Mathematical Geology, Vol. 32, No. 6, 2000

Short Note

Effective Hydraulic Conductivity and Transmissivity for Heterogeneous Aquifers[1]

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Regional scale models of groundwater flow and transport often employ domain discretizations with grid blocks larger than typical scales of field data. For heterogeneous formations, this difference in scales is often handled by using effective (upscaled) parameters. We investigate the problem of upscaling hydraulic conductivity and transmissivity from a small scale of measurement to a larger scale of grid blocks. Transmissivity statistics is expressed in terms of statistics of hydraulic conductivity, and expressions for the effective (upscaled) hydraulic conductivity K_{eff} *and transmissivity* T_{eff} *for steady state flow in confined heterogeneous aquifers are derived by means of stochastic averaging and perturbation analysis. These expressions reveal that the commonly used relation* $\mathrm{T}_{eff} = \mathrm{BK}_{eff}$*, where* B *is the confined aquifer thickness, is not generally valid.*

KEY WORDS: groundwater, upscaling, effective hydraulic conductivity, transmissivity, stochastic.

INTRODUCTION

Models for interpreting experimental data usually assume that, at least on a measurement scale, flow takes place in a homogeneous environment. Under this assumption, hydraulic conductivity $K(\mathbf{x})$ represents a quantity averaged over some support volume ω_1 centered around point $\mathbf{x} = (x_1, x_2, x_3)^T$. If the support volume ω_1 is comparable to an aquifer thickness, $B(x_1, x_2)$ (as is the case for fully penetrating wells), then transmissivity associated with this support volume is defined as BK. However, K is usually associated with much smaller measurement volumes, and local transmissivity of heterogeneous formations is defined as $T = \int_0^B K\,dx_3$, where x_3 is the vertical coordinate. Thus, transmissivity represents

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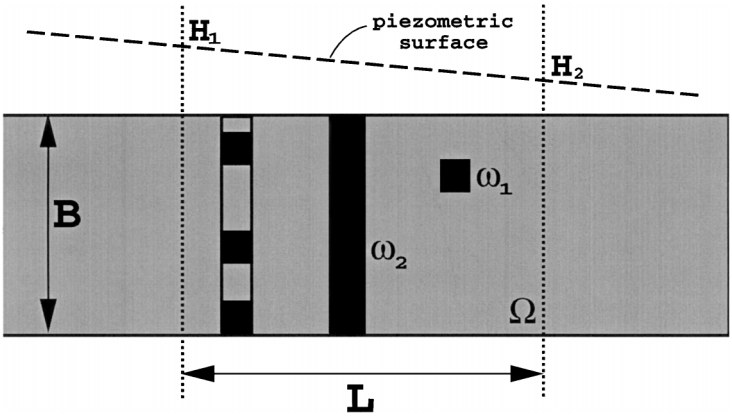

Figure 1. Schematic representation of support scales for hydraulic conductivity ω_1 and transmissivity ω_2 within a grid block Ω (length L and thickness B) of a confined aquifer.

a quantity averaged over some local observation scale $\omega_2 > \omega_1$ (Fig. 1), so that the smaller scale variability of hydraulic conductivity is neglected.

Effective, or upscaled, parameters are often used for numerical modeling of groundwater flow and transport in heterogeneous aquifers. Such models require assigning hydraulic conductivities or transmissivities to large grid blocks, while experimental data are usually available at a much smaller scale of core or well-log measurements. These parameters can be obtained by standard inverse methods, which is equivalent to the common groundwater modeling practice of taking the deterministic form of Darcy's law for granted, associating it with some effective or equivalent property and estimating its spatial distribution by model calibration against measured heads and fluxes (Zimmerman and others, 1998). A detailed discussion of these methodologies and their drawbacks is given by Guadagnini and Neuman (1998). An alternative approach, which we pursue in this paper, consists of estimating effective or equivalent parameters by stochastically derived analytical formulae (e.g., Matheron, 1967; Dagan, 1989; Paleologos, Neuman, and Tartakovsky, 1996; Tartakovsky and Neuman, 1998).

It was demonstrated numerically (Dykaar and Kitanidis, 1993) and proven analytically (Desbarats and Bachu, 1994) that the accepted method of defining transmissivity as a vertical average,

$$T(x_1, x_2) = \int_0^B K(\mathbf{x})\, dx_3 \tag{1}$$

overestimates flow rates in the horizontal plane. To overcome this problem,

Desbarats and Bachu (1994) employed a generalized power averaging (Desbarats, 1992, 1994)

$$T(x_1, x_2) = \int_0^B K^{\omega}(\mathbf{x})\, dx_3 \tag{2}$$

where ω is a fitting parameter. While useful for many practical applications, (2) lacks physical justification, and estimating an appropriate ω may be difficult (Desbarats and Bachu, 1994). Dagan (1989, p. 357) suggested another generalization of (1),

$$T = BK_{\text{eff}} \tag{3}$$

where K_{eff} is the effective hydraulic conductivity. For perfectly layered aquifers, (3) reduces to (1) exactly, and these two definitions are practically identical when B is "much larger" than the vertical correlation scale, l_v (Dagan, 1989, p. 358). It remains to answer the question of how large is large enough, and to provide a simple closed-form expression for K_{eff} in the presence of boundaries.

In this paper, we investigate the relationship between the effective (upscaled) hydraulic conductivity K_{eff} and transmissivity T_{eff} for randomly heterogeneous confined aquifers of either deterministically or randomly varying thickness. To facilitate this comparison, we start by expressing statistics of transmissivity in terms of conductivity statistics.

TRANSMISSIVITY STATISTICS

It is customary to treat hydraulic conductivity K as a random field (e.g., Dagan, 1989) characterized by a joint (multivariate) probability density function or, equivalently, its joint ensemble moments. Thus, hydraulic conductivity $K(\mathbf{x})$ varies not only across the real space coordinates $\mathbf{x}$, but also in probability space (this variation may be represented by another "coordinate" $\boldsymbol{\xi}$, which, for simplicity, we suppress). Whereas spatial moments are obtained by sampling $K(\mathbf{x})$ in real space (across $\mathbf{x}$), ensemble moments are defined in terms of samples collected in probability space (across $\boldsymbol{\xi}$).

In line with the current trend in stochastic hydrogeology, we assume that log hydraulic conductivity $Y(\mathbf{x}) = \ln K(\mathbf{x})$ forms a statistically homogeneous Gaussian field with constant mean $\langle Y \rangle$ and variance $\sigma_Y^2 \equiv \langle Y'(\mathbf{x})Y'(\mathbf{x})\rangle$, and two-point Gaussian anisotropic covariance function, $C_Y(\mathbf{x}, \mathbf{y}) = \sigma_Y^2 \rho_Y(r)$,

$$\rho_Y(r) = e^{-r^2} \qquad r^2 = \frac{(x_1 - y_1)^2 + (x_2 - y_2)^2}{l_h^2} + \frac{(x_3 - y_3)^2}{l_v^2} \tag{4}$$

where l_h and l_v are the horizontal and vertical correlation scales, respectively. This particular choice of the correlation function ρ_Y is for mathematical convenience only and is not crucial to the methodology used in this paper.

Our aim is to express the statistics of log transmissivity $Z = \ln T$ in terms of the statistics of Y. (The statistics of random transmissivity T is derived in the Appendix.) If a spatial distribution of the aquifer thickness $B(x_1, x_2)$ is known with certainty (deterministic), first-order (in σ_Y^2) approximations of the mean log transmissivity $\langle Z \rangle$, geometric mean $T_G = \exp(\langle T \rangle)$, variance σ_Z^2, and correlation function ρ_Z are given by (Appendix)

$$\langle Z \rangle = \ln(BK_G) + (1 - \beta)\frac{\sigma_Y^2}{2} \tag{5}$$

$$T_G = B\left[1 + \frac{1-\beta}{2}\sigma_Y^2\right]K_G \tag{6}$$

and

$$\sigma_Z^2 = \beta\sigma_Y^2 \qquad \rho_Z(r_h) = \exp\left(-r_h^2\right) \qquad r_h^2 = \frac{(x_1 - y_1)^2 + (x_2 - y_2)^2}{l_h^2} \tag{7}$$

respectively. Here $K_G = \exp(\langle K \rangle)$ is the geometric mean of K,

$$\beta(\lambda_v) = \lambda_v^2\left[\sqrt{\pi}\lambda_v^{-1}\,\mathrm{erf}\left(\lambda_v^{-1}\right) + \exp\left(-\lambda_v^{-2}\right) - 1\right] \tag{8}$$

and $\lambda_v = l_v/B$.

Thus the constructed random field of log transmissivity Z is dependent upon a number λ_v of the vertical correlation scales l_v in the total thickness B of an aquifer. This dependence manifests itself through the correction factor $\beta(\lambda_v)$, which is depicted in Figure 2. Because $\beta < 1$, it follows from (7) that the log transmissivity Z, as inferred from the given statistics of the log conductivity Y, exhibits smaller spatial variation than Y. A lack of the vertical correlation of hydraulic conductivity ($l_v = 0$) results in $\sigma_Z^2 = 0$.

A procedure for deriving the ensemble mean and (co)variance of $Z = \ln T$ for randomly varying B is outlined in the Appendix.

It is clear that if T is defined on a support volume ω_2 through the spatial averaging (1) of K (associated with a smaller scale ω_1), log-normality of K does not imply log-normality of T. Alternatively, if transmissivity and conductivity are defined on the same support scale, then $T = BK$, and unless B is random, log-normality of K also implies log-normality of T.

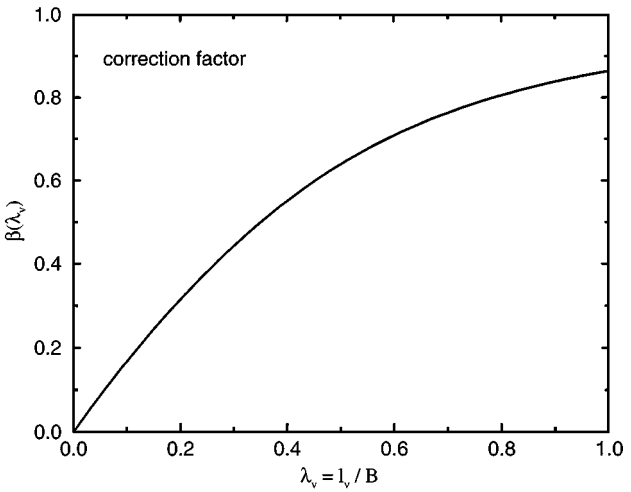

Figure 2. Correction factor β as a function of the number of vertical correlation scales l_v in the total thickness B of an aquifer.

EFFECTIVE TRANSMISSIVITY VS. EFFECTIVE CONDUCTIVITY

Consider upscaling of Darcy's law, $\mathbf{q} = -K\nabla h$ ($\mathbf{q}$ being flux and h being hydraulic head), from its support scale ω_1 to a larger grid-block Ω (Fig. 1). Following Dagan (1989) and Neuman and Orr (1993), we define effective conductivity K_{eff} of a randomly heterogeneous grid-block Ω as a coefficient of proportionality in the mean flow equation, $\langle \mathbf{q} \rangle = -K_{\text{eff}} J$, where $\langle \mathbf{q} \rangle$ is the mean flux and $J = (H_2 - H_1)/L$ is the mean hydraulic head gradient. Up to first order in σ_Y^2, it is given by (Paleologos, Neuman, and Tartakovsky, 1996)

$$\frac{K_{\text{eff}}(\mathbf{x})}{K_G} = 1 + \sigma_Y^2 \left[\frac{1}{2} - \kappa_d(\mathbf{x}) \right] \qquad \kappa_d(\mathbf{x}) = \int_{\Omega_d} \rho_Y(r) \frac{\partial^2 G_d(\mathbf{x}, \mathbf{y})}{\partial x_1 \partial y_1} d\mathbf{y} \tag{9}$$

where G_d is the Green's function for d-dimensional Laplace equation in Ω subject to appropriate homogeneous boundary conditions. The dimensionality d is determined by dimensionality of flow. Paleologos, Neuman, and Tartakovsky (1996) and Tartakovsky and Neuman (1998) demonstrated that, in d-dimensions, κ monotonically increases from 0 to $1/d$ with the size of Ω relative to the correlation scales l_h and l_v. In particular, κ reaches 90% of its asymptotic value of $1/3$ at $\lambda_h = \lambda_v = 0.1$, where $\lambda_h = l_h/L$.

Defining effective transmissivity T_{eff} in a similar manner leads to

$$\frac{T_{\text{eff}}(\mathbf{x})}{T_G} = 1 + \sigma_Z^2\left[\frac{1}{2} - k_{d-1}(\mathbf{x})\right] \qquad k_{d-1}(\mathbf{x}) = \int_{\Omega_{d-1}} \rho_Z(r)\frac{\partial^2 G_{d-1}(\mathbf{x},\mathbf{y})}{\partial x_1 \partial y_1}\,d\mathbf{y} \tag{10}$$

with $\kappa_{d-1} \approx 1/(d-1)$ at $\lambda_h = 0.1$. These findings are in agreement with numerical results of Dykaar and Kitanidis (1993). These unambiguous definitions of the effective conductivity K_{eff} and transmissivity T_{eff} clearly conserve mean Darcian flux through the grid block Ω.

Whereas an anisotropy ratio l_h/l_v and a number of vertical correlation scales in the aquifer thickness λ_v are determined by the physical processes, the choice of a grid-block size L in the horizontal plane (x_1, x_2) is up to a modeler. Our analysis shows that one can use well-established values for upscaled parameters (Matheron, 1967; Gelhar and Axness, 1983; and Dagan, 1989),

$$\frac{K_{\text{eff}}}{K_G} = 1 + \frac{\sigma_Y^2}{6} \qquad \frac{T_{\text{eff}}}{T_G} = 1 \tag{11}$$

so long as $\lambda_h = \lambda_v < 0.1$. If the size of a grid block is large enough to satisfy this criteria, but $\lambda_h \neq \lambda_v$, Equation 30 of Tartakovsky and Neuman (1998) might be used instead.

The effective transmissivity T_{eff} in (10) is expressed in terms of the statistical moments of log transmissivity Z. These can be obtained either directly from field measurements of transmissivity T, or from the statistics of log conductivity Y. To facilitate the comparison between effective conductivity and transmissivity, we employ the latter approach.

Substituting (6) into (11) yields an expression for the effective transmissivity in terms of the statistical moments of log conductivity,

$$T_{\text{eff}} = B\left[1 + \frac{1-\beta}{2}\sigma_Y^2\right]K_G \tag{12}$$

It follows from (11) and (12) that, for the traditional practice of setting $T_{\text{eff}} = BK_{\text{eff}}$ to be valid, it is necessary that $\beta = 2/3$ or (see Fig. 2) $\lambda_v \approx 0.53$. The latter clearly contradicts the condition for validity of (11), $\lambda_v < 0.1$, so that $T_{\text{eff}} \neq BK_{\text{eff}}$.

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APPENDIX: STATISTICAL MOMENTS OF LOG-TRANSMISSIVITY

If log-conductivity Y is a Gaussian and statistically homogeneous random field, the definition of T leads to an exact expression for its mean $\langle T \rangle$ in a randomly heterogeneous aquifer of deterministically varying thickness B

$$\langle T \rangle = e^{\langle Y \rangle} \int_0^B \left\langle e^{Y'(\mathbf{x})} \right\rangle dx_3 = BK_G \exp\left(\frac{\sigma_Y^2}{2}\right) \tag{A1}$$

and a first-order (in σ_Y^2) approximation of its covariance function, $C_T(r_h) \equiv \langle T'(x_1, x_2) T'(y_1, y_2) \rangle$,

$$C_T(r_h) = \int_0^B \int_0^B \langle K'(\mathbf{x}) K'(\mathbf{y}) \rangle \, dx_2 dy_2 = K_G^2 \sigma_Y^2 \int_0^B \int_0^B \rho_Y(r) \, dx_2 dy_2 + O\left(\sigma_Y^4\right) \tag{A2}$$

Substituting (4) into (A2) yields

$$C_T(r_h) = K_G^2 \sigma_Y^2 \alpha(l_v, B) \rho_T(r_h) \tag{A3}$$

where $\rho_T(r_h) = \exp(-r_h^2)$, $r_h^2 = [(x_1 - y_1)^2 + (x_2 - y_2)^2]/l_h^2$, and

$$\frac{\alpha(l_v, B)}{l_v^2} = \sqrt{\pi}\frac{B}{l_v}\,\mathrm{erf}\left(\frac{B}{l_v}\right) + \exp\left(-\frac{B^2}{l_v^2}\right) - 1 \tag{A4}$$

First-order (in σ_Y^2) approximation of the transmissivity variance σ_T^2 is obtained from (A3) by setting $r_h = 0$.

Ensemble mean of log-transmissivity $\langle Z \rangle$ is derived through the Taylor expansion

$$\langle Z \rangle = \langle \ln T \rangle = \ln\langle T \rangle - \frac{1}{2}\frac{\sigma_T^2}{\langle T \rangle^2} + O\left(\frac{\langle T'(x_1)^3 \rangle}{\langle T \rangle^3}\right) \tag{A5}$$

Substituting (A1) and (A3) into (A5), and retaining the terms up to σ_Y^2, leads directly to (5). It follows from (5) that

$$T_G \equiv \exp(\langle Z \rangle) = BK_G \exp\left[\frac{1-\beta}{2}\sigma_Y^2\right] \tag{A6}$$

Approximating (A6) up to first order in σ_Y^2 gives (6).

To derive an expression for the (co)variance of log-transmissivity, we notice that, up to first order in σ_Z^2, $C_T(r_h) = T_G^2 C_Z(r_h)$. It then follows from (A3) that $T_G^2 C_Z(r_h) = K_G^2 \sigma_Y^2 \alpha \rho(r_h)$. Utilizing (A6), and retaining the terms up to σ_Y^2, yields (7).

When the thickness B of a confined aquifer varies randomly in space, (A1) takes the form

$$\langle T \rangle = K_G f(B) \qquad f(B) = \left\langle \int_0^B e^{Y'(\mathbf{x})}\, dx_3 \right\rangle \tag{A7}$$

Representing $B = \langle B \rangle + B'$, expanding $f(B)$ in Taylor's series about $\langle B \rangle$, and retaining the terms of the first order in the variance σ_B^2 of B, yields

$$\langle T \rangle = \langle B \rangle K_G \exp\left(\frac{\sigma_Y^2}{2}\right) + \langle K'(\langle B \rangle) B'(x_1) \rangle \tag{A8}$$

The last term in (A8) represents cross-covariance between aquifer's thickness B and hydraulic conductivity K evaluated at the average elevation of the aquifer top. If these two quantities are uncorrelated [as data of Desbarats and Bachu (1994) indicate], then (A8) reduces to (A1) upon replacing B with its expected value $\langle B \rangle$. Analogously, one can obtain expressions for the second ensemble moment of Z.