Title

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Journal
Stochastic Environmental Research and Risk Assessment, 8(1)

ISSN
1436-3240

Authors
Loaiciga, HA
Leipnik, RB
Hudak, PF
et al.

Publication Date
1994-03-01

DOI
10.1007/bf01581388

Peer reviewed

Stochastic Hydrology and Hydraulics 8, 1–17 © Springer-Verlag 1994

Effective hydraulic conductivity of nonstationary aquifers

H. A. Loaiciga

Department of Geography and Environmental Studies, University of California, Santa Barbara, CA 93106, USA

R. B. Leipnik

Department of Mathematics, University of California, Santa Barbara, CA 93106, USA

P. F. Hudak

Department of Geography, University of North Texas, Denton, TX 76203, USA

M. A. Marino

Department of Land, Air and Water Resources and Department of Civil Engineering, University of California, Davis, CA 95616, USA

Abstract: Assuming that the ln hydraulic conductivity in an aquifer is mathematically approximated by a spatial deterministic "surface", or trend, plus a stationary random noise, we treat the problem of finding what the effective hydraulic conductivity of that aquifer is. This problem is tackled by spectral methods applied to a type of diffusion equation of groundwater flow, together with suitable coordinate transformations. Analytical (exact) solutions in terms of elementary functions are presented for one- and three-dimensional finite and infinite domains. Stability criteria are obtained for the solutions, in terms of a critical parameter, that turns out to involve the product of correlation scale and trend gradient. For the case of finite and symmetrical domains, additional provisions to insure the stability of numerical calculations of effective hydraulic conductivity are provided. Effective hydraulic conductivity is an important property, with potential applications in the calibrations of groundwater and transport numerical models.

Key words: Stochastic diffusion equations, effective hydraulic conductivity, correlation scale, heterogeneous aquifers, spectral representation

1 Introduction

The mathematical foundations of stochastic processes can be traced back to Bachelier (1900), who introduced the concept of a martingale. Langevin (1908) introduced the first formal stochastic differential equation to describe the motion of a particle subject to "Brownian" impacts, the latter named after Robert Brown, a botanist who first described the erratic motion of small particles immersed in a fluid in 1829. Einstein (1905), derived the deterministic differential equation, in fact a diffusion equation, describing the distribution of solute particles in a stationary fluid. Einstein's 1905 paper briged a significant gap at the time, since it demonstrated the linkage between a random process, namely, Brownian motion, and the the physical distribution of solute particles in a fluid. The linkage was a simple diffusion (deterministic) equation. A convergence was shaping between the experimental and theoretical work of A. Fick, L. Boltzmann and others in the second half of the 19th century in solute diffusion, and the incipient theory of stochastic processes at the turn of the 20th century. It would take nearly 40 years after Einstein's 1905 work for the mathematical relationship between Brownian motion and diffusion processes to be generalized and rigorized probabilistically.

Progress continued to be made in the interim, and, for example, Ornstein and Uhlenbeck (1930) provided a solution to Langevin's stochastic differential equation based on the widely known Ornstein-Uhlenbeck process. Both Brownian and Markovian processes (the latter introduced by Markov in 1906) played a role in the theory. Wiener (1923) provided rigorous treatment to the Brownian motion process, that Kolmogorov (1940) expanded in a fundamental paper on the general Markov process. By the early 1940's a good deal of work being done on stochastic differential equations revolved around the following Itô (1944) stochastic difference equation:

$$dX_t = \mu(t, X_t)dt + \sigma(t, X_t) \cdot dB_t \tag{1}$$

where X_t is a n-dimensional martingale process defined in positive continous time t, driven by the d-dimensional Brownian process B_t; μ and σ are n x 1 and n x d coefficient vector and matrix, respectively. The vector μ and matrix σ are of particular significance in relating the solution of the stochastic differential equation in equation (1) to the diffusion process of primary interest to this paper, as will be. shown later.

2 Stochastic difference equations, Itô and Stratonovich calculus

Itô (1944) introduced a class of integrals, in fact, thereafter named after him as Itô integrals (or more generally, Itô calculus), to integrate the difference equation (1) (known as Itô's stochastic differential equation) with respect to time. Formally,

$$X_t - X_{t_0} = \int_{t_0}^{t} \mu(s, X(s))ds + \int_{t_0}^{t} \sigma(s, X(s))\, dB(s) \tag{2}$$

where the initial condition X_{t_0} is independent of the Brownian process $dB(t)$. The first integral in the right-hand side of equation (2) can be defined as a Riemann integral in the mean square sense under suitable conditions (Soon, 1973). The second integral in the right-hand side of equation (2) involving the Brownian process, however, is meaningless either in the mean square or the classical sense as a Riemann integral, but it can be handled by Itô integration, defined as follows:

$$\int_{t_0}^{t} \sigma(s, X(s))dB(s) = \lim_{n\to\infty;\Delta t\to 0} \sum_{k=0}^{n-1} \sigma(t_k, X_{t_k})[B_{t_{k+1}} - B_{t_k}] \tag{3}$$

in which $\Delta t = \max(t_{k+1} - t_k)$, k = 0, 1, 2, ..., n-1, and the limit in equation (3) denotes convergence in mean square (Loaiciga and Marino, 1990).

The Itô stochastic differential differential equation (1) has been considered in groundwater hydrology, written in a slightly different way as follows (Loaiciga and Marino, 1987a; 1987b):

$$\frac{dX_t}{dt} = \mu(t, X_t) + \sigma(t, X_t)\, \xi \tag{4}$$

in which ξ is a white noise process (that can be interpreted as special type of derivative of Brownian motion, i.e., $\xi \equiv dB_t/dt$, since Brownian processes are not differentiable in the classical sense). With an added observation process (i.e., $Y_t = \Psi X_t + w_t$, where Ψ is an observation matrix and w is white noise), equation (4) denotes the well-known state-space model of Kalman and Bucy (1961). This is widely used in stochastic hydrology (Loaiciga and Marino, 1987a,b; Graham and McLaughlin, 1989), and arises after numerical discretization of the continuous equations of groundwater flow and mass transport.

In applied hydrologic work, equation (4) is integrated numerically, mostly via the statespace filtering method of Kalman and Bucy (1961). At a more fundamental level, stochastic Itô integration has been important in furthering the theory of stochastic differential equations, although applications, in fields such as biology, and computer simulations can be found in Arnold (1974), Wong and Zakai (1969), Turelli (1978), Sussman (1978), and Gard (1988). One of the most intriguing paradoxes of stochastic calculus concerns the existence of two different, yet mathematically consistent, approaches for the integration of stochastic difference equations. One approach is that by Itô (1944) whereby the stochastic difference equation (4) is rigorously written as in equation (1), and then integrated according to equations (2) and (3). The other, more recent, approach is due to Stratonovich (1964), wherein equation (4) is rigorously written as follows (von Weizsacker and Winkler, 1990):

$$dX_t = \mu(t, X_t)dt + \sigma(t, X_t)dB_t + 1/2\, d\sigma(t, X_t)dB_t \tag{5}$$

Notice in equation (5) that Stratonovich calculus introduces the last term in the right-hand side of equation (5), resembling the chain rule of classical calculus (except for the 1/2 term) applied on its right-hand side. Once written as in equation (5), it is obvious that the integration of this equation leads to a result different to that obtained from integrating the Itô stochastic differential equation

(1). Yet, both Itô's and Stratonovich's solutions are mathematically consistent. A significant body of literature exists on this intriguing paradox concerning the Itô and Stratonovich approaches, which are connected by the "switching theorem" (von Weizsacker and Winkler, 1990).

3 Stochastic differential equations and diffusion problems

Much of the discussion thus far presented would seem rather esoteric if it were not for a truly remarkable connection between deterministic diffusion equations, quite important in groundwater hydrology, and stochastic difference equations of the Itô type. A less conclusive and general connection has been hinted at already in citing of Einstein's (1905) work. The following result due to Itô (1944; 1951) establishes the fundamental link between deterministic diffusion problems and the stochastic differential equation (1). Consider the deterministic diffusion equation:

$$L[\phi(t,\mathbf{x})] = \frac{\partial\phi(t,\mathbf{x})}{\partial t} - \left[\sum_{i=1}^{n} \mu_i(t,\mathbf{x}) \frac{\partial\phi(t,\mathbf{x})}{\partial \mathbf{x}_i} + 1/2 \sum_{i,j=1}^{n} a_{i,j}(t,\mathbf{x}) \frac{\partial\phi^2(t,\mathbf{x})}{\partial x_i\, \partial x_j}\right] = 0 \tag{6}$$

where L represents a diffusion operator;, μ_i and $\mathbf{a}_{i,j}$ are components of a deterministic coefficient (drift) vector, μ, and deterministic positive definite (diffusion) matrix, a, respectively. Itô's (1944; 1951) fundamental result states (see, e.g., von Weizsacker and Winkler, 1990) that, under suitable conditions, solutions $\mathbf{X}_t$ to the stochastic differential equation (1) are diffusion processes, i.e., there is an L and a ϕ(t, $\mathbf{x}$) such that L(ϕ(t, $\mathbf{X}_t$) satisfies equation (6). (The necessary and sufficient condition is that the driving noise in equation (1) have independent and stationary increments, as Brownian noise does). Furthermore, the diffusive matrix **a** in equation (6) is such that its square root is the coefficient matrix in the Itô stochastic differential equation (1), specificallly, $\mathbf{a} = \sigma\, \sigma^T$, where T denotes the transpose. Therefore, the fundamental Itô theorem just stated reveals the remarkable fact that for every deterministic diffusion process of the form in equation (6), there is a related Itô stochastic differential equation whose solution (which is unique for a given initial condition of the driving noise and positive definite matrix σ in equation (1)) satisfies the diffusion process in question. We call this result the stochastic-deterministic duality of diffusion processes. (See Nelson (1967) and Prugovecki (1984) for important applications.)

4 A stochastic diffusion equation with random parameters

Consider the following steady-state groundwater flow equation with random hydraulic conductivity K($\mathbf{x}$) (tensorial index notation is used):

$$\frac{\partial}{\partial x_i}\left[K(\mathbf{x}) \frac{\partial\phi(\mathbf{x})}{\partial x_i}\right] = 0 \tag{7}$$

where $\mathbf{x}$ denotes a three-dimensional coordinate vector; and $\phi(\mathbf{x})$ is the hydraulic head. In the approach of Loaiciga et al (1993), adopted herein, K($\mathbf{x}$) is a stochastic parameter whose distribution is conveniently expressed in terms of the log-hydraulic conductivity, Y = lnK. (Equation (7) is a stochastic differential diffusion equation with random parameters.) It is assumed, furthermore, that the log-conductivity is composed of a deterministic, although spatially variable, trend T plus a zero-mean random noise f with spatial statistical structure. Specifically, $Y(\mathbf{x}) = T(\mathbf{x}) + f(\mathbf{x})$. The field variable $\phi(\mathbf{x})$, is modeled as the sum of a deterministic mean H($\mathbf{x}$) and a zero-mean random noise h, i.e., $\phi(\mathbf{x}) = H(\mathbf{x}) + h(\mathbf{x})$. Substitution of these decompositions of log-conductivity and hydraulic head in terms of a deterministic structural and a random component into equation (7), plus further manipulation of the resulting expression can be shown to lead to the following deterministic partial differential equation governing the mean hydraulic head H (equation (8)) and to a stochastic partial differential equation for the hydraulic head perturbation h (equation (9)) (note that the stochastic structure of the perturbation f is specified extraneously):

$$\frac{\partial^2 H}{\partial x_i \partial x_i} + b_i \frac{\partial H}{\partial x_i} + E\left\{\frac{\partial f}{\partial x_i}\frac{\partial h}{\partial x_i}\right\} = 0 \tag{8}$$

where $b_i = \partial T/\partial x_i$; and E denotes expectation;

$$\frac{\partial^2 h}{\partial x_i \partial x_i} + b_i \frac{\partial h}{\partial x_i} + \frac{\partial f}{\partial x_i}\frac{\partial H}{\partial x_i} + \left\{\frac{\partial f}{\partial x_i}\frac{\partial h}{\partial x_i} - E\left(\frac{\partial f}{\partial x_i}\frac{\partial h}{\partial x_i}\right)\right\} = 0 \tag{9}$$

From equations (8) and (9) it can be seen that they are coupled (H and h appear in both equations). Given that the probabilistic nature of f is specified, equations (8) and (9) form a system of linear simultaneous equations. Therefore, equations (8) and (9) require a simultaneous solution. One possible approach to solve the coupled mean and perturbation equations, is: (i) assume the products of perturbation gradients are zero in equations (8) and (9); (2) proceed to solve the mean equation (8); (iii) use that solution in equation (9) and solve the latter (i.e., find the covariance of h); (iv) having the covariance of h derive the expected value of the product of perturbation gradients in equation (8); (v) re-solve the mean equation (8) with the term involving the product of perturbation gradients obtained in (iv) included; (vi) with the revised solution to the mean equation proceed to re-solve the perturbation equation (9) with the terms in brackets involving products of perturbation gradients included. These series of steps can be iterated until an adequate convergence criterion is met. Regrettably, there is no theoretical proof at this time that such an iterative scheme will converge to a solution nor that a solution to equations (8) and (9) exists. Loaiciga et al (1993) followed the solution approach just outlined successfully to obtain an approximate analytical solution to the mean and perturbation equations in a one-dimensional flow domain.

By and large, however, it is customarily assumed that the terms in brackets in equations (8) and (9) are negligible, of "order σ_f^2", $O(\sigma_f^2)$, where σ_f^2 is the variance of f, and $\sigma_f^2 << 1$ by assumption. The latter assumptions are synonymous to the widely used "first-order" or "small-perturbations" analysis of stochastic groundwater. Loaiciga and Marino (1990), have shown that the order of magnitude (as measured by the standard deviation) of the nonlinear product of perturbation gradients in equations (8) and (9) is not always proportional to σ_f^2 as is generally assumed. Their (approximate) expression for the standard deviation of the term in brackets in equation (9) is:

$$\sigma_2 = \left\{\sigma''_{fh}(0)^2 + \sigma''_{ff}(0)\,\sigma''_{hh}(0)\right\}^{1/2} \tag{10}$$

in which $\sigma''_{fh}(0)$ denotes the second derivative of the cross-covariance of the perturbation of lnK, f, and hydraulic head, h, evaluated at $\tau = 0$, where τ is a separation vector; analogous definitions hold for the second derivatives of the covariances of f (σ_{ff}) and hydraulic head (σ_{hh}). Empirical evidence (see, e.g., Gelhar et al, 1993) on the field variability of f is not at all conclusive either that the assumption $\sigma_f^2 << 1$ is valid in many highly heterogenous conditions. Therefore, there is at present a significant theoretical gap on the understanding of the solutions to equations (8) and (9) in heterogenous 2- and 3-dimensional aquifers.

5 Effective hydraulic conductivity in one-dimensional domains

Assuming an exponential model for the covariance of the disturbance of lnK ($\sigma_{ff}(\tau) = \sigma_f^2 \exp(-|\tau|/\lambda)$, where τ is the separation vector, and λ is the correlation scale of lnK), and using a spectral method of solution for the perturbation equation (9), Loaiciga et al (1993) have shown that the effective hydraulic conductivity, K_e, which relates mean specific discharge to minus the mean hydraulic gradient, is given by the following expression in one-dimensional domains:

$$K_e = e^T \left[1 - \frac{\sigma_f^2}{b\lambda + 1}\right] \tag{11}$$

where $b = dT/dx$ denotes the one-dimensional trend gradient.

It is seen from equation (11) that the condition for nonnegative effective hydraulic conductivity is $\sigma_f^2 < b\lambda + 1$, and that a singular point exists at $b\lambda = -1$. Notice then how in the presence of a trend in lnK, the restriction on the variance of lnK perturbation involves the critical product of parameters $b\lambda$. (The parameter $b\lambda$ plays an important role in 2- and 3-dimensional analysis also.) The expression in equation (11) also shows that, since the trend T is in general spatially variable, so is the effective hydraulic conductivity. If the trend of lnK can be adequately identified from data, it is possible to construct a spatially dependent effective hydraulic conductivity field directly from equation (11). In 2- and 3-dimensional domains this is potentially useful in calibrating numerical models of groundwater flow and mass transport. Most of the hydraulic head and aquifer properties data collected in the field represent averages or "effective" values over extended spatial domains. Numerical simulation models are also coarse and discrete spatial approximations to continuous processes. It seems reasonable, therefore, that in seeking calibrating parameters for such numerical simulation models, to focus on the theoretical effective conductivity relating the mean or average groundwater flow discharge to the mean hydraulic gradients. Average effective hydraulic conductivities over finite-difference ceils and finite elements can be calculated (e.g., by integration) from the continous-space function K_e.

6 Effective hydraulic conductivity in 3-dimensional domains

Novel results in stochastic groundwater hydrology for the effective hydraulic conductivity in finite and infinite 3-dimensional domains are developed in this and following sections. (Results for 2-dimensional domains are being derived, but, somewhat counterintuitively, involve more advanced functions than those which appear in three dimensions.) The spectral method used by Loaiciga et al (1993) to derive solutions such as that given in equation (11) can be extended to the solution of stochastic diffusion groundwater equations in three-,dimensions. Loaiciga et al (1993) showed that the mean specific discharge $\bar{q}_i$ in the i-th coordinate axis (i = 1, 2, 3) is given by the following expression (where **J** is the mean hydraulic gradient vector whose components are $J_i = \partial H/\partial x_i$, i = 1, 2, 3; k_i is the ith component of the wave-number vector **k**; is the ith component of the log-conductivity trend gradient vector **b**; **R** is the complete three-dimensional space; $j^2 = -1$; $k^2 = \mathbf{k}\cdot\mathbf{k}$; $\mathbf{k}\cdot\mathbf{b}$; $\mathbf{k}\cdot\mathbf{J}$ are inner vectorial products):

$$\bar{q}_i = -e^T \left[J_i + \frac{j\,\sigma_f^2 \lambda^3}{\pi^2} \int_{\mathbf{R}} \frac{k_i\,[\mathbf{k}\cdot\mathbf{b} + j\,k^2][\mathbf{k}\cdot\mathbf{J}]}{[(k^2)^2 + (\mathbf{k}\cdot\mathbf{b})^2](1 + \lambda^2 k^2)^2}\, d^3\mathbf{k} \right] \tag{12}$$

The remainder of this paper presents a method for the analytical exact evaluation of the integral in equation (12).

6.1 The integral class $I_{l,n,p,q}$ and the evaluation method

Let us define the following generic integral:

$$I_{l,n,p,q}\,(\mathbf{b},\ \mathbf{J},\ \lambda,\ \mathbf{S}) = \int_{\mathbf{S}} \frac{k_p^l\, F(k^2,\ \mathbf{k}\cdot\mathbf{b})\, (\mathbf{k}\cdot\mathbf{J})^n}{[(k^2)^2 + (\mathbf{k}\cdot\mathbf{b})^2](1 + \lambda^2 k^2)^{q/2}}\, d^3\mathbf{k} \tag{13}$$

where F is a suitably defined function; **S** is a spherical region in **k**-space with center at the origin and of radius ρ; l, n, p, q are index integers suitably chosen for any given function F. The functions F that appear in the integral of equation (13) are typically quite simple. For example, if $F(k^2,\mathbf{k}\cdot\mathbf{b}) = \mathbf{k}\cdot\mathbf{b} + j\,k^2$, l = 1, n = 1, p = i (i = 1, 2, 3), and q = 4, then $I_{l,n,p,q}$ so defined is the integral in equation (12). The integration method presented herein does not strongly depend on the nature of F, given that F depends only on k^2 and $\mathbf{k}\cdot\mathbf{b}$. The integration method to be developed does apply to more general integrals than those represented by equation (13), such as those that might arise in anisotropic porous media.

The basic strategy in the development of the integradon method is to find geometric transformations of the vectors **b**, **k**, and **J** to reduce the triple integrals of interest to single integrals with elementary functions as integrands. Conical and spherical trigonometry will play a central role in carrying out these geometric transformations. The single integrals that emerge are slowly convergent, or divergent but renormalizable by subtraction and domain truncation. They were introduced by Euler (1748) under the name of "dilogarithms", further developed by Spence (1809), and perfected by Kummer (1840), who reduced them to trigonometric series studied by Clausen (1832) in relation to diffusion problems. In the period 1880 to 1950 these integrals were much neglected, but were revived as a systematic matter by Lewin (1981), presumably because of their occasional appearance in electrical, electromagnetic, and thermodynamic problems, as well as in quantum electrodynamics, a prolific source of physically important but exceptionally puzzling integradon problems (Feynman, 1948; Kallen, 1950).

The devices required to carry out the integrals of this paper (see equation (12)) - integration by parts, partial fractions, trigonometric and rational substitution, and differentiation with respect to a parameter-, are all very familiar but the number of times that these must be employed to get through a typical $I_{l,n,p,q}$ problem is distressing. Finally, even the answers have many disparate terms, more than usual in classical or quantum electrodynamics. The relative sizes of these terms depend on the relations between three or four parameters, leading to a large number of potentially different "regimes". All these features militate against a straightforward three-dimensional numerical integration strategy- numerical analysis enters rather at the later stage of evaluation of the slowly convergent Clausen series.

6.2 A differential relation for the integral class $I_{l,n,p,q}$

If the function $F(k^2, \mathbf{k}\cdot\mathbf{b})$ in the integral of equation (13) is an even function of $\mathbf{k}\cdot\mathbf{b}$, assign F the parity $\nu = 0$, and if it is an odd function of $\mathbf{k}\cdot\mathbf{b}$, assign it the parity $\nu = 1$. Consider the effect of the transformation $\mathbf{k} \rightarrow -\mathbf{k}$ on the integral of equation (13). If the integration region $\mathbf{S}$ is invariant under this transformation, it is seen from equation (13) that if $l + n + \nu$ is odd, then $I_{l,n,p,q} = 0$, and if $l + n + \nu$ is even, then $I_{l,n,p,q}$ is likely to be nonzero. The dependence of equation (13) on l and p can be clarified by differentiation of a two-index family of integrals, $G_{n,q}$, l times with respect to J_p, the pth component of the mean vector gradient $\mathbf{J}$. Let

$$G_{n,q} = \int_{\mathbf{S}} \frac{F(k^2,\ \mathbf{k}\cdot\mathbf{b})\ (\mathbf{k}\cdot\mathbf{J})^n}{[(k^2)^2\ +\ (\mathbf{k}\cdot\mathbf{b})^2](1\ +\ \lambda^2k^2)^{q/2}}\ d^3\mathbf{k} \tag{14}$$

Clearly, $G_{n,q} = I_{0,n,p,q}$ (which is independent of p). Differentiation of $G_{n,q}$ in equation (14) l times with respect to J_p establishes that

$$\frac{\partial^l G_{n,q}}{\partial J_p^l} = \frac{n!}{(n-l)!}\, I_{l,n-l,p,q} \tag{15}$$

so, that by letting $n' = n - \ell$, then:

$$I_{l,n',p,q} = \frac{(n')!}{(n'+l)!}\,\frac{\partial^l G_{n'+l,q}}{\partial J_p^l} \tag{16}$$

Thus, if $G_{n,q}$ is known as a function of $\mathbf{J}$ for some specific F, formal differentiation as indicated above yields $I_{l,n-l,p,q}$.

Further progress is difficult unless the integral $I_{l,n,p,q}$ is particularized. Let us focus on the example

$$I_{1,1,p,4} = \int_{\mathbf{S}} \frac{k_p(\mathbf{k}\cdot\mathbf{b}\ +\ jk^2)(\mathbf{k}\cdot\mathbf{J})}{[(k^2)^2\ +\ (\mathbf{k}\cdot\mathbf{b})^2](1\ +\ \lambda^2k^2)^2}\ d^3\mathbf{k} \tag{17}$$

which enters the integral in equation (12). Obviously, $I_{1,1,p,4}$ is a sum of two integrals of the $I_{l,n,p,q}$ type for different choices of F. The first integral has $l = 1$, $n = 1$, $q = 4$, $F_1 = \mathbf{k}\cdot\mathbf{b}$, $\nu = 1$ (i.e., F_1 is and odd function of $\mathbf{k}\cdot\mathbf{b}$, thus the parity 1 assigned to it), and, therefore, $l + n + \nu = 3$; so, if the region of integration $\mathbf{S}$ is a sphere with center at the origin. then the first integral is zero. The second integral has $l = 1$, $n = 1$, $q = 4$, $F_2 = j\ k^2$, with parity $\nu = 0$, and, therefore, $l + n + \nu = 2$; so, the second integral probably does not vanish.

With the choice of F as in equation (17), the following relation exists between the two-index integral $G_{2,4}$ and $I_{1,1,p,4}$, according to the result of equation (16):

$$\begin{aligned} I_{1,1,p,4} &= \frac{1}{2}\,\frac{\partial G_{2,4}}{\partial J_p} \\ &= \frac{1}{2}\,\frac{\partial}{\partial J_p}\int_{\mathbf{S}} \frac{j\ k^2(\mathbf{k}\cdot\mathbf{J})^2}{[(k^2)^2\ +\ (\mathbf{k}\cdot\mathbf{b})^2](1\ +\ \lambda^2k^2)^2}\ d^3\mathbf{k} \end{aligned} \tag{18}$$

Note that $I_{1,1,p,4}$ is the integral that appears in equation (12). Therefore, if $G_{2,4}$ is known, its derivative with respect to J_p gives the integral of equation (12). In the next section the triple integral of equation (18) is reduced to a single integral written in terms of elementary functions, which is then evaluated exactly in terms of dilogarithms and Clausen functions. The reduction method from triple to single integrals is quite general for treating integrals of the type defined by equation (13), and is easily modified to two dimensions. The triple integrals of this paper appear quite often in the solution of stochastic groundwater differential equations (see Loaiciga et al (1993)). It will be shown later on that numerical integration is not advisable even for the reduced single integral. Instead, analytical evaluation expressible in terms of Clausen series is the best method to ultimately integrate equation (13) in general, and equation (12) in particular, the subject matter of this paper.

7 Biplanar and biconical coordinate transformations

7.1 Biplanar radial coordinates

The integrand of equation (18) is the quotient of a quartic in k_1, k_2, k_3 by an octic in k_1, k_2, k_3. Straightforward algebraic methods are impractical in such cases. Define the biplanar radial coordinates $r = \sqrt{k^2}$, $u = \mathbf{k}\cdot\mathbf{b}$, $\nu = \mathbf{k}\cdot\mathbf{J}$, that appears attractive based on the structure of the integrand in equation (18). Integration of $G_{2,4}$ in the r, u, ν coordinates requires the Jacobian, $J_{r,u,\nu}$, of the transformation from **k** space to r, u, ν space. It is assumed that the vectors **b** and **J** are neither parallel nor antiparallel for calculations to be non-degenerate in biplanar radial coordinates. After careful analysis of the geometry of the r, u, ν space, it follows that the absolute value of the Jacobian of the transformation is (with $\mathbf{c} = \mathbf{b} \times \mathbf{J}$ the vector product of **b** and **J**; and $w^2 = ||w||^2 = \mathbf{w}\cdot\mathbf{w}$ for any vector **w**, **w** = **b**, **c**, **J**):

$$|J_{r,u,\nu}| = \frac{r}{\sqrt{r^2\, c^2 + 2u\, \nu\, \mathbf{b}\cdot\mathbf{J} - \nu^2 b^2 - u^2 J^2}} \tag{19}$$

The integral $G_{2,4}$ of equation (18) in r, u, ν coordinates becomes:

$$G_{2,4} = \int_{\Omega} j\, \frac{r^2\nu^2}{\sqrt{(r^4 + u^2)(1+\lambda^2 r^2)^2}}\, \frac{r\, dr\, du\, d\nu}{\sqrt{r^2c^2 + 2u\nu\, \mathbf{b}\cdot\mathbf{j} - b^2\nu^2 - J^2u^2}} \tag{20}$$

where Ω is the set of triples (r, u, ν) such that $r^2c^2 > b^2\nu^2 + J^2u^2 - 2\mathbf{b}\cdot\mathbf{J}\, u\nu$ and $r \leq \rho$, where ρ has been defined as the radius of the region of integration **S**.

7.2 Biconical radial coordinates

The goal is to integrate equation (20) for ρ finite as well as in infinite domain, $\rho \to \infty$. Evidently, $G_{2,4}$ depends on c^2, b^2, J^2, λ, ρ, and $\mathbf{b}\cdot\mathbf{J}$. But $c^2 = ||\mathbf{b}\times\mathbf{J}||^2 = b^2J^2 - (\mathbf{b}\cdot\mathbf{J})^2$, so either c^2 or $(\mathbf{b}\cdot\mathbf{J})^2$ can be dropped, and $G_{2,4}$ is determined, for example, by b, J, $\mathbf{b}\cdot\mathbf{J}$, λ, and ρ. These five parameters can be somewhat reduced as seen later.

For fixed r, $b^2\nu^2 - 2\mathbf{b}\cdot\mathbf{J}\, u\nu + J^2u^2 < r^2c^2$ is the interior of an elliptical region in (u, ν) space. As r varies with 0 to ρ, the regions are geometrically similar, with the same principal axes. Thus the region Ω is a solid elliptical cone. This geometry suggests replacement of the biplanar radial coordinate system with a biconical radial system, wherein (u, ν) is replaced by angular variables, A, B, leading to a three-dimensional system (r, A, B). Specifically, $u = \mathbf{k}\cdot\mathbf{b} = br\cos B$, $\nu = \mathbf{k}\cdot\mathbf{J} = Jr\cos A$, supplemented by a third angular quantity θ defined by $\mathbf{b}\cdot\mathbf{J} = bJ\cos\theta$, which remains fixed in later calculations.

Clearly, A, B, θ are the angles between the edges **b**, **k**, **J** of a trihedron, where **k** is variable and **b**, **J** are fixed. (The angles A, B, θ can be chosen to vary in the interval $[0, \pi]$.) Since $r = \sqrt{k^2}$, it is evident that the coordinates r, A, B constitute a type of spherical coordinate system. Further simplifications arise in passing from (r, u, ν) space to (r, A, B) in equation (20). The absolute value of the Jacobian of the transformation r, u, $\nu \to$ r, A, B is given by $|J_{r,A,B}| = bJr^2|\sin A||\sin B|$. Substitution of the biconical radial coordinates and their absolute Jacobian in equation (20) transforms the integral to:

$$G_{2,4} = J^2 \int_{\Omega} j\, \frac{r^4\cos^2 A\, |\sin A||\sin B|}{\Delta(A,B,\theta)(r^2+b^2\cos^2 B)(1+\lambda^2r^2)^2}\, dr\, dA\, dB \tag{21}$$

where $\Delta(A,B,\theta) = \sqrt{\sin^2\theta + 2\cos\theta\cos A\, \cos B - \cos^2 A - \cos^2 B}$.

The formula for Δ(A, B, θ) can be much simplified by the use of the co-angle α to A, which goes back to Ptolemy (Braunmuhl, 1900). The co-angles (α,β,γ) to (A, B, θ) are the angles betwen the three planes determined by the pairs of vectors (**k**, **J**), (**k**, **b**), and (**b**, **J**). Ptolemy's formula (2nd Century AD) $\cos A = \cos B\cos\theta + \cos\alpha\, \sin B\, \sin\theta$ and its analogs are useful in determining (α,β,γ) from (A, B, θ). One key result is that $\Delta(A, B, \theta) = |\sin\theta||\sin B||\sin\alpha|$, showing that Δ(A, B, θ) is separable in (r, α, B) coordinates.

7.3 Biconical mixed coordinates

The last in the series of geometric transformations aimed at simplifying the original triple integrals in Cartesian space, is to derive the Jacobian $J_{r,\alpha,B}$ of the transformation from biconical radial coordinates (r, A, B) to the mixed biconical coordinates (r, α, B). The absolute value of this Jacobian can be shown to be $|J_{r,\alpha,B}| = |\sin\alpha||\sin B||\sin\theta|/|\sin A|$, which upon substitution in equation (21) along with the results for $\Delta(A, B, \theta)$ and Ptolemy's formula for cosA, yields:

$$G_{2,4} = J^2 \int_{\Omega} j \frac{r^4|\sin B| \cos^2 A}{(r^2 + b^2\cos^2 B)(1+\lambda^2 r^2)^2} \, dr \, d\alpha \, dB \tag{22}$$

where $\Omega = (0 \le \alpha \le 2\pi;\ 0 \le B \le \pi;\ 0 \le r \le \rho)$ is the integration region; and $\cos^2 A = \cos^2 B \cos^2\theta + 1/2 \cos\alpha \sin 2B \sin 2\theta + \cos^2\alpha \sin^2 B \sin^2\theta$.

Equation (22) is integrated with respect to α from 0 to 2π to reduce it to a double integral on r, B:

$$\begin{aligned} G_{2,4} = {} & 2\, j\, \pi J^2 \cos^2\theta \int_0^{\rho}\int_0^{\pi} \frac{r^4 \sin B \cos^2 B}{(r^2 + b^2\cos^2 B)(1+\lambda^2 r^2)^2} \, dB \, dr \\ & + j\, \pi J^2 \sin^2\theta \int_0^{\rho}\int_0^{\pi} \frac{r^4 \sin^3 B}{(r^2 + b^2\cos^2 B)(1+\lambda^2 r^2)^2} \, dB \, dr \\ = {} & j\, \pi J^2 (2\cos^2\theta\, G_c + \sin^2\theta\, G_s) \end{aligned} \tag{23}$$

in which G_c and G_s are defined as the appropriate double integrals in equation (23). The final step in reducing the triple integrals to single integrals is to integrate equation (23) with respect to B. In doing so, the substitution of variable $t = \cos B$ proves convenient, to yield the single integral:

$$\begin{aligned} G_{2,4} = {} & 2\, j\, \pi J^2 \cos^2\theta \int_0^{\rho} \frac{2r^4}{(1+\lambda^2 r^2)^2 b^2} \left[1 - \frac{r}{b}\tan^{-1}\left(\frac{b}{r}\right)\right] dr \\ & + j\, \pi J^2 \sin^2\theta \int_0^{\rho} \frac{2r^4}{b(1+\lambda^2 r^2)^2} \left[\frac{1}{r}\tan^{-1}\left(\frac{1}{b}\right) - \frac{1}{b}\left(1 - \frac{r}{b}\tan^{-1}\left(\frac{b}{r}\right)\right)\right] dr \end{aligned} \tag{24}$$

The first and second integrals in the right-hand side of equation (24) represent the G_c and G_s integrals, respectively, of equation (23) integrated over B. The G_c integral when separated into $(2/b^2) \int_0^{\rho} [r^4/(1+\lambda^2 r^2)^2]\, dr$, which is easily integrated, and $(-2/b^3) \int_0^{\rho} [r^5/(1+\lambda^2 r^2)^2] \tan^{-1}(b/r)\, dr$, which is not at all easy, and not found in any of the usual tables of integrals, is seen to have two parts which diverge as $\rho \to \infty$, but their "divergent parts" cancel. The part of the G_s integral that does not involve G_c, also not found in the usual tables, converges (although slowly) as $\rho \to \infty$. Notice that equation (24) is a single integral written in terms of elementary functions. Because of the presence of divergent parts in equation (24) (that mutually cancel out, fortunately) and the slow convergence of some of the parts of equation (24), further analytical evaluation is called for rather than numerical integration. In the next section the single integrals in equation (24) are evaluated exactly.

8 Evaluation of single, radial, integrals of stochastic analysis

8.1 Dilogarithms, Spence functions, and Clausen series

Let us introduce Euler's dilogarithm (Euler, 1748):

$$\mathrm{Li}_2(z) = -\int_0^{z} \frac{\ln(1-z_1)}{z_1} \, dz_1 \tag{25}$$

with $z \neq 1$. For $|z| \leq 1$, $Li_2(z) = \sum_1^\infty z^n/n^2$ converges, and so $Li_2(1) = \sum_1^\infty 1/n^2 = \pi^2/6$. The first Spence function (Spence, 1809) is defined by:

$$Ti_2(z) = \int_0^z \frac{\tan^{-1}u}{u}\,du \tag{26}$$

The second Spence function is given by:

$$Ti_2(z,k) = \int_0^z \frac{\tan^{-1}u}{u + k}\,du \tag{27}$$

Finally, there is the Clausen function (Clausen, 1832):

$$Cl_2(\theta) = \sum_{n=1}^{\infty} [\sin(n\theta)/n^2] \tag{28}$$

Obviously, $Li_2(e^{j\theta}) = \sum_1^\infty e^{jn\theta}/n^2 = \sum_1^\infty (\cos(n\theta)/n^2) + j\,Cl_2(\theta)$. A bizarre web of idendties relates these functions to themselves, to each other, and to suitable logarithms. Lewin's (1981) book cites many hundreds of such idendties. Clausen's function (1832) enters several diffusion problems, when they are solved using Fourier series. The final single integrals of section 3 involve inverse tangents, as do the Spence functions. To bring those integrals within convenient range of the Spence functions, let us introduce three new dimensionless quantities $s = b/r$, $m = b\lambda$, and $\epsilon = b/\rho$, where $\epsilon \leq s$ for $r \leq R$. Define:

$$K_{p,q}(\epsilon, m) = \int_\epsilon^\infty s^q(s^2 + m^2)^{-p}\,ds \tag{29}$$

and

$$K_{p,q} = \int s^q(s^2 + m^2)^{-p}\,ds \tag{30}$$

as the corresponding indefinite integral, so that $K_{p,q}(\epsilon, m) = K_{p,q}|_\epsilon^\infty$. Define also:

$$H_q(\epsilon, m) = \int_\epsilon^\infty \frac{s^q \tan^{-1}s}{(s^2 + m^2)^2}\,ds \tag{31}$$

whose indefinite integral is H_q. It follows from these definitions and equation (24) that the latter equation can be written as follows:

$$\begin{aligned} G_{2,4} = {} & 2j\pi J^2 b^3 \sin^2\theta \left[\int_\epsilon^\infty \frac{\tan^{-1}s}{s(s^2 + m^2)^2}\,ds - \int_\epsilon^\infty \frac{ds}{s^2(s^2 + m^2)^2}\,ds + \int_\epsilon^\infty \frac{\tan^{-1}s}{s^3(s^2 + m^2)^2}\,ds\right] \\ & + 4j\pi J^2 b^3 \cos^2\theta \left[\int_\epsilon^\infty \frac{ds}{s^2(s^2 + m^2)^2} - \int_\epsilon^\infty \frac{\tan^{-1}s}{s^3(s^2 + m^2)^2}\,ds\right] \\ = {} & 2j\pi J^2 b^3 \sin^2\theta\, G_s' + 4j\pi J^2 b^3 \cos^2\theta\, G_c' \end{aligned} \tag{32}$$

where

$$G_c' = K_{2,-2}(\epsilon, m) - H_{-3}(\epsilon, m) \tag{33}$$

and

$$G_s' = H_{-1}(\epsilon, m) - K_{2,-2}(\epsilon, m) + H-3(\epsilon, m) \tag{34}$$

Since $\tan^{-1}s = s - \frac{s^3}{3} + O(s^5)$ for small s, and $\tan^{-1}s = \frac{\pi}{2} - \frac{1}{s} + O(s^{-3})$ for large s, the above integrals converge, though slowly. For $\rho \to \infty$, $\epsilon \to 0$, finite limits exist, and that suffices in many applications. This is the case of infinite aquifer domain. However, in laboratory simulations or other finite-domain instances, results for finite ρ would be important. Also, the integration technique developed herein involves separation of integrals in equation (32) into terms that diverge as $\rho \to \infty$ (although they cancel out when considered simultaneously), so one must avoid taking $\rho \to \infty$ prematurely.

8.2 The $K_{p,q}$ and H_q integrals

Integration of equation (30) for p = 2 and q = -2 gives the following result:

$$K_{2,-2} = \frac{1}{2sm^2(s^2 + m^2)} - \frac{3}{2m^4 s} - \frac{3}{2|m|^5} \tan^{-1} \frac{s}{|m|} + \text{const} \tag{35}$$

in which "const" denotes constant of integration in the indefinite case. The definite integral $K_{2,-2}(\epsilon,m) = K_{2,-2}|_\epsilon^\infty$. Evidently, $K_{2,-2}$ has a singularity at s = 0, but k will be shown below that the singularity is canceled out when $K_{2,-2}$ and H_{-3} are considered together (see equations (33 and (34)). This is important since the case s = 0 corresponds to an infinite flow domain, a classical case in stochastic groundwater analysis.

The second integral needed is H_{-1}, which from equations (29) and (30) is seen to be given by $H_{-1} = \int \tan^{-1}s/[s(s^2 + m^2)^2]ds = \int \tan^{-1}s \, dK_{2,-1}$. Carrying out the integration yields:

$$\begin{aligned} H_{-1} = {} & \tan^{-1}s \left[\frac{1}{2m^2(s^2 + m^2)} - \frac{1}{2m^4} \ln\left(\frac{s^2 + m^2}{s^2}\right)\right] \\ & - \frac{1}{2m^2} \left[\frac{1}{m^2 - 1} \left(\tan^{-1}s - \frac{1}{|m|} \tan^{-1} \frac{s}{|m|}\right)\right] \\ & + \frac{1}{2m^4} (N_m - N_0) + \text{const} \end{aligned} \tag{36}$$

where

$$N_m = \int \frac{\ln(s^2 + m^2)}{s^2 + 1} ds \tag{37}$$

is expressible in terms of the Clausen (Cl_2) functions introduced previously. It is clear from equation (37) that H_{-1} has no singularity at s = 0, since $(\tan^{-1}s)\ln(s) \to s \ln(s) \to 0$ as $s \to 0$.

Following the same integration routine, one obtains the third integral $H_{-3} = \int \tan^{-1}s \, dK_{2,-3}$ intervening in the key single integral of equation (32):

$$\begin{aligned} H_{-3} = {} & -\frac{1}{2m^4} \tan^{-1}s \left(\frac{1}{s^2} + \frac{1}{s^2 + m^2}\right) + \frac{1}{m^6} \tan^{-1}s \ln\left(\frac{s^2 + m^2}{s^2}\right) \\ & - \frac{1}{2m^4} \left(\frac{1}{s} + \tan^{-1}s\right) + \frac{1}{2m^4(m^2 - 1)} \left[\tan^{-1}s - \frac{1}{|m|} \tan^{-1} \frac{s}{|m|}\right] \\ & - \frac{1}{m^6} (N_m - N_0) \end{aligned} \tag{38}$$

There is a non-removable singularity at s = 0 in H_{-3} due to the term $(-1/2m^4)$ $[(\tan^{-1}s)/s^2 + 1/s]$. Clearly, $(\tan^{-1})/s^2 = 1/s + f(s)$ where f(s) is analytic near s = 0. Therefore, the singularity at s = 0 is that of $-1/m^4 s$. From equation (42) $K_{2,-2}$ has the same singularity at s = 0 as does $1/[2sm^2(s^2 + m^2)] - 3/(2m^4 s) = (-1/m^4 s)[1 + s^2/2(s^2 + m^2)]$, or equivalently, as $-1/m^4 s$. Hence, the singularity of G_c' at s = 0 is removable via the decomposition of equations (33) and (34), from which it is evident that the singular terms of $K_{2,-2}$ and H_{-3} cancel each other. This was the only troublesome theoretical point concerning singularities in the evaluations of G_c' and G_s' in equation (32).

The remaining practical point in the evaluation of G_c', and G_s' is the integral N_m of equation (37). For future reference, note that the integral

$$\int \frac{ds}{(1 + s^2)(s^2 + m^2)} = \frac{1}{m^2 - 1} \left[\tan^{-1}s - \frac{1}{|m|} \tan^{-1} \frac{s}{|m|}\right] + \text{const} \tag{39}$$

appears in H_{-1} and H_{-3}. The integral itself is continuous at $m^2 = 1$, yielding $\int ds/(1 + s^2)^2 = (1/2)\ [\tan^{-1}s + s/(s^2 + 1)] + \text{const}$. Its evaluation is singular at $m^2 = 1$, but this singularity is removable by L'Hospital's rule, yielding

$$\lim_{m \to 1} \frac{1}{2m} \left[\frac{1}{m^2} \tan^{-1} \left(\frac{s}{|m|}\right) + \frac{s}{m(m^2 + s^2)}\right] = 1/2 \left[\tan^{-1}s + \frac{s}{1 + s^2}\right] \tag{40}$$

as expected. The integrals so far considered have a removable singularity at $m = \pm 1$, quite in contrast to the one-dimensional flow problem that had a nonremovable singularity at $m = b\lambda = -1$. The stochastic integrals have been reduced entirely to elementary functions, except for the integral N_m appearing in H_{-1} and H_{-3}. This difficult integral is evaluated next, establishing the existence of the stochastic integral $G_{2,4}$ for all values of the parameter m except for $m = 0$, for which $K_{2,-2}$, H_{-1} and H_{-3} are not defined.

8.3 The N_m integral

For the purpose of evaluation of the integral $G_{2,4}$ in equation (32), N_m and N_0 are needed. For the analysis of singularities the case $m = \pm 1$, i.e., $N_{\pm 1}$ is relevant (recall that singularities existed at $m = \pm 1$ in the one-dimensional case). These integrals have been derived in terms of dilogarithms, Clausen functions and Spence functions. Although they are inconvenient for computation (they are very slowly convergent), avoiding them is expensive and hazardous. From Grobner and Hofreiter (1957, Erster Teil, p. 112):

$$N_0(s) = 2\ln|s|\tan^{-1}s - 2Ti_2(s) + \text{const} \tag{41}$$

$$N_{\pm 1}(s) = 1/2\ln[4(1 + s^2)] \tan^{-1}s + \frac{j}{2} \left[Li_2 \left(\frac{1 + js}{2}\right) - Li_2 \left(\frac{1 - js}{2}\right)\right] + \text{const} \tag{42}$$

Lewin (1981) presents tables for the Spence functions and dilogarithms appearing in equations (41) and (42), which are numerically slowly convergent. (The expression for N_0, $N_{\pm 1}$, and N_m in terms of Clausen functions requires an identity of Kummer, 1840.) The formula for N_m is due to Newman (1847; Lewin (1981), pp. 243-252, which we have simplified):

$$\begin{aligned} N_m(s) = {} & 2\tan^{-1}s \ln(1 + |m|) - \tan^{-1} \left[\frac{2s|1 - |m||}{(1 + |m|)(1 + s^2) + |1 - |m||(1 - s^2)}\right] \cdot \\ & \ln \frac{|1 + |m||}{|1 - |m||} + 1/2Cl_2 \left[2\tan^{-1} \left(\frac{2s|1 - |m||}{(1 + |m|)(1 + s^2) + |1 - |m||(1 - s^2)}\right)\right] \\ & + 1/2Cl_2 \left[4\tan^{-1}s - 2\tan^{-1} \left(\frac{2s|1 - |m||}{(1 + |m|)(1 + s^2) + |1 - |m||(1 - s^2)}\right)\right] \\ & - Cl_2(2\tan^{-1}s) \end{aligned} \tag{43}$$

Using L'Hospital's rule in equation (43) it can verified that $N_m(s)$ has a removable discontinuity at $m = \pm 1$. This establishes then that the three-dimensional stochastic groundwater results do not exhibit discontinuous singularides at the point $m = \pm 1$, quite in contrast to the one-dimensional case. From equation (43) it can be established that

$$N_m|_0^\infty = \pi \ln(1 + |m|) \tag{44}$$

a useful result in evaluating the integral (32) for the case of an infinite flow domain (i.e., $\rho \to \infty$).

At this point all the pieces needed to evaluate the fundamental radial integral (32) have been derived. Summary of results is given in the next section.

9 Summary of results

The effective conductivity depends directly on equation (32) as seen in equation (12). In turn, the radial integral (32) was expressed in terms of $K_{2,-2}$ (see equation 35)), H_{-1} (see equation (36)), and H_{-3} (see equation (38)). The latter two integrals involve the term N_m - N_0, and a expression for N_m in terms of (tabulated) Clausen functions was given in equation (43). The only singularity in the groundwater integrals occurs for the value of the parameter $m = b\lambda = 0$, a case of little interest herein since it corresponds to the presence of no trend in the log-conductivity field. All the previous work is summarized next, giving the expression for effective hydraulic conductivity in the presence of trends. This is done for the case of finite and infinite flow domains. Recall the following notation defining important parameters in the analysis: $b = ||\mathbf{b}||$; $J = ||\mathbf{J}||$; $m = b\lambda$; $\epsilon = b/\rho$; and $\theta = \cos^{-1}[(\mathbf{b}\cdot\mathbf{J})/bJ]$; ρ is the radius of the flow domain. The variable $s = br$.

9.1 Effective hydraulic conductivity in finite domains, $\epsilon \neq 0$

Equation (18) indicates that the mean specific discharge $\bar{q}_i$ is related to the derivative of the radial integral $G_{2,4}$, which in turn is shown in equation (32) in terms of integrals involving $K_{2,-2}$, H_{-1}, and H_{-3} all of which were developed in section 8. Substitution of $G_{2,4}$ into equation (18) plus differentiation of the resulting expression with respect to the mean gradient J_i permits factoring of the gradient J_i out of the brackets in equation 12. The resulting term within brackets in that equation multiplied by e^T is the equivalent hydraulic conductivity, K_e, that relates the mean specific discharge to minus the mean hydraulic gradient in the ith direction. The effective hydraulic conductivity is independent of direction as seen next, i.e., is isotropic, but it is space-dependent and hence heterogeneous. After proper rearrangement of the individual integrals in $G_{2,4}$, the effective hydraulic conductivity is:

$$K_e = e^T \left\{1 - Y\left[(4\cos^2\theta - 2\sin^2\theta)(K_{2,-2}|_\epsilon^\infty - H_{-3}|_\epsilon^\infty) + 2\sin^2\theta\, H_{-1}|_\epsilon^\infty\right]\right\} \tag{45}$$

where $Y = \sigma_f^2\lambda^3 b^3/\pi$.

Notice that in equation (45) has been expressed in terms of the difference $K_{2,-2}|_\epsilon^\infty$ - $H_{-3}|_\epsilon^\infty$ since individual singularities cancel each other through such difference as established in section 8. Naive evaluation of $K_{2,-2}$ and H_{-3} separately would fail for the case of infinite flow domain, $\rho \rightarrow 0$, due to the singularity at $s = 0$ already established. It is seen in equation (45) that the effective hydraulic conductivity equals the geometric mean e^T times a factor (the term in brackets in equation (45)) introduced by the trend in In conductivity.

The effective hydraulic conductivity in equation (45) is isotropic and heterogeneous. The angle θ in equation (45) varies simply as a result of the possible spatial variation of the trend gradient vector $\mathbf{b}$ and/or the mean hydraulic gradient vector $\mathbf{J}$. θ is the angle between the trend gradient and the mean hydraulic gradient. Evidently, for each three-dimensional location $\mathbf{x}$ there will be corresponding values $T(\mathbf{x})$, $b(\mathbf{x})$ and, thus, $K(\mathbf{x})$. Obvious simplifications occur when the trend T is linear on $\mathbf{x}$, in which case b becomes a constant. If, in addition, the mean hydraulic gradient is constant, then the spatial dependence of effective hydraulic conductivity is due exclusively to the spatial variations in the trend T.

Because of the slow convergence of the (tabulated, Ashour and Sabri, 1956)) Clausen functions and the special numerical precautions needed to prevent singularities when $\rho \rightarrow \infty$, the evaluation of K_e for given trend T is nontrivial.

9.2 Effective hydraulic conductivity in infinite domains, $\rho \rightarrow \infty$, $\epsilon \rightarrow 0$

The case of an infinite domain, perhaps the one that has received greatest attention in stochastic groundwater analysis, follows from the results for finite domain by taking the limit as $\epsilon \rightarrow 0$ in equation (45). This leads to significant simplifications for the resulting effective hydraulic conductivity, that is now expressible in terms of simple elementary functions of θ and m. The resulting limiting value of K_e for $\epsilon \rightarrow 0$ is:

$$\frac{K_e}{e^T} = 1 - Y\,(4\cos^2\theta - 2\sin^2\theta)\,\frac{\pi}{m^6}\left[\ln(1+|m|) + \frac{|m|}{4}\,\frac{(m^2 - 2|m| - 4)}{1+|m|}\right]$$
$$- 2Y\sin^2\theta\left[\frac{\pi}{2m^4}\ln(1+|m|) - \frac{\pi}{4|m|^3(1+|m|)}\right] \tag{46}$$

where Y was defined after equation (45). It is evident from equation (46) that K_e does not present discontinuous singularities for nonzero values of m = b . However, detailed analysis shows that the derivatives with respect to m are discontinuous at $m = \pm 1$. Note also that in equation (46) b and λ appear together as the parameter $m = b\lambda$. Loaiciga et al (1993) showed that the condition $\sigma_f^2 < b\lambda + 1$ was necesary for the feasibility of stochastic analysis in one-dimensional flow domains (see equation (11)). Clearly, the product of trend gradient magnitude and correlation scale is central to stochastic analysis in the presence of trends.

10 Example calculations of effective hydraulic conductivities

Figure 1 shows the three-dimensional plot of vertically averaged hydraulic conductivity in a semi-consolidated, fractured, claystone aquifer of the Casmalia Hills, Santa Barbara County, California, extensively studied by Hudak (1991). The heterogeneous nature of this random realization (plotted from thousands of granulometric field-measurements) is clear, with values ranging over three orders of magnitude In three-dimensions, the log-conductivity field was fitted by a second order polynomial (quadric surface) to yield a trend T(x, y, z) = -50.6 + 0.0556y + 0.252z + $0.000003x^2$ - $0.000019y^2$ - 0.000065xz - 0.000132yz, where $\mathbf{x}' = (x, y, z)$, with all spatial dimensions in meters. The components of the trend gradient vector **b** are linear functions of at least one of the spatial coordinates in each case. The other two parameters needed in fitting the effective hydraulic conductivity are σ_f^2 (estimable by several alternative methods), and λ, the correlation scale. This last parameter is estimable by several methods (Hudak et al, 1993). For the present example, the estimates for the log-conductivity variance and the correlation scale are 14.24 (an unusually large value) and 16.25 m, respectively, completing the data needs required in equation (46) for developing a three-dimensional field of effective hydraulic conductivity. Because of the large variability of lnK, evident from an estimated σ_f^2 in excess of 10 (recall that in first order analysis it is assumed that $\sigma_f^2 << 1$!!), the Casmalia data is particularly difficult to model. Evidently, better behaved data sets are advisable to implement and test the results of this work. In this regard, our data can be considered borderline for this purpose.

A computer program was written for equation (46) to generate field of effective hydraulic conductivity assuming a constant direction of the mean hydraulic gradient. Recall that when either one or both of the vectors **b** and **J** are space-dependent the angle θ between them needs to be calculated for any location **x** considered in the calculations. Figures 2 and 3 show the plots of effective hydraulic conductivity for fixed depths z = 60 m and z = 90 m. It is clear some sort of an east-west "ridge", that seems to be accentuated with depth. Because of the extremely large variance of lnK, we suspect that calculations based on equation (46) unduly reduced the calculated K_e, and the relative uniform distribution of effective hydraulic conductivity over extensive areas of Figures 2 and 3 is suspect. Note that in equation (46), the term Y is directly proportional to σ_f^2. Therefore, the larger σ_f^2 the smaller K_e is, provided that all other terms multiplied by Y are positive.

At this point the authors are seeking additional data sets to conduct further analysis of the theory developed herein. The Borden data set on lnK (Woodbury and Sudicky (1991)) is quite extensive and is not hindered by the extreme variability observed in the Casmalia lnK data set. Unfortunately, the Borden data was collected along vertical cross-sections, and they are, therefore, two-dimensional. The 3-dimensional results of this paper cannot be directly specialized to two dimensions. Two-dimensional effective hydraulic conductivities are, in fact, more difficult to derive than the 3-dimensional counterparts. This is an unfortunate situation, traceable to the the integer q talcing the value q = 3 in equation (14) in two-dimensional analysis, which introduces a non-rational function in the denominator of equation (14), and with it additional complications not encountered in the three-dimensional case. Nevertheless, the decompositions used in this paper are suitable for two-dimensional analysis, taking account of geometry and the resulting elliptic functions. The authors are developing the 2-dimensional results for effective hydraulic conductivity at present.

11 Summary and conclusions

A detailed analysis was made of the use of biconical integration in developing analytical and exact values of effective hydraulic conductivity. The results of our study apply to groundwater flow regimes where the conductivity field is nonstationary, in this case arising from spatial trends. Several key conclusions of our study are:

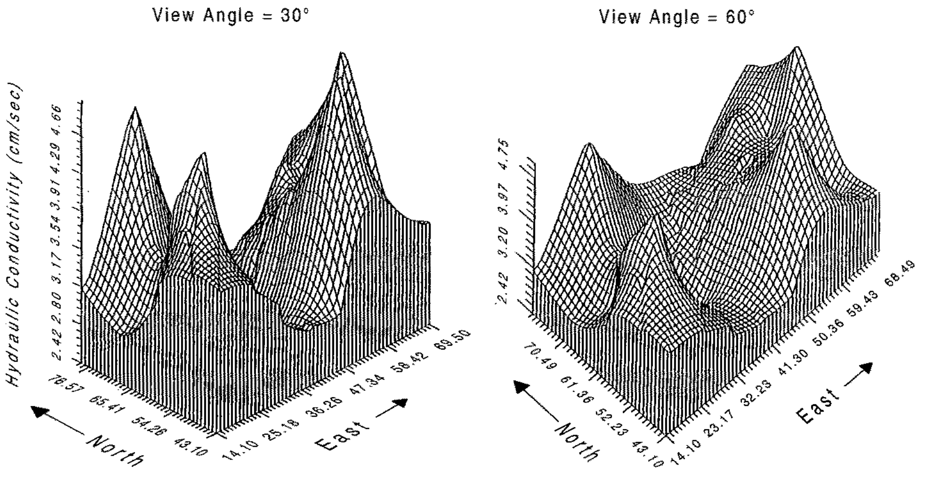

Figure 1. Two three-dimensional views of vertically averaged hydraulic conductivity for the semiconsolidated claystone of the Casmalia Hill aquifer, Santa Barbara County, California

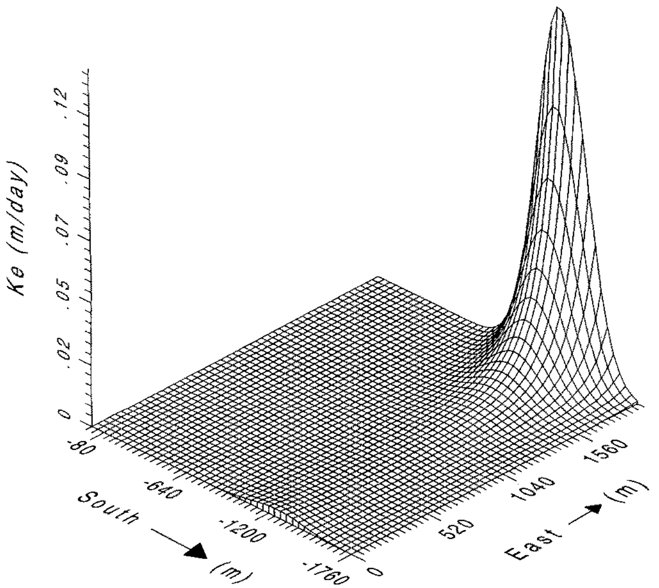

Figure 2. Effective hydraulic conductivity at depth z = 60 m at the Casmalia aquifer

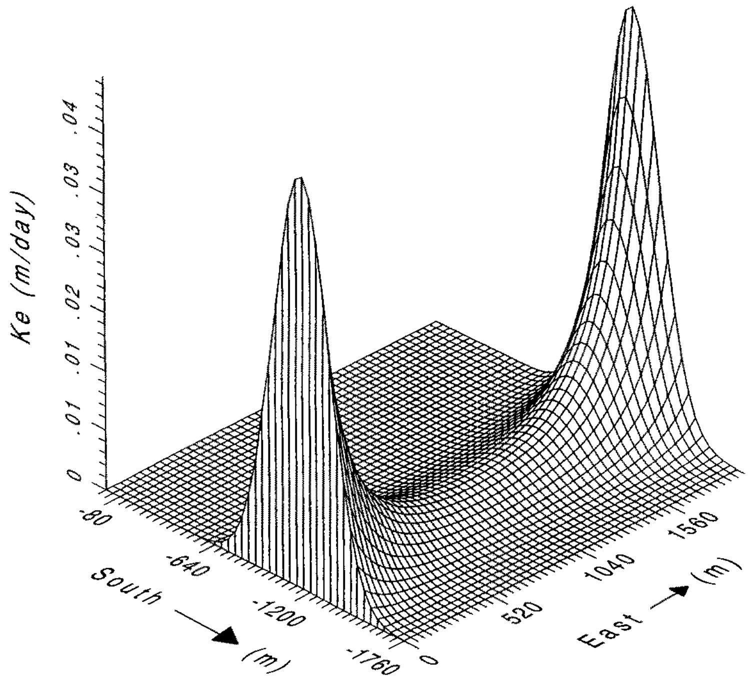

Figure 3. Effective hydraulic conductivity at depth z = 90 m at the Casmalia aquifer

1. Singularities in the results of one-dimensional groundwater analysis are removed when passing to three-dimensions. Specifically, effective conductivity and head vanances are defined for $m = b\lambda = \pm 1$ in the three dimensional case. The parameter m has been shown to play a key role in one-dimensional and three-dimensional stochastic, nonstationary, groundwater flow analysis.
2. The integrals that appear in three-dimensional stochastic groundwater flow analysis are not very suitable for straightforward numerical integration in full three-dimensional space. Instead, numerical calculation should enter at a later stage, after the triple integrals have been reduced to single radial integrals and they have been arranged so that individual singularities cancel each other. Even then, in the finite flow domain case the resulting expressions (Clausen and Spence functions) are slowly convergent. In the case of an infinite flow domain the equation for effective hydraulic conductivity simplifies greatly, and is expressible in terms of elementary trigonometric and logarithmic functions.
3. The three-dimensional effective hydraulic conductivity is isotropic and heterogeneous. Its numerical value depends on the angle θ formed between the trend gradient vector **b** and the mean hydraulic gradient **J**; other intervening hydrogeologic parameters are the variance of log-conductivity, its correlation scale, log-conductivity trend and gradient of the trend. For the case of a finite domain of radius ρ the formula for effective hydraulic conductivity depends on a number of slowly convergent series involving the trend gradient and the conductivity correlation scale. The classical case of infinite flow domain was developed exactly with no need for numerical approximations.
4. Calculations of effective hydraulic conductivity for the Casmalia data indicate that for large σ_f^2 the effective hydraulic conductivity can be underestimated relative to intuitive results. In spite of this difficulty, rather exotic three-dimensional plots of K_e were developed that suggest differences of over one order of magnitude in K_e for fixed depth.

5. The types of exact results for nonstationary stochastic groundwater flow analysis presented herein are novel in the field. The method of integration and reduction to single radial integrals developed herein was illustrated with the calculation of K_e. However, this method is generic for this kind of nonstationary groundwater analysis, and, for example, the triple integrals associated with the variance of hydraulic head can be treated by the same method used to reduce the triple effective conductivity integrals. This method involves biplanar radial, biconical radial, and mixed biconical radial coordinate transformations. Differences in the various triple integrals that emerge in the nonstationary groundwater flow analysis come at a later stage, after they have been reduced to single radial integrals, and even then the differences in the integrands appear minor, though numerically they are not so minor.

The tools of applied mathematics, apart from the stochastic equations, used to solve the problems of this paper have existed since the second half of the 19th century; however, their application to solve the difficult triple integrals of nonstationary groundwater analysis, and specifically, the introduction of biplanar and biconical coordinates constitutes a new contribution. It has been shown that exact results are obtainable for the kind of hard problems treated herein, and that in many respects these analytical solutions are preferable to numerical methods of approximation.

Acknowledgements

Support for this research was provided by the Kearney Foundation through grant 92-09, and by the National Science Foundation through grant NSF-SES-88-109-17 to the National Center for Geographic Information and Analysis of the Department of Geography, University of California, Santa Barbara.

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