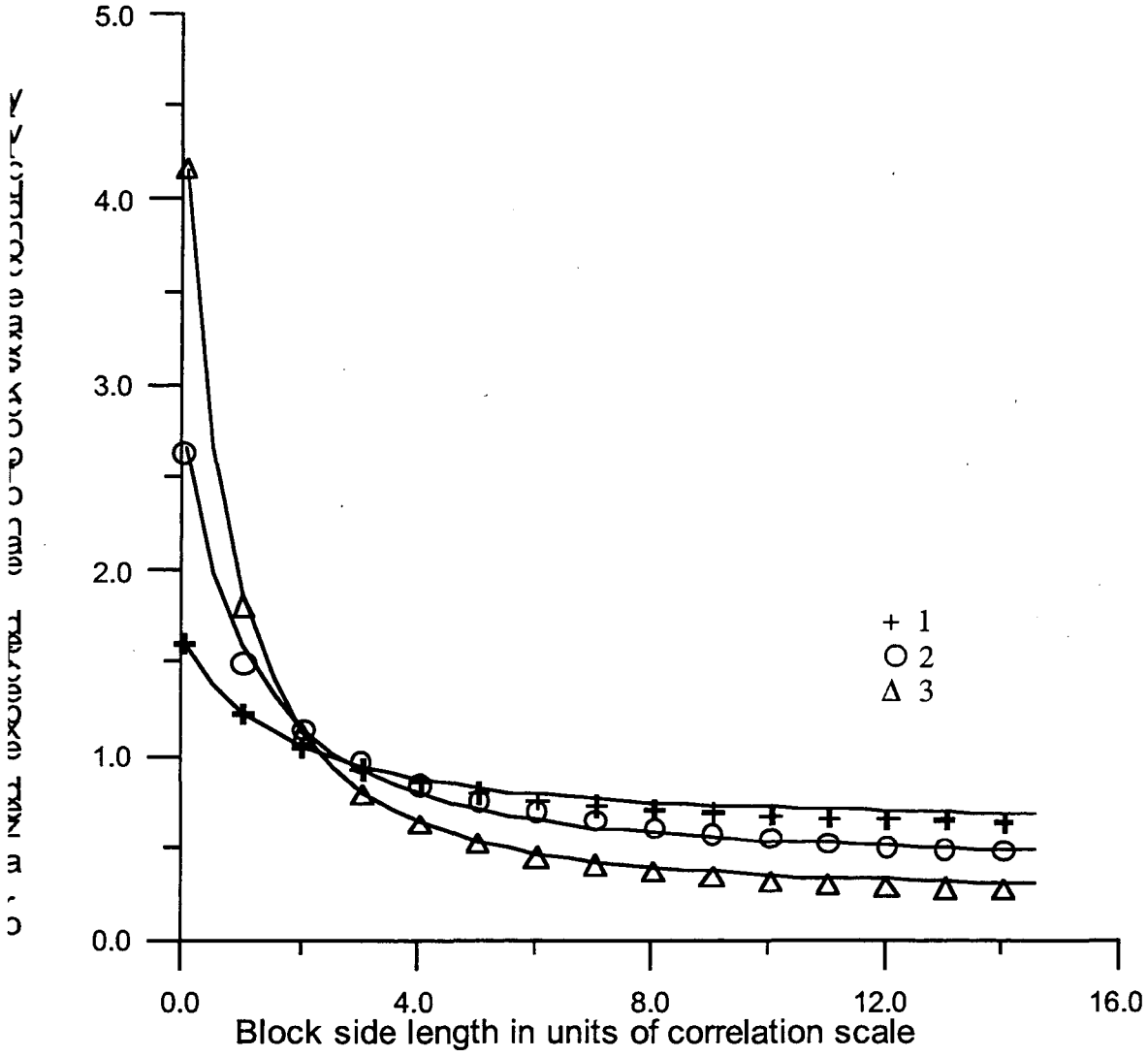

Figure 4. The expected mean of block-scale conductivity for the one-dimensional flow case. Lines are analytically calculated values and symbols are numerically calculated values. Curves are labeled by the values of log conductivity variance. All data were normalized by dividing them by the geometric mean.

process with σ^2 values equal to 1, 2 and 3. The expected mean and the expected coefficient variance C_v also were calculated analytically by using the upscaling equations for the one-dimensional flow case, i.e.,:

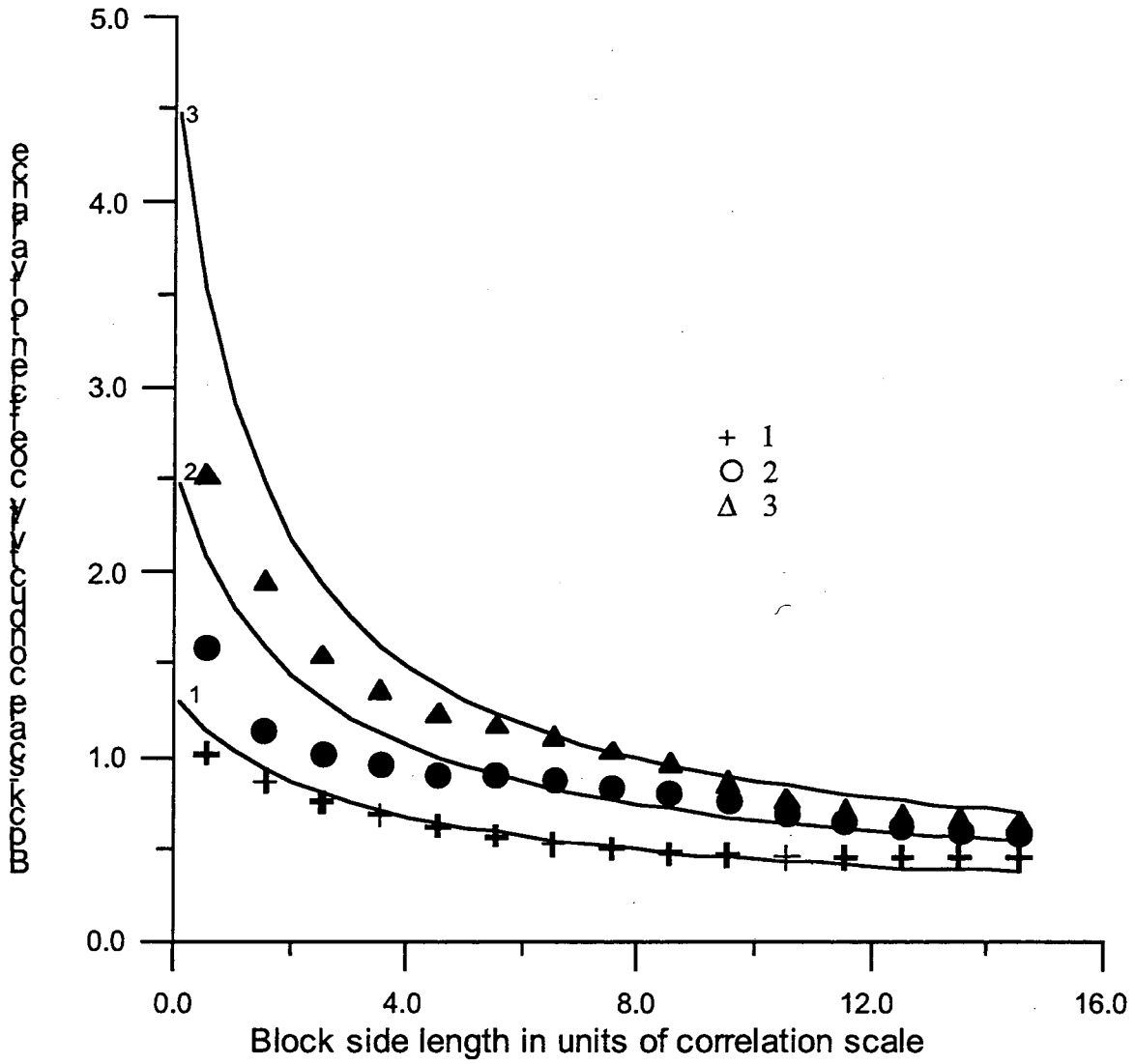

Figure 5. The coefficient of variance of block-scale conductivity for the one-dimensional flow case. Lines are analytically calculated values and symbols are numerically calculated values. Curves and symbols are labeled by the values of log conductivity variance.

$$k_b = k_g \exp\left[\sigma^2(\frac{1}{2} - g_{scale})\right] = k_g \exp\left[\sigma^2\left(\varphi(\frac{b_1}{\lambda}) - \frac{1}{2}\right)\right], \tag{31a}$$

$$C_v = \frac{\sqrt{Var[k_b]}}{k_b} = \sqrt{\exp\left(\sigma^2 \varphi(\frac{b_1}{\lambda})\right) - 1}. \tag{31b}$$

Figure 4 shows a very agreement of numerical and analytical results for all used σ^2 values. The agreement for the coefficient of variance is good for $\sigma^2 = 1$ for any size of block side length. For larger σ^2 values the agreement of numerical and analytical data begins to be good when the block-size value exceeds four times the correlation scale. Note that for analytical calculations of the expected mean, we used the correlation scale for log local conductivity and got a very good agreement between numerical and analytical results. According to these results, it is believable that the scale of log is really the effective scale for averaging hydraulic conductivity.

3.2 Two-dimensional flow

Rubin and Gomez-Hernandez [1990] and *Gomez-Hernandez* [1991] investigated the block-scale transmissivity using numerical simulation of steady-state flow on a fine grid after averaging the numerical result over blocks that have a size larger than the grid cell size. The steady-state two-dimensional flow in a rectangular aquifer with stochastic local-scale transmissivity field was simulated. The boundary conditions imposed were: no flow along the boundary parallel to one axis; and constant heads in each of the boundaries parallel to the other axes. The local-scale transmissivity was defined as a stochastic process with an isotropic exponential correlation function and lognormal distribution. The

size of the simulated domain $L_1 \times L_2$ was equal to 6.5 $\times$ 6.5 times the log transmissivity correlation scale. To numerically simulate the aquifer it was subdivided into a grid with the length of each side of the grid cell equal to 0.1 of the correlation scale. For a constant value of the mean of log local transmissivity and different values of variance, 200 realizations of the transmissivity field for each variance value were simulated using a turning band method in the grid nodes. For each realization, the steady-state flow was modeled by the finite difference method, using this numerical grid and the mentioned boundary conditions. Then, the values of block-scale transmissivity were computed for different block sizes by using the discrete version of eq. (2) for two-dimensional flow, and blocks of different sizes growing outwards from the center of the simulated domain. The mean and the variance of block-scale transmissivity were obtained for different block sizes by averaging over all 200 realizations for each local-scale transmissivity variance value.

Figure 6 compares the numerically calculated mean of the block-scale transmissivity and analytically predicted values of the expected mean as a function of the block side length and the variance of log local-scale transmissivity. The two-dimensional version of eq. (5) was used for the analytical prediction of the expected mean. To calculate the g_{scale} values for two-dimensional exponential correlation using eq. (11b), the effective correlation scale was increased 1.25 times. All numerical and analytical results were normalized by dividing by the effective value for two-dimensional uniform flow. One can see from Figure 6 that the comparison results show a good agreement of analytical

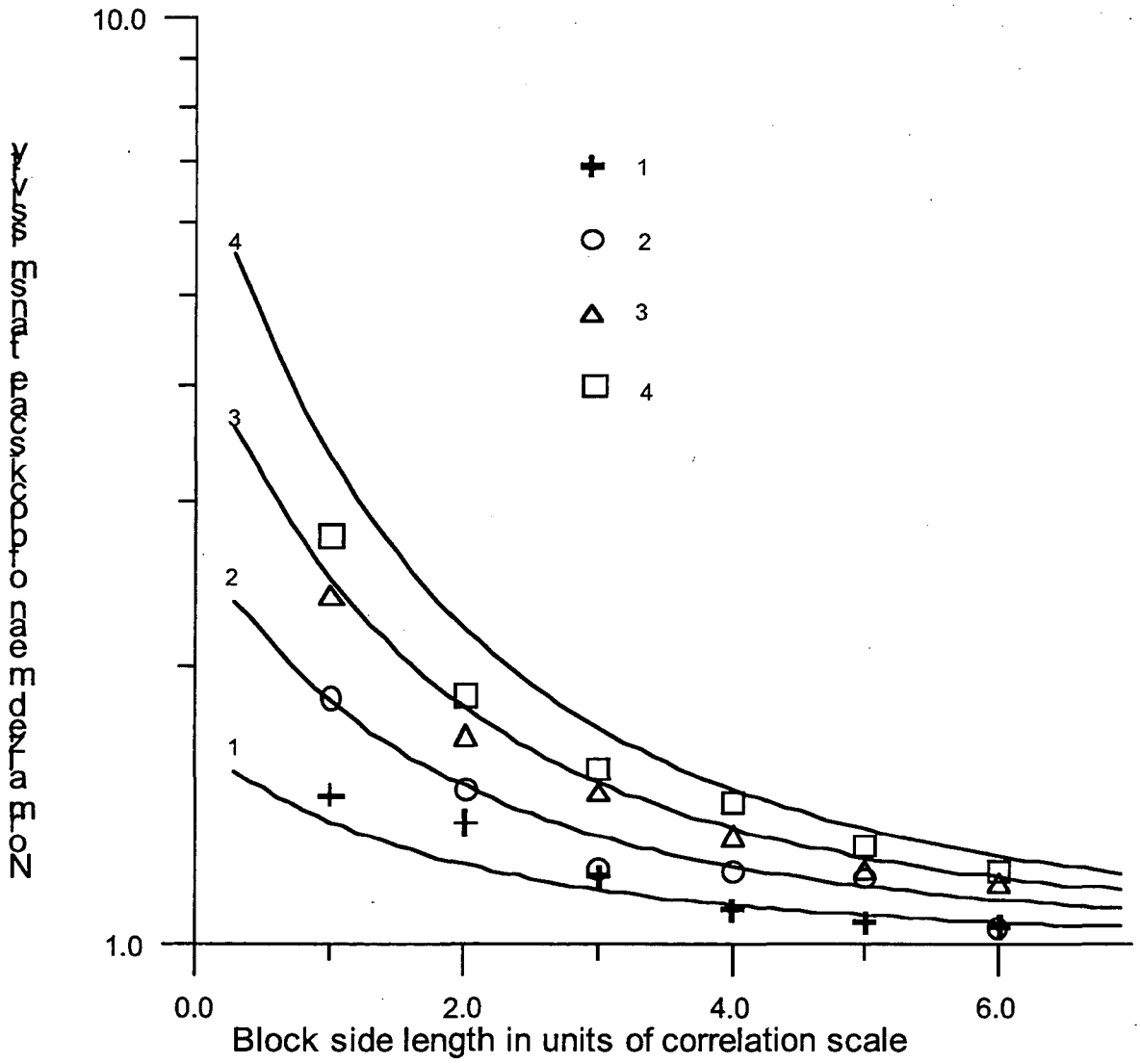

Figure 6. The expected mean of block-scale transmissivity for the two-dimensional flow case. Lines are analytically calculated values and symbols are numerically calculated values. Curves are leveled by the values of log conductivity variance. All data were normalized by dividing by the geometric means.

prediction with numerical data up to variances equal to 3. The errors of prediction for variance equals 4 are not significant for block side lengths exceeding two times the correlation scale.

Figure 7 shows the same graph for the coefficient of variance of block-scale transmissivity. As in the one-dimensional case, the coefficient of variance of the block-

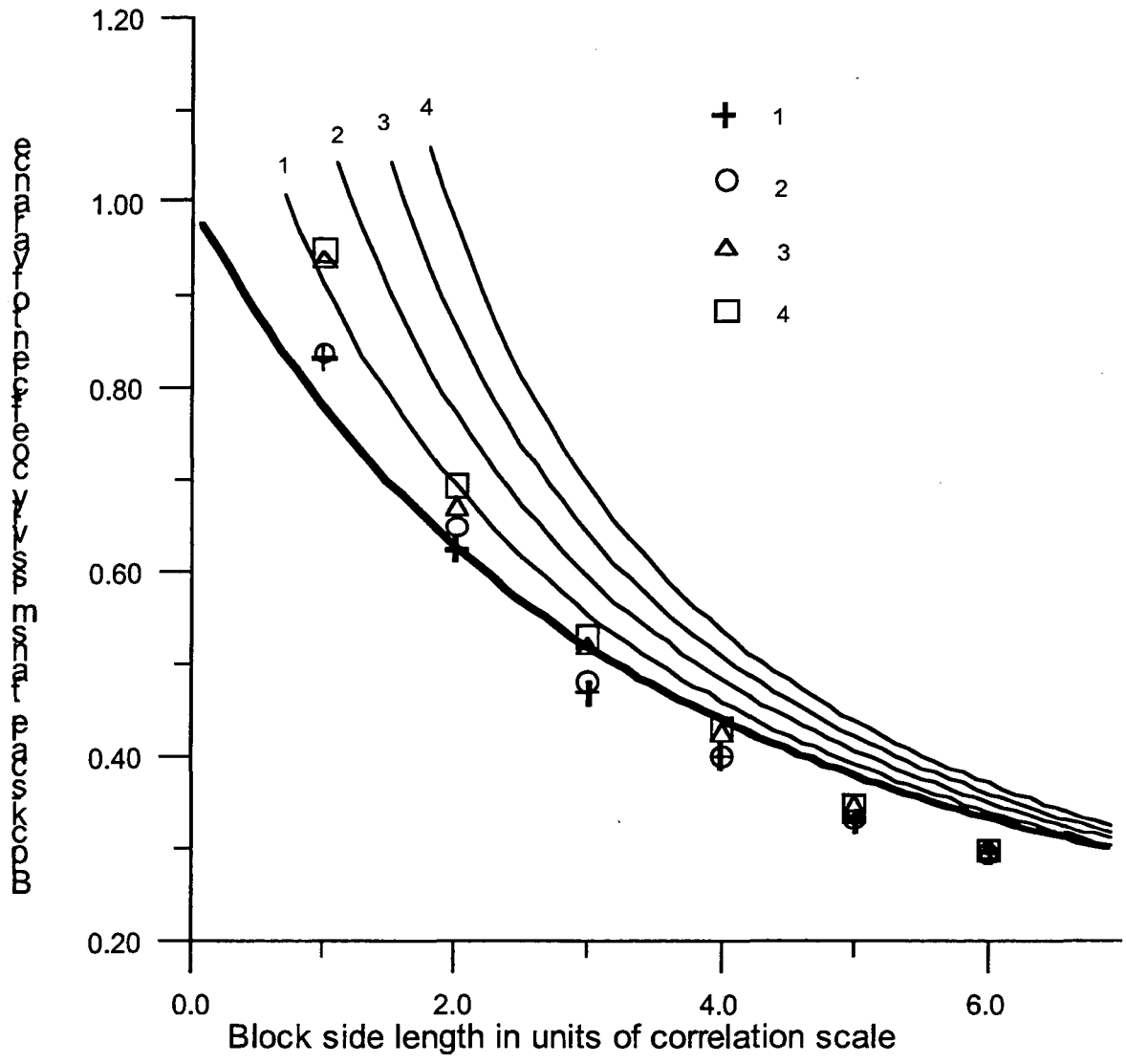

Figure 7. The coefficient of variance of block-scale transmissivity for the two-dimensional flow case. Lines are analytically calculated values and symbols are numerically calculated values. Curves and symbols are labeled by the values of log conductivity variance.

scale values is less predictable analytically than the expected mean. One the possible reason for the numerical values being smaller than the analytical ones is that the flow domain was equal to 6.5 × 6.5 times the correlation scale. This means that the variance of log transmissivity for this finite domain was less that the ensemble variance by a factor of $(1-\zeta_2(6.5))$, which gives a value of about 90% for the ensemble variance.

3.3 Three-dimensional flow

Dukaar and Kitanidis [1993] investigated the block-scale transmissivity using the numerical method based on general Taylor-Aris moment analysis. This method allows to find out the effective parameters of two-dimensional flow by solving specially determinated periodic three-dimensional flow problem and then integrating the results into the vertical direction. Thus, in this paper the block-scale transmissivity was determinated using a three-dimensional spatially variable local hydraulic conductivity tensor and locally variable three-dimensional flow. The stationary Gaussian log conductivity variation process with the Gaussian covariation function was used for generating a three-dimensional local hydraulic conductivity field. A number of experiments for determining effective grid transmissivity were performed for various block sizes and log conductivity variances. For each block size and variance of log conductivity the expected block-scale transmissivity mean and the variation coefficient were obtained by averaging the results of over 10 realizations.

The series of experiments discussed in this subsection examined the influence of aquifer thickness on block-scale transmissivity. The expected block-scale transmissivity mean was found for the aquifer thickness (L_3) change from 1 to 30 times the correlation scale, and for a constant horizontal block size equal to 30 times the correlation scale. Figure 8 shows the comparison of analytical and numerical values of the mean block-scale transmissivity. Analytical values of transmissivity were determined as $L_3 \cdot k_b$, where the block-scale conductivity k_b values were calculated for the given block size equal to

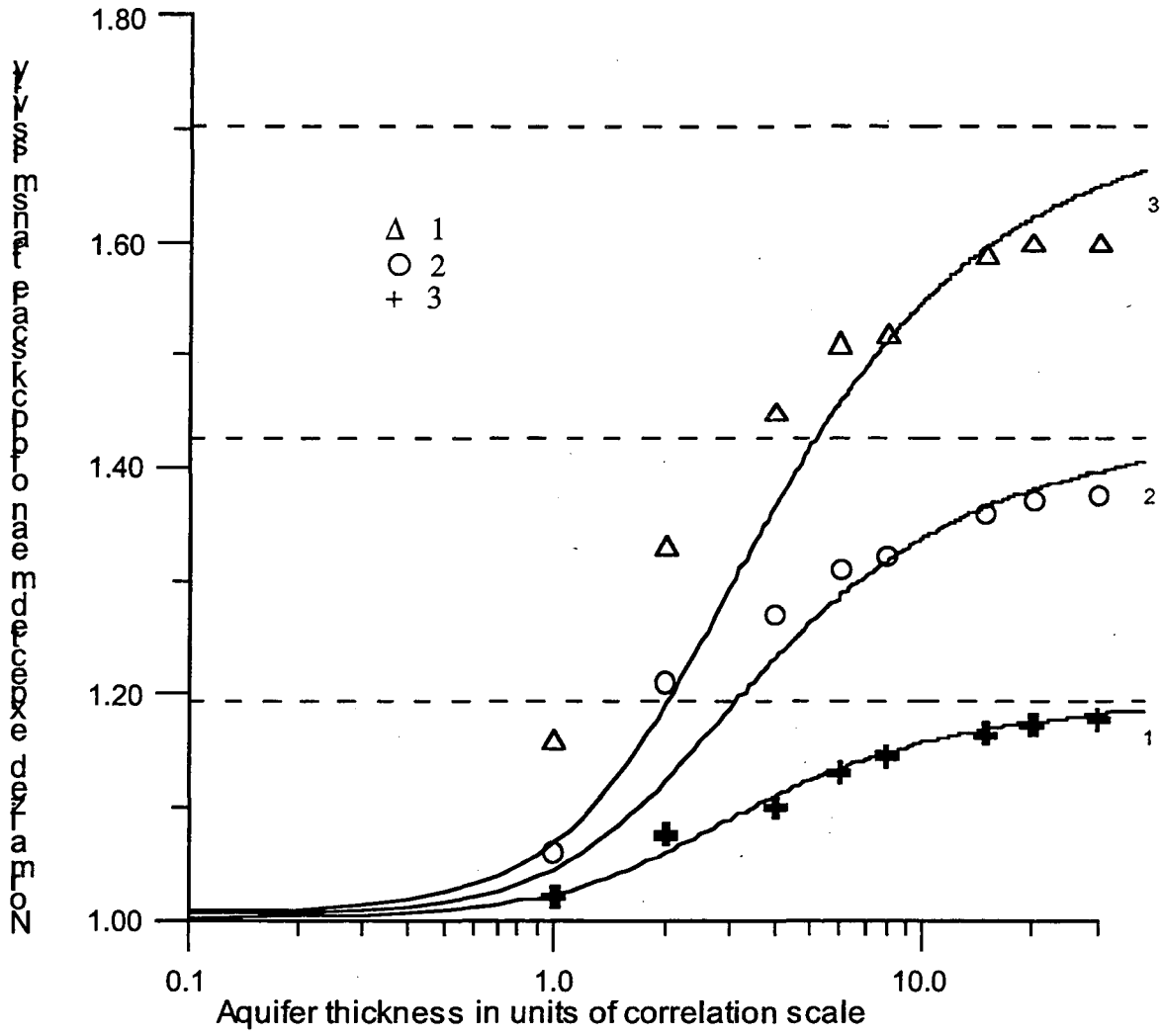

Figure 8. The expected mean of block-scale transmissivity for three-dimensional flow case. Lines are analytically calculated values and symbols are numerically calculated values. Curves are labeled by the values of log conductivity variance. All data were normalized by dividing by the geometric mean. The horizontal block length equals to 30 times the correlation scale.

$30\times30\times L_3$ times the correlation scale. All data were normalized by dividing by the effective value for two-dimensional uniform flow. From Figure 8 one can find a very good agreement between numerical and analytical data for the variance equals to 1 and satisfactory agreement for variances equal to 2 and 3.

Figure 9 shows an agreement of numerical and analytical calculations of the coefficient of variation of block transmissivity for variance of log conductivity equals to 2 and two different values of the aquifer thickness: 10 and 4 times the correlation scale, respectively.

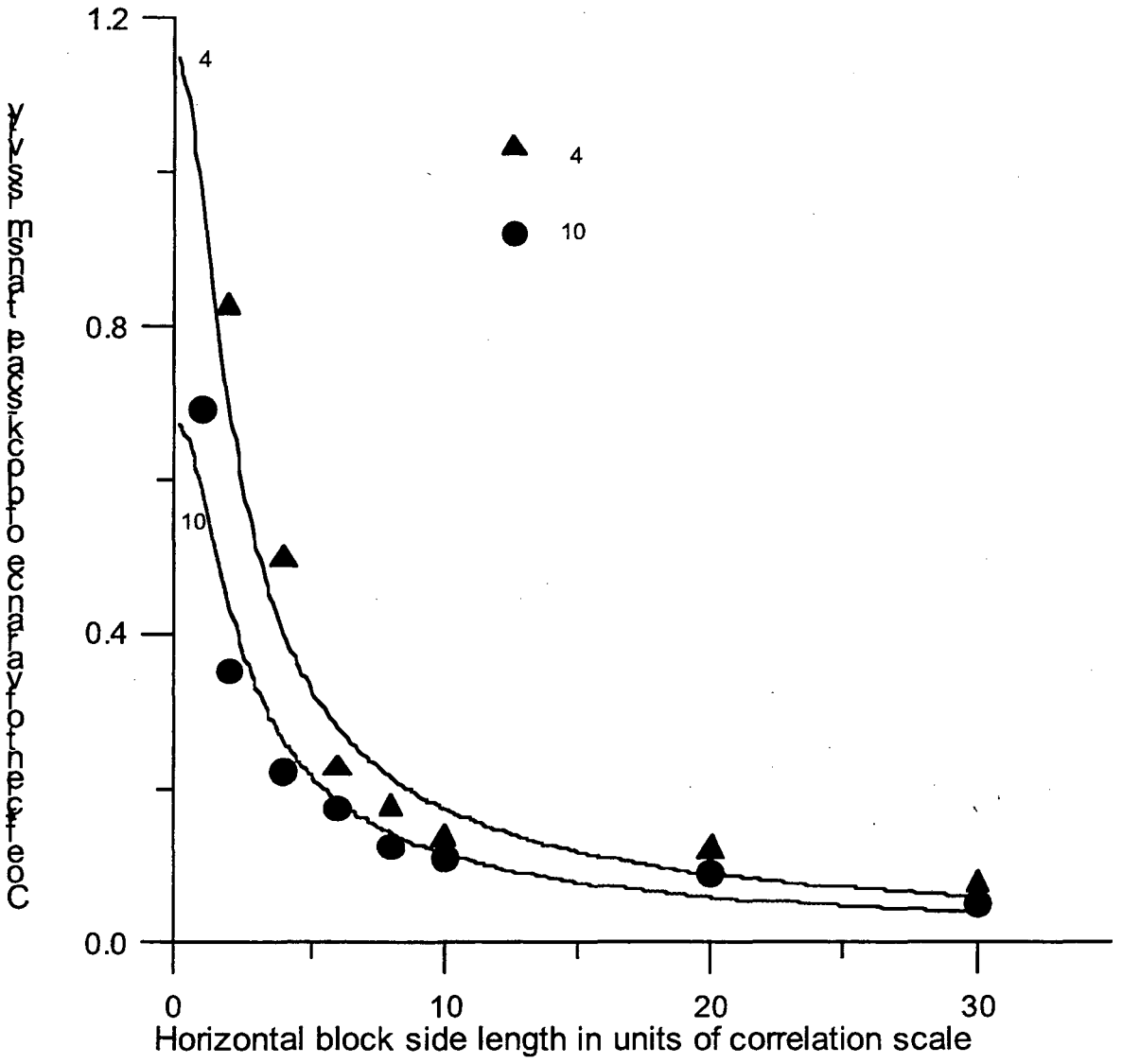

Figure 9. The coefficient of variance of block-scale transmissivity for three-dimensional flow case. Lines are analytically calculated values and symbols are numerically calculated values. Curves and symbols are labeled by the values of aquifer thickness in units of correlation scale. The log conductivity variance equals to 3 for cases in this figure.

Desbarats [1992b] used results of three-dimensional numerical simulations of steady-state flow in a heterogeneous medium with the exponential correlation of log local-scale conductivity to estimate the expected mean of block-scale conductivity and the value of power-averaging exponent for a rectangular flow domain. Then he computed the values of block-scale transmissivity for different block sizes by using the discrete version of eq. (2) for three-dimensional flow. To investigate the effect of the geometry of flow domain on the power-averaging exponent ω, he numerically estimated the ω values for the domain that had constant side lengths in two directions ($b_2 = b_3 = 3$ times the correlation scale) and increased the side length along the main flow direction (b_1) from 0 to 20 times the correlation scale. Analytically, the value of the exponent can be predicted by using eq. (29) for the three-dimensional flow case and given block side lengths.

Figure 10 shows the comparison of the numerical and analytical results. One can see from this figure a good agreement of analytical data and numerical experiments for the relatively cubic blocks. However, when the transversal block length increases, the difference between analytical and numerical data also increases. The reason for this can be found in the numerical data and in the analytical estimations. Note that for the exponential structure of correlation we use the symmetric-exponential correlation function to approximate. That is why the bounding lines (dashed) are shown in Figure 9. The bounding lines were calculated taking into account eqs. (17) and (18). One can see from this figure that the numerical data are bound by these lines.

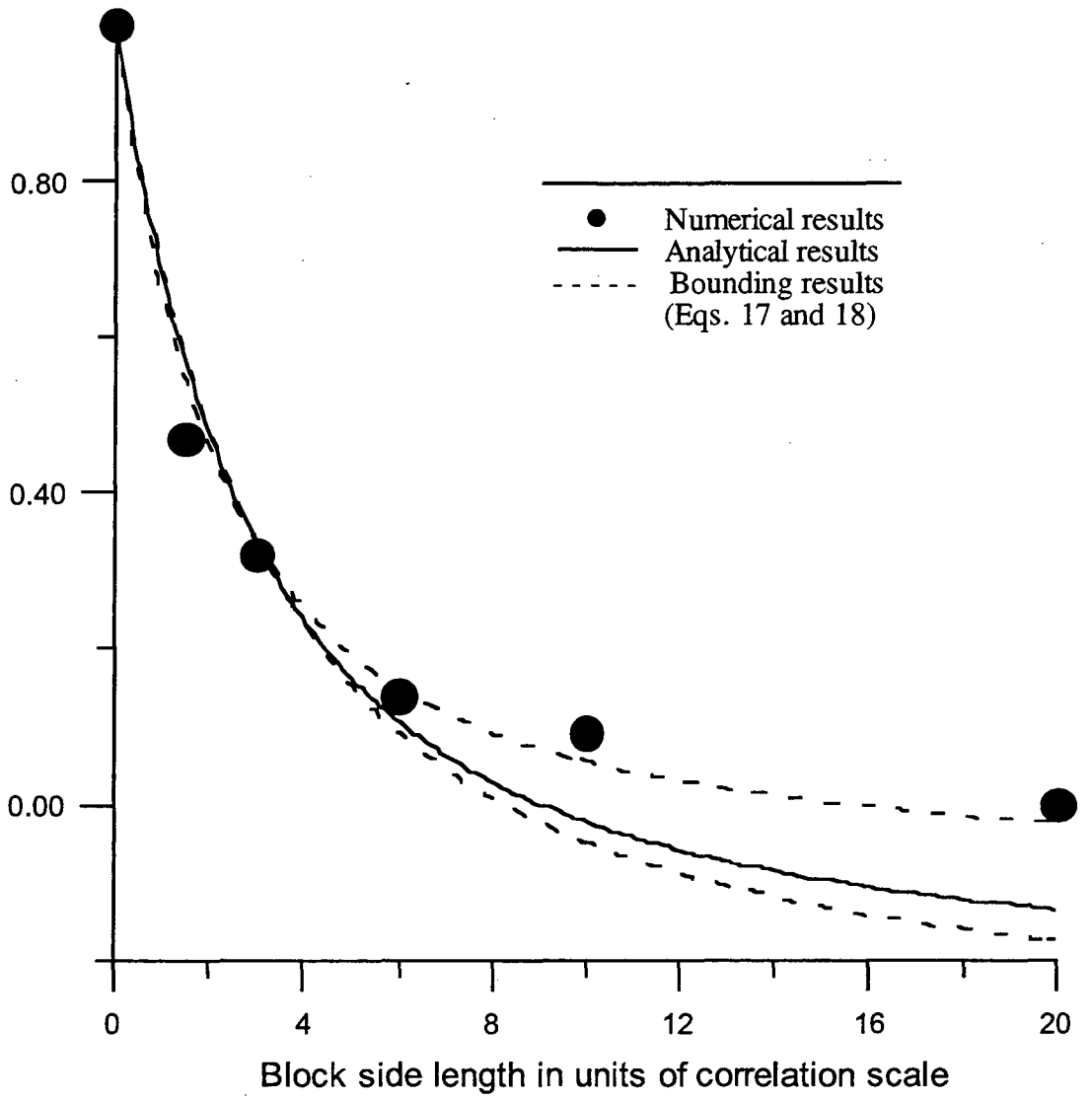

Figure 10. Power-averaging exponent value versus the block side length along the main flow direction for the constant block-length transverse flow.

Thus, in this section the comparison of the proposed upscaling equations for the block-scale conductivity with numerical data shows that analytical estimates (using eq. (5)) of the expected mean of block-scale conductivity agree well with numerical data for all physical dimensions of flow and local-scale hydraulic log conductivity variances up to 3. Although the coefficient of variance of block-scale conductivity predicted by eq. (6b) does

not agree so well with the numerical data for small block sizes, asymptotically the method gives satisfactory results for large blocks. Thus, the verification presented here show that the proposed upscaling equations can be used to estimate block-size conductivities.

4. Discussion and conclusion

Present development of upscaling properties of a stochastic heterogeneous medium from the local-scale data to a larger scale can be useful for a broad range of applications of stochastic theory investigating flow in confined domain. Let us discuss some problems where we can see applications of the approach discussed in this paper.

4.1 Computational stochastic subsurface hydrodynamics

Direct numerical simulation of processes is used to understand flow and transport phenomena in a strongly heterogeneous medium. Examples of such an approach can be found in *Tsang et. al.* [1988], *Tompson and Gelhar* [1990]. The basic approach here is to simulate flow and transport in a heterogeneous medium by using a very fine numerical grid to obtain the representative fields of head and flow velocity; that is, the model of natural velocity fluctuation. *Van Lent and Kitanidis* [1996] stated, that typically a discretization of 5-10 nodes per correlation scale is required and it should be even finer as the log of local conductivity variance increases.

A typical example where this approach can be used is a three-dimensional contaminant plume spreading in uniform flow in a heterogeneous medium [*Tompson and Gelhar,* 1990]. For example, the size of the modeling flow domain is an important critical number in examining transversal and longitudinal macrodispersion. On the one hand the domain size should significantly exceed the correlation scale (by one or two orders of magnitude). However, precise modeling of the flow field requires a very fine resolutions of the grid (by an order of magnitude of 10^{-1} and 10^{-2} on the correlation scale). Trying to satisfy these two criteria one can run into computational problems because of the need of billions of grid nodes. A reasonable way to resolve this problem is to decrease the domain size of the transversal-to-flow section (relative the longitudinal direction). Using the upscaling equations discussed in this paper, one can determine how this domain compares to the uniform media. Table 1 show the ratio of the expected means of block-scale hydraulic conductivity for $\sigma^2 = 3$ and for a flow domain having a the constant length L_1=50 times the correlation scale in one direction, and different domain sizes in the other two directions. The k_1 value was calculated when the main flow direction is along L_1; the k_2 value was calculated for the case when the main flow direction is along L_2. Here k_{ef} is the effective value for a three-dimensional uniform medium. One can see from the table that the influence of apparent anisotropy of a bounded flow domain can be significant for a non-cubic domain with the small (less than 0.2-0.3) ratio of the domain size in the longitudinal direction to the size in the transversal direction.

Table 1. Comparison of the expected conductivity in the longitudinal direction k_1 and the transverse direction k_2, and the effective value for uniform flow k_{ef} for a rectangular flow domain.

Domain Dimensions $L_1 \times L_2 \times L_2$	k_1/k_2 Gaussian correlation	k_1/k_2 Exponential correlation	k_1/k_{ef} Gaussian correlation	k_2/k_{ef} Exponential correlation
50×1×1	0.091	0.130	0.208	0.266
50×5×5	0.534	0.455	0.662	0.598
50×10×10	0.769	0.690	0.840	0.784
50×15×15	0.861	0.806	0.906	0.868
50×20×10	0.910	0.871	0.939	0.913
50×30×10	0.960	0.941	0.973	0.961
50×40×40	0.985	0.978	0.990	0.985
50×50×50	1.00	1.00	1.00	1.00

Another useful application is to use the power-averaging method to calculate interface conductivity between grid nodes for simulating flow in a heterogeneous medium. The values of interface conductivity can be calculated by using simulated values of conductivity in two neighboring nodes along a given direction. For the cubic blocks, the exponent ω value should be 1/3.

4.2 Upscaling and downscaling from local data to the transmissivity of an aquifer

Another possible application is an upscaling and downscaling from local data to the aquifer transmissivity, which is averaged over aquifer thickness. Sometimes the value of aquifer transmissivity should be estimated by using core-scale data measured in a vertical section of an aquifer. To achieve this, the power-averaging method with the

exponent value defined by eqs. (30a) and (30b) can be used for upscaling from the point-measured conductivity to the aquifer transmissivity.

Sometimes field data present the opposite problem; that is, data on spatial variation of transmissivity are available, but one needs to know the variation at the local-scale level. This problem, of course, cannot be solved correctly for a general case, because the scale of the measuring tools here is larger than the scale of the local data. However, the method developed in this paper can be useful for one particular important problem: to estimate the variance of log local-scale conductivity σ^2 by the use of the known value of log transmissivity variance σ^2_T obtained from the field data. Let us assume the variance of transmissivity to be equal to that of the local-scale value. According to the obtained upscaling equation for the variance, these values are related by:

$$\sigma_T^2 = \varsigma_{scale}\sigma^2 . \tag{32}$$

The problem is that, as a rule, we do not know exactly what is the real volume of the "block," which is represented by the transmissivity measuring point. Formally we know that in the vertical direction it is the aquifer thickness L_3. To obtain the size of this "block" in a horizontal direction, we can use the autocorrelation function to perform the averaging over a block random function (Appendix A). The integral correlation scale of this function I is equal to the sum of the block horizontal size and the correlation scale of random function λ. Thus, obtaining from the variogram analysis of the field transmissivity data its horizontal correlation scale I_h, one can rewrite eq. (32) as:

$$\sigma_T^2 = \sigma^2\varphi(\frac{L_3}{\lambda})\varphi^2(\frac{I_h}{\lambda} - 1) . \tag{33a}$$

Taking into account that for a large u $\varphi(u) \approx 2/u$ we obtain the relationship between variances and correlation scales of local-scale conductivity and transmissivity:

$$\sigma^2 \approx 0.25\sigma_T^2\varphi^{-1}(\frac{L_3}{\lambda})\left(\frac{I_h}{\lambda}-1\right)^2. \tag{33b}$$

Thus, to estimate local-scale conductivity variance one needs the variance and the correlation scale of field-measured transmissivity data.

4.3 Summary and conclusion

This paper presents the development of a relationship between the local-scale hydraulic conductivity and the conductivity hydraulically averaged over a block, i.e., block-scale hydraulic conductivity. The block-scale conductivity is considered to be a stochastic function, and a semianalytical method is used to obtain the expected mean and the variance of this function. The results are summarized as follows:

1. The equation for the expected mean of the block-scale conductivity has the form $k_{ef} = k_g \exp\left[\sigma^2(\frac{1}{2} - g_{scale})\right]$ for a given lognormal distribution of local-scale hydraulic conductivity with isotropic autocovariance. The equation for the variance of the log of the block-scale conductivity has the form $Var[Y_b(\mathbf{x})] = \sigma^2 \cdot \varsigma_{scale}$. The upscaling functions g_{scale} and ζ_{scale} are different for the cases of quasi-parallel and convergent flows. In the case of quasi-parallel flow, the equation for the upscaling function is obtained by using perturbation analysis, followed by extrapolation of the result to a large variance of local hydraulic conductivity.

2. The derived equation for the block-scale conductivity completely described the result for the flow domain within limits of small and large values of the ratio of block size to the local hydraulic conductivity correlation scale (for any spatial flow dimensions). Comparison of these analytical results with numerical calculations of the expected mean and variance of the block-scale conductivity, given in recent technical literature, shows good agreement over a broad range of log local-scale conductivity variance for all physical dimensions of the flow domain.
3. An equation of effective transmissivity for uniform flow in an aquifer whose thickness is comparable to the correlation scale of local hydraulic conductivity is proposed on the basis of asymptotic solutions of the upscaling function. The value of effective transmissivity thus obtained depends on the ratio of correlation scale to aquifer thickness, and lies between the effective conductivities of the two- and three-dimensional cases. An equation for effective transmissivity of aquifer with different correlation scales of local conductivity in the horizontal and the vertical directions is also proposed.
4. The spatial power-averaging method of local-scale conductivity data described by earlier authors is developed in this paper, and an analytical equation for the averaging exponent is obtained. This equation gives for three dimensional flow the value of 1/3, which agrees with the Landau and Lifshitz (1960) conjecture. However, for a flow domain which is infinite horizontally but of a limited size in the vertical direction, the averaging exponent is found to be between 0 and 1/3. In general, the value of the

exponent depends on the ratio of the aquifer thickness and the correlation scale of local conductivity.

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Nomenclature

n	spatial dimension of flow, where $n = 1$ or $n = 2$ or $n = 3$, [-]
$\mathbf{x}(x_1..,x_n)$	Cartesian coordinate system, [L]
$\mathbf{L}(L_1..,L_n)$	size of flow domain, [L]
$\mathrm{b}(b_1..,b_n)$	size of blocks covering the flow domain, [L]
$K(\mathbf{x})$	spatial variable local hydraulic conductivity, [L/T].
$K_b(\mathrm{x})$	block-scale hydraulic conductivity, [L/T]
$Y(\mathbf{x})$	stationary random field, where $Y(\mathbf{x}) = \ln K(\mathbf{x})$, [-]
μ	mean value of $Y(\mathbf{x})$, where $\mu = E[Y(\mathbf{x})]$, [-]
σ^2	log conductivity variance, where $\sigma^2 = Var[Y(\mathbf{x})]$, [-]
$\rho(\mathrm{u})$	log conductivity autocorrelation function, [-]
λ	integral correlation scale of log conductivity, [L]
k_g	geometric mean of local hydraulic conductivity, where $k_g = \exp(\mu)$, [L/T]
k_{ef}	effective value of hydraulic conductivity for uniform flow (L/T).
k_b	expected mean of block-scale conductivity, where $k_b = \mathrm{E}[K_b(\mathbf{x})]$, [L/T]
g_{scale}	upscaling function, [-]
ς_{scale}	upscaling function, [-]
ω	averaging exponent, [-]

APPENDIX A: Block Covariation Function for Gaussian Stochastic Process

Let us consider a stationary random function $Y(\mathbf{x})$ with Gaussian autocorrelation:

$$Cov_y = \sigma^2 \prod_{i=1}^{n} \exp(-x_i^2 / \lambda_i^2) \ , \tag{A.1}$$

where n = 1,2,3 is a space dimension of Y, x_i a separation along i-axis, and λ_i the correlation scale.

The covariation function $Cov(x, B)$ averaged over blocks of random function $Y(\mathbf{x})$ can be represented in the form:

$$Cov(x, B) = \sigma^2 \prod_{i=1}^{n} Cov_0(x_i / \lambda_i, B_i / \lambda_i), \tag{A.2}$$

where B_i is a block-side length along the i- direction and the partial covariation $Cov_0(x / \lambda, B / \lambda)$ is

$$Cov_0(\frac{x}{\lambda}, \frac{B}{\lambda}) = B^{-2} \int_{X-0.5B}^{X+o.5B} \int_{X+x-0.5B}^{X+x+0.5B} \exp\left[-(\theta_1 - \theta_2)^2 / \lambda^2\right] d\theta_1 d\theta_2 \ . \tag{A.3}$$

Upon integrating (A3) we obtain the equation for partial covariation as a function of dimensionless block side length $\overline{B} = B / \lambda$, and dimensionless separation $\overline{x} = x / \lambda$:

$$\begin{aligned} Cov_0(\overline{x}, \overline{B}) = 0.5\overline{B}^{-1} \{ & \sqrt{\pi}[(x_0 + 1) erf(\overline{x} + \overline{B}) - 2x_0 erf(\overline{x}) + (x_0 - 1) erf(\overline{x} - \overline{B})] \\ & + \overline{B}^{-1}[\exp(-(\overline{x} + \overline{B})^2) - 2\exp(-\overline{x}) + \exp(-(\overline{x} - \overline{B})^2)]\}; \quad x_0 = x / B \end{aligned} \tag{A.4}$$

For the zero separation eq. (A.4) is going to be equal to eq. (19):

$$Cov_0(0, \overline{B}) = \varphi'(\overline{B}) . \tag{A.5}$$

The autocorrelation function $\rho(\overline{x}, \overline{B})$ of a value averaged over the block can be calculated as:

$$\rho(\overline{x}, \overline{B}) = \prod_{i=1}^{n} \frac{Cov_0(\overline{x}_i, \overline{B}_i)}{\varphi(\overline{x}_i)}. \tag{A.6}$$

For a small ratio of the block-side length to the correlation scale, eq. (A.6) is Gaussian autocorrelation, and for a ratio of more than 5-7, the equation for autocorrelation function can be rewritten in the simple form:

$$R\,(\overline{x}, \overline{B}) = \prod_{i=1}^{n} (1 - x_i / B_i) \quad \text{or} \quad 0 \quad \text{for} \quad x_i > B_i \tag{A.7}$$

The correlation scale along each direction of averaged process equals to $\lambda_i + B_i$.

APPENDIX B: Integral Scale of Spatial Covariance of Lognormal Distributed Random Function

Let us analyze the spatial correlation scale for stationary random function *K(x)* for the given normal distribution of $Y = \log(k)$ with the expected mean μ, the variance σ^2, and the spatial covariance $Cov_Y = \sigma^2 r(x)$. Here *r(x)* is the function of the separation between the points. Using the moment-generating function for a normal random variable

$$M(n) = E[\exp(nY)] = \exp(n\mu + \sigma^2 n^2 / 2), \tag{B.1}$$

the second spatial moment $Cov_k(x)$ will be:

$$Cov_k(x) = \exp(2\mu + \sigma^2)[\exp(\sigma^2 r(x)) - 1], \tag{B.2a}$$

and for the normalized autocorrelation function $\rho_k(x)$ dependent on distance and variance:

$$\rho_k(x) = \frac{\exp[\sigma^2 r(x)] - 1}{\exp(\sigma^2) - 1}. \tag{B.2b}$$

It is clear from the structure of eq. (B.2b) that for the small values of variance $\sigma^2 \to 0$ the normalized autocorrelation function ρ_k(x) is almost the same as function ρ (x). However, for the large variance these functions can be very different. Let us inspect the difference between autocorrelation functions $\rho(x)$ and ρ_k(x) for two spatial autocorrelation functions of Y(x): i.e., exponential covariance, $\rho(x) = \exp(-x / \lambda)$; and Gaussian covariance, $\rho(x) = \exp[-(0.25\pi x / \lambda)$. We will use the ratio of the spatial integral scales equals to

$$I = \frac{\int_0^\infty \rho_k(x)dx}{\int_0^\infty \rho(x)dx}. \tag{B.3}$$

The results of the integration of eq. (B.3) are shown in Figure 11. One can see that for the exponential structure of covariance for the realistic values of variance σ^2 of about 1–3, the integral scale for K(x) changes from 0.767 to 0.433 times the scale for Y(x). For the Gaussian correlation the difference between the K(x) and Y(x) scales is much smaller.

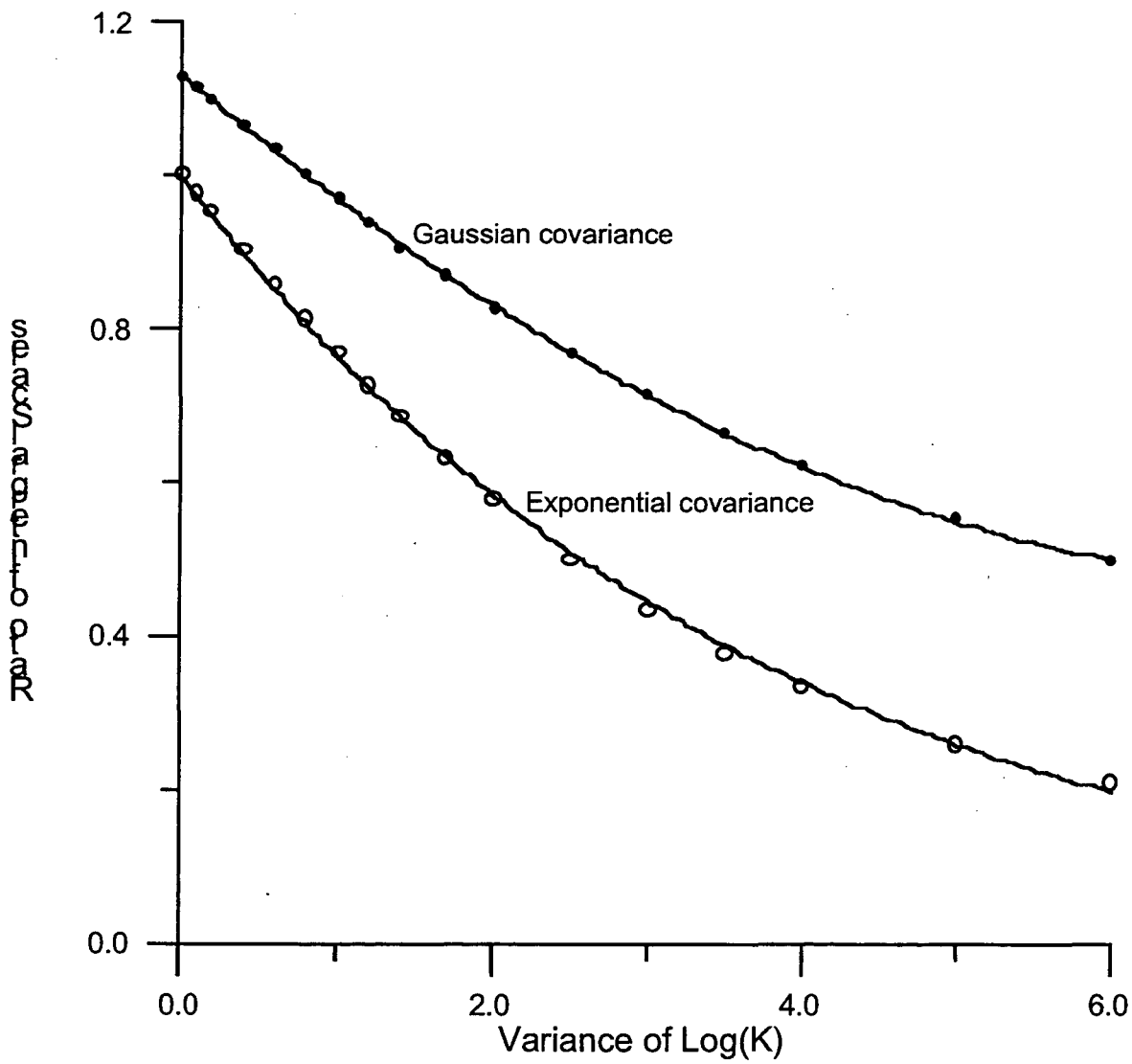

Figure 11. Ratio of the spatial integral scales (Equation B.3) as a function of the variance of log (K) for the two autocorrelation structures.

The calculations of integral scale show that for the exponential structure of autocovariance of Y(x), the autocorrelation function (B.2b) for K(x) can be approximated by the exponential function $\rho_k \approx \exp(-x / \lambda_k)$ with the integral scale λ_k equal to:

$$\lambda_k \approx \lambda \exp(-0.272\sigma^2). \tag{B.4}$$

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