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Perturbation and Gaussian methods for stochastic flow problems

M. H. Nachabe* & H. J. Morel-Seytoux

Department of Civil Engineering, Colorado State University, Fort Collins, Colorado 80523, USA

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Most applications of stochastic ground water modeling rely on a perturbation assumption; the magnitude of the randomly distributed parameters in the governing equation should be small to obtain a valid solution. A Gaussian method was developed to solve the ground water flow equation with random hydraulic conductivity distribution. In the Gaussian method, the moment generating function for multivariate normally distributed random variables was used to express joint high order moments of hydraulic head and conductivity in terms of low order moments. A set of coupled partial differential equations for the moments of the hydraulic head were formulated. The number of unknowns in the Gaussian method was the same as in the perturbation method, however the 'closure problem' was solved without the truncation of high order terms. Comparison with an exact analytical solution suggested that the Gaussian method can be more appropriate in the case of short correlation length. The Gaussian and the perturbations methods can be equivalent for the case of steady-state flow. For transient ground water flow, the two methods are different. The Gaussian method preserves the known lognormal spatial frequency distribution of the conductivity in the field.

Key words: stochastic subsurface hydrology, multivariate normal distribution, perturbation method.

1 INTRODUCTION

In the last two decades, the interest in stochastic ground water hydrology has increased tremendously. This growing interest was driven by the complex heterogeneity of aquifer's parameters, and by the lack of knowledge of the exact spatial distribution of these parameters (e.g. McLaughlin & Wood;[11] Gelhar[7]). Nachabe and Morel-Seytoux[13] and Morel-Seytoux and Nachabe[12] argued that the stochastic framework provided a mean to upscale the physical process from a macroscopic level, order 1 to 10 m, to a megascopic scale, order of 1 km or larger. The megascopic scale is more suitable for numerical models than the macroscopic scale.

In the stochastic framework, the hydraulic conductivity is considered a realization of a lognormal spatial random function. Therefore, its joint frequency distribution is multivariate normal and is fully characterized by the first two order moments: the mean, or the expected value of the conductivity random variable, and the covariance function, a probabilistic measure of spatial correlation. By adopting this mathematical representation, the ground water flow equation becomes a stochastic differential equation with random coefficients. Consequently, one is interested in determining the spatial probabilistic distribution of the hydraulic head or, less ambitiously, one may be satisfied by determining the first two order moments of the hydraulic head random process.

In this paper, a new approach is presented to solve the ground water flow equation with random parameters. A closed set of deterministic partial differential equations is derived for the moments of the head random process by hypothesizing that the head and the logarithm of the hydraulic conductivity are derived from a joint normal distribution. As opposed to perturbation methods (e.g. Sagar;[15] Dagan;[3] McLaughlin & Wood,[11]) the Gaussian distribution method retains all the high order moments of the random variables, i.e. the expectation of the product of more than two random variables. For transient ground water flow, the

*Correspondence should be addressed to: University of Colorado at Boulder, Campus Box 428, Boulder, CO 80309-0428, USA.

perturbation and Gaussian methods provide different formulations. The Gaussian method evolves into a perturbation method if the magnitudes of the random variables are small.

2 THEORY

2.1 Review of solutions procedures

A variety of procedures have been utilized to solve the ground water equation with random parameters. Dettinger and Wilson[4] divided the various solution procedures into two main groups: full distribution analyses, and first and second moments analyses. Given the cumulative distribution function of all the input parameters, the full distribution methods attempt to specify completely the probability distribution of the resulting hydraulic head without introducing an assumption concerning the magnitude of the random processes. A popular method to obtain probability density functions is the Monte Carlo approach which requires the performance of numerous flow simulation, with the parameters in each simulation generated at random from their respective probability distribution. In ground water hydrology, the Monte Carlo approach was utilized by Warren and Price,[16] Freeze,[5] and Smith and Freeze.[16] However, Dettinger and Wilson[4] noted that discretization of the hydraulic conductivity random process reduces its variance and increases its correlation length. To avoid this numerical error, the frequency distribution function of the random field should be integrated over the spatial domain, e.g. Rubin and Gomez-Hernandez.[14]

Most first two moments methods, whether in the spectral domain or the actual physical domain, are adaptations of the perturbation theory. The variance of the random variable is assumed small to obtain a valid solution. The spectral approach generates analytical solutions but, in general, is unable to handle the nonstationarity associated with the boundary conditions (e.g. Gelhar[6]). Li and McLaughlin[10] devised a new spectral approach that can handle nonstationarity. This approach retained the attractive features of spectral analysis, however the perturbation assumption was used implicitly in the derivations.

Perturbation solutions in the physical domain were developed by Dagan[3] who used Green's functions to achieve analytical solutions. Sagar[15] adopted a Galerkin finite element approximation to develop a numerical solution scheme based on a perturbation assumption. It is easily shown that the perturbation solution is a Neuman series expansion that generates a sequential system of partial differential equations. The solution of this system of equations, which is usually truncated to the first order, converges to the actual solution when the magnitude of the random parameter is small. Even though there is no solid criterion for the range of validity of a perturbation method, Gutjahr and Gelhar,[7] who compared the perturbation solutions with Monte Carlo simulations, suggested that, in the case of steady-state flow in an infinite spatial domain, the perturbation solution provided good results even for large standard deviations in input parameters. The closest study to the spirit of this paper is that of Gutjahr.[8] Gutjahr[8] attributed this good match between perturbation analysis and Monte Carlo simulations to the theoretical proof that if the joint distribution between the hydraulic head and the conductivity random variables is multivariate normal, the perturbation analysis is exact regardless of the magnitude of the random variables. Gutjahr's[8] finding was restricted to the case of no aquifer storage and infinite domain. However, in this paper, the utility of the Gaussian method will be extended for the case of transient ground water flow.

McLaughlin and Wood[11] formulated a set of deterministic partial differential equations for the moments of the hydraulic head. In general this approach generates an infinite set of deterministic equations that should be solved simultaneously (Beran[1]). McLaughlin and Wood[11] addressed this issue by truncating the high order moments, i.e. the moments resulting from the product of more than two random variables. In the Gaussian method, all the high order moments appearing in the governing flow equation will be expressed in terms of the first and second order known moments using the moment generating function. Then, the Gaussian and the perturbation methods will be compared.

First, to familiarize our readers with the calculus of moments equations, in the following section is presented a simple flow problem for which an exact analytical solution exists without invoking a perturbation or a Gaussian assumption. This tutorial problem will provide insights into the limitations of the Gaussian method.

3 COMPARISON OF THE GAUSSIAN SOLUTION WITH AN EXACT ANALYTICAL SOLUTION

In one dimension, the governing differential equation for the hydraulic head under steady-state conditions has the form

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(K_r \frac{\mathrm{d}H_r}{\mathrm{d}x}\right) = 0 \tag{1}$$

where x is the spatial coordinate, K_r is the hydraulic conductivity, and H_r is the hydraulic head. The subscript 'r' indicates that the variable is random. Following the general consensus in stochastic ground water modeling, K_r is considered a lognormal spatial random function. The logarithm of K_r is written as

$$\ln K_r(x) = \overline{\ln K_r}(x) + \theta(x) \tag{2}$$

where $\overline{\ln K_r}(x)$ is the expected value of $\ln(K_r)$ and $\theta(x)$ is the stochastic element with an expected value of zero. If the expectation operator is defined by $E(\cdot)$ then mathematically $E(\theta(x)) = \overline{\theta(x)} = 0$. Inverting eqn (2) for K_r yields

$$K_r(x) = K_g(x)\exp(\theta(x)) \tag{3}$$

where $K_g(x)$ is defined as

$$K_g(x) = \exp\overline{(\ln(K_r(x))} \tag{4}$$

Similarly, $H_r(x)$ is partitioned into two components, $H(x)$ the expected value of $H_r(x)$ and $h(x)$ the stochastic element with an expected value of zero. Symbolically

$$H_r(x) = H(x) + h(x) \tag{5}$$

where

$$E(H_r(x)) = \overline{H_r(x)} = H(x) \text{ and } E(h(x)) = \overline{h(x)} = 0$$

One is interested in determining $H(x)$ and the covariance $C_{hh'}(x,x')$ of h. For the sake of simplicity in the following derivation, assume that the hydraulic conductivity random function is a stationary stochastic process in both its mean, i.e. $K_g(x) = K_g =$ constant, and covariance function, i.e. $C_{\theta\theta'}(x,x') = C_{\theta\theta'}(x-x')$ where θ' is the random component of the hydraulic conductivity at location x'. The boundary condition on eqn (1) is one of a prescribed deterministic head H_0 at $x = 0$ and of a prescribed water flux q throughout the system.

3.1 Exact analytical solution

Integration of eqn (1) twice in space and use of the boundary conditions yields the solution

$$H(x) + h(x) = H_0 - q\int_0^x \frac{q}{K_g e^{\theta(x)}}\,dx \tag{6}$$

Taking expectations on both sides of eqn (6) yields

$$H(x) = H_0 - \frac{q}{K_g}\int_0^x E(e^{-\theta(x)})\,dx \tag{7}$$

Because the expectation and integral operators are linear ones, interchange of order of operation is permissible. Substituting $E(e^{-\theta(x)})$ by its equivalent evaluated in the Appendix, $H(x)$ becomes

$$H(x) = H_0 - \frac{q}{K_h}x \tag{8}$$

where $K_h = K_g\exp(-\sigma_\theta^2/2)$ is the harmonic average of the conductivity lognormal distribution. The covariance $C_{hh'}(x,x')$ solution is obtained by multiplying eqn (6) by $h'(x')$ and taking expectation. The result is

$$C_{hh'}(x,x') = \frac{q^2 e^{\sigma_\theta^2}}{K_g^2}\left(\int_0^x\int_0^{x'} e^{C_{\theta\theta'}(\xi-\xi')}\,d\xi\,d\xi' - xx'\right) \tag{9}$$

For a stationary hydraulic conductivity covariance

$$C_{\theta\theta'}(\xi,\xi') = C_{\theta\theta'}(\xi-\xi') = \sigma_\theta^2\,\rho_{\theta\theta'}(\xi-\xi') \tag{10}$$

where ρ, the correlation function of the hydraulic conductivity, depends on the difference between the spatial arguments ξ and ξ'. The variance of the head is secured from eqn (9) by setting $x = x'$, mathematically

$$(\sigma_h^2(x))_e = C_{hh'}(x,x')|_{x'=x}$$
$$= \left(\frac{q}{K_h}\right)^2\left\{\int_0^x\int_0^x e^{\rho_{\theta\theta'}\sigma_\theta^2}\,d\xi\,d\xi' - x^2\right\} \tag{11}$$

The subscript e, was used to indicate that the solution is exact.

An exact analytical solution was achieved for this simple problem, but in general deriving expressions for the moments by inverting a multi-dimensional random operator for transient flow is complicated unless some type of approximation is introduced. In the following section, the governing stochastic equation in (1) was manipulated to obtain deterministic equations for the moments of the head. In this formulation, a joint multivariate normality assumption between the head and the conductivity will be invoked to demonstrate some limitations on the Gaussian method. A similar approach will also be used later in the case of three dimensional and transient flow.

3.2 Analytical solution by the Gaussian method

Substituting K_r and H_r in eqns (3) and (5) and the constant flux boundary condition into eqn (1) yields

$$\frac{dH}{dx} + \frac{dh}{dx} = -\frac{q}{K_g}e^{-\theta} \tag{12}$$

The governing deterministic equation for the first moment of the head is obtained by taking the expectation of eqn (12). After interchanging the order of operators between differentiation and expectation (e.g. Blanc-Lapierre & Fortet[2]) the result is

$$\frac{dH}{dx} = -\frac{q}{K_g}\overline{e^{(-\theta)}} = -\frac{q}{K_h} \tag{13}$$

Integrating (13) with respect to x and substituting the boundary condition $H = H_0$ at $x = 0$ yields

$$H(x) = H_0 - \frac{q}{K_h}x \tag{14}$$

The first moment solution was identical to the exact one in eqn (8). To initiate a governing deterministic equation for the covariance of the head, eqn (12) expressed at location x' is multiplied by $h(x)$. Because $h(x)$ is a variable dependent on x only, it can be taken inside the derivative with respect to x' (Blanc-Lapierre & Fortet[2]) with the result

$$\frac{\mathrm{d}\,hh'}{\mathrm{d}x'} + h\frac{\mathrm{d}H'}{\mathrm{d}x'} = -\frac{q}{K_g}h\,\mathrm{e}^{-\theta'} \tag{15}$$

The expectation of eqn (15) yields

$$\frac{\mathrm{d}\,\overline{hh'}}{\mathrm{d}x'} = \frac{\mathrm{d}\,C_{hh'}}{\mathrm{d}x'} = -\frac{q}{K_g}(\overline{h\,\mathrm{e}^{-\theta'}}) \tag{16}$$

Equation (16) is one differential equation in two unknowns, namely $C_{hh'}$ and the high order moment $E(h\,\mathrm{e}^{-\theta'})$. If h and θ' are assumed multivariate normal random variables then this higher order moment is expressed in terms of lower order ones using the moment generating function (eqn (A.10) in the Appendix). Symbolically, the result is

$$\overline{h\,\mathrm{e}^{-\theta'}} = -C_{h\theta'}\,\mathrm{e}^{\frac{\sigma_\theta^2}{2}} \tag{17}$$

The relationship in eqn (17) is then substituted into eqn (16) with the result

$$\frac{\mathrm{d}C_{hh'}}{\mathrm{d}x'} = \frac{q}{K_g\,\mathrm{e}^{\frac{-\sigma_\theta^2}{2}}}C_{h\theta'} \tag{18}$$

Because at $x = 0$ the head takes a deterministic value, the boundary condition on the covariance of the head is

$$C_{hh'}(x, 0) = 0 \tag{19}$$

The cross covariance moment on the right hand side of eqn (18) is unknown. An equation for this moment is obtained by multiplying (12) by θ' and taking expectation

$$\frac{\mathrm{d}C_{h\theta'}}{\mathrm{d}x} = -\frac{q}{K_g}\overline{\theta'\,\mathrm{e}^{-\theta}} \tag{20}$$

The boundary condition on the cross covariance moment equation is

$$C_{h\theta'}(0, x') = 0 \tag{21}$$

Because the hydraulic conductivity random process is assumed multivariate normal, the high order moment on the right hand side of eqn (20) is expressed in terms of the second order moment (eqn (A.10) in the Appendix) with the result

$$\overline{\theta'\,\mathrm{e}^{-\theta}} = -\mathrm{e}^{\frac{\sigma_\theta^2}{2}}C_{\theta\theta'} \tag{22}$$

Substituting this last relationship into eqn (20) yields after integrating eqn (20) with respect to x and using the boundary condition in eqn (21)

$$C_{h\theta'}(x, x') = \frac{q}{K_g\,\mathrm{e}^{-\frac{\sigma_\theta^2}{2}}}\int_0^x C_{\theta\theta'}(\xi, x')\,\mathrm{d}\xi \tag{23}$$

Finally, substituting this cross covariance moment into eqn (18), integrating with respect to x', and using the boundary condition in eqn (19), the expression for the covariance of the head becomes

$$C_{hh'}(x, x') = \left(\frac{q}{K_h}\right)^2\int_0^x\int_0^{x'} C_{\theta\theta'}(\xi, \xi')\,\mathrm{d}\xi\,\mathrm{d}\xi' \tag{24}$$

The variance of the head is inferred from eqn (24) by setting $x' = x$ and replacing $C_{\theta\theta'}$ by its equivalent from eqn (10)

$$(\sigma_h^2(x))_a = C_{h,h'}(x, x')|_{x'=x}$$

$$= \left(\frac{q}{K_h}\right)^2\int_0^x\int_0^x \sigma_\theta^2\,\rho_{\theta\theta'}(\xi, \xi')\,\mathrm{d}\xi\,\mathrm{d}\xi' \tag{25}$$

The subscript a is used to indicate that the solution is approximate.

3.3 Comparison of two solutions

For this simple flow problem, the first moment of the head, $H(x)$ in (14), was the same as the exact solution in eqn (8). The expression for the variance of h in eqn (25) is compared with the exact one in eqn (11) (repeated here for convenience)

$$\sigma_h^2(x)|_e = C_{hh'}(x, x')|_{x'=x}$$

$$= \left(\frac{q}{K_g\,\mathrm{e}^{-\frac{\sigma_\theta^2}{2}}}\right)^2\left\{\int_0^x\int_0^x \mathrm{e}^{\rho_{\theta\theta'}\sigma_\theta^2}\,\mathrm{d}\xi\,\mathrm{d}\xi' - x^2\right\} \tag{11}$$

Again, the only distinction in the derivation of these expressions is that in the approximate one, a multivariate normality assumption between h and θ was assumed. If the product $(\rho\sigma_\theta^2)$ in the exact solution is small then retaining the first term in a Taylor series expansion of the exponential argument is justified and the resulting solution becomes identical to the Gaussian solution in (25). A small $(\rho\sigma_\theta^2)$ implies a small variance for θ or a short correlation length. However, because the correlation coefficient, ρ, is always less than one, the Gaussian method might remain valid for a larger variance of θ. Of course this will also depend on the correlation length of the hydraulic conductivity.

These conditions for the normality of head, short correlation length and small σ_θ^2, coincided with the findings of the one dimensional Monte Carlo simulations of Smith and Freeze.[16] Smith and Freeze demonstrated that in a bounded domain the head was more likely to be normally distributed for shorter correlation length. In general, in large scale numerical simulations of ground water flow, the correlation length can be order of magnitudes smaller than the aquifer spatial domain. The analytical solution presented here explained the findings of Smith and Freeze without numerical simulations. Actually, the conditions for the equivalence of the exact and Gaussian solutions, had broader implications than the findings of Smith and Freeze.[16] It indicates that h is multivariate normal and that h and θ are joint multivariate normal. The requirement for h and θ to be jointly normal was not explored by the Monte Carlo simulations before.

4 DERIVATION OF MOMENT EQUATIONS FOR MULTI-DIMENSIONAL TRANSIENT GROUND WATER FLOW

In this section, partial differential equations are developed for the moments of the head in the general case of transient ground water flow. The governing flow equation in three dimensions has the form

$$\nabla.[K_r \nabla H_r)] + N = S\frac{\partial H_r}{\partial t} \tag{26}$$

where, $\nabla.$ is the divergence operator, N is the aquifer volumetric recharge (water volume per unit aquifer volume per unit time), t is time, and S is the specific storage (volume of water released from storage per unit volume of aquifer per unit decline in head), K_r and H_r are the hydraulic conductivity and head random variables. The source of randomness in this equation is the conductivity which is considered a lognormal spatial random function. Substituting K_r and H_r by their equivalent expressions in (3) and (5) into eqn (26), the ground water flow equation takes the form

$$\nabla.[K_g \mathrm{e}^{\theta} \nabla H] + \nabla.[K_g \mathrm{e}^{\theta} \nabla h] = S\frac{\partial H}{\partial t} + S\frac{\partial h}{\partial t} - N \tag{27}$$

The moments of the conductivity were presumably known. If the head and the conductivity are jointly normal, the remaining three unknowns, to fully characterize their joint frequency distribution, are the first two moments of the head $H(\mathbf{x}, t)$ and $C_{hh'}(\mathbf{x}, \mathbf{x}', t)$, and the cross covariance moment between the head and the conductivity $C_{h\theta'}(\mathbf{x}, \mathbf{x}', t)$. Hence, in the Gaussian method, the moment generating function is used to express high order moments in terms of first and second order moments. It is convenient to rewrite the second term on the left hand side of eqn (27) in the fashion

$$\nabla.(K_g \mathrm{e}^{\theta} \nabla h) = \nabla.[K_g(\nabla h \mathrm{e}^{\theta'})_{\mathbf{x}'=\mathbf{x}}] \tag{28}$$

In eqn (28) the argument $\mathbf{x}'$ is set equal to $\mathbf{x}$ after the gradient operation is carried out and before the divergence operator is applied. Substituting eqn (28) into eqn (27) and summing the resulting equation over the ensemble of possible realizations i.e. taking expectation (Beran;[1] Blanc-Lapiere & Fortet[2]), yields

$$\nabla.(K_g \overline{\mathrm{e}^{\theta}} \nabla H) + \nabla.[K_g(\overline{\nabla h \mathrm{e}^{\theta'}})_{\mathbf{x}'=\mathbf{x}}] = S\frac{\partial H}{\partial t} - N \tag{29}$$

If $\theta'(x')$ and $h(x)$ are jointly multivariate normal, the expectations of the high order moments are expressed linearly in terms of lower order ones using the moment generating function. The result is

$$\nabla.(K_a \nabla H) + \nabla.[K_a(\nabla C_{h\theta'})_{\mathbf{x}'=\mathbf{x}}] = S\frac{\partial H}{\partial t} - N \tag{30}$$

where K_a is the arithmetic average of the conductivity defined symbolically as

$$K_a = K_g \mathrm{e}^{\frac{\sigma_\theta^2}{2}} \tag{31}$$

Equation (30) becomes the classical deterministic equation for the head H if θ, the random component of the conductivity, is zero. This partial differential equation has two unknowns, H and $C_{h\theta'}$. Another partial differential equation that involves the cross covariance moment is developed by multiplying eqn (27) by $\theta'(\mathbf{x}')$, the random component of the hydraulic conductivity at location $\mathbf{x}'$, and taking the variables that are dependent on $\mathbf{x}'$ and $\mathbf{x}''$ inside the derivative with respect to $\mathbf{x}$

$$\nabla.[K_g \theta' \mathrm{e}^{\theta} \nabla H] + \nabla.[K_g(\nabla \mathrm{e}^{\theta''} \theta' h)_{\mathbf{x}''=\mathbf{x}}] = S\theta' \frac{\partial H}{\partial t} + S\frac{\partial h\theta'}{\partial t} - N\theta' \tag{32}$$

The sum of eqn (32) over the ensemble of possible realizations yields, after expressing the high order moments in terms of low order ones

$$\nabla.[K_a C_{\theta\theta'} \nabla H] + \nabla.[K_a \nabla C_{h\theta'}] + \nabla.[K_a C_{\theta\theta'}(\nabla C_{h\theta'})_{\mathbf{x}'=\mathbf{x}}] = S\frac{\partial C_{h\theta'}}{\partial t} \tag{33}$$

The system of deterministic equations in (30) and (33) involves two unknowns, $H(\mathbf{x}, t)$ and $C_{h\theta'}(\mathbf{x}, \mathbf{x}', t)$. These two equations are coupled and need to be solved simultaneously.

Similarly, an equation for $C_{hh'}(\mathbf{x}, \mathbf{x}', t)$ is developed by using (27) twice at locations $\mathbf{x}$ and $\mathbf{x}'$. Equation (27) at location $\mathbf{x}$ is multiplied by $h'(\mathbf{x}')$, and at location $\mathbf{x}'$ by $h(\mathbf{x})$. Taking expectation and adding the two equations yields after using the results in the Appendix

$$\begin{aligned} &\nabla.[K_a \nabla C_{hh'}] + \nabla'.[K_a \nabla' C_{hh'}] + \nabla.[K_a C_{h'\theta} \nabla H] \\ &\quad + \nabla'.[K_a C_{h\theta'} \nabla' H'] + \nabla.[K_a C_{h'\theta}(\nabla C_{h\theta'})_{\mathbf{x}'=\mathbf{x}}] \\ &\quad + \nabla'.[K_a C_{h\theta'}(\nabla' C_{h'\theta})_{\mathbf{x}=\mathbf{x}'}] = S\frac{\partial C_{hh'}}{\partial t} \end{aligned} \tag{34}$$

Equation (34) which involves the unknown $C_{hh'}(\mathbf{x}, \mathbf{x}', t)$ is linear. In what follows, we demonstrate the conditions under which the Gaussian method will be equivalent to a perturbation method.

4.1 Comparison with perturbation methods: Case of transient flow (McLaughlin & Wood[11])

In the Gaussian method, the system of equations in (30), (33), and (34) describes the non-stationary spatial and temporal joint frequency distribution of the head and conductivity. While these equations are different from the ones developed by McLaughlin and Wood,[11] it is easily shown that the Gaussian approach will reduce to a perturbation method if the variances of h and θ random variables are assumed small. The assumption of small random variables in perturbation methods can then be used to neglect products of more than two random variables.

The Taylor series expansion of eqn (31) yields after neglecting all high order moments

$$K_a \cong K_g\left(1+\frac{\sigma_\theta^2}{2}\right) \tag{35}$$

The substitution of eqn (35) into eqns (30), (33), and (34) yields after neglecting moments resulting from the product of more than two random variables

$$\nabla.\left[K_g\left(1+\frac{\sigma_\theta^2}{2}\right)\nabla H\right]+\nabla.[K_g(\nabla C_{h\theta'})_{\mathbf{x}'=\mathbf{x}}] = S\frac{\partial H}{\partial t}-N \tag{36}$$

$$\nabla.[K_g C_{\theta\theta'}\nabla H]+\nabla.[K_g\nabla C_{h\theta'}] = S\frac{\partial C_{h\theta'}}{\partial t} \tag{37}$$

$$\nabla.[K_g\nabla C_{hh'}]+\nabla'.[K_g\nabla' C_{hh'}]+\nabla.[K_g C_{h'\theta}\nabla H] + \nabla'.[K_g C_{h\theta'}\nabla' H'] = S\frac{\partial C_{hh'}}{\partial t} \tag{38}$$

The system of eqns (36), (37), and (38), obtained under the assumption that the magnitudes of the random variables are small, is different from the original system of equations derived with the Gaussian methods. This last system of equations is equivalent to the one developed by McLaughlin and Wood.[11] Hence, the two methods are different. However, the Gaussian method will evolve into a perturbation method if the magnitude of the random variables are small. The two methods involve the same number of unknowns, $H(\mathbf{x},t)$, $C_{h\theta'}(\mathbf{x},\mathbf{x}',t)$ and $C_{hh'}(\mathbf{x},\mathbf{x}',t)$, and will require similar computations. However, the Gaussian method retains the known lognormal probabilistic structure of the hydraulic conductivity distribution that is usually observed in the field.

4.2 Comparison with perturbation methods: Case of steady-state flow (Gutjahr[8])

For the particular case of steady-state flow and no aquifer recharge, i.e. $S=0$ and $N=0$ in eqn (27), it is possible to obtain a formulation for which the Gaussian and the perturbation methods are equivalent. This particular case which was investigated earlier by Gutjahr[8] using spectral analysis, can be proven here for these strict flow conditions.

Neglecting the storage and the recharge terms and substituting for

$$\nabla e^\theta = e^\theta\nabla\theta \tag{39}$$

in eqn (27) yields

$$\nabla.[K_g\nabla H]+\nabla.[K_g\nabla h]+K_g(\nabla\theta)(\nabla H) + K_g(\nabla\theta)(\nabla h) = 0 \tag{40}$$

An equation involving the moments H and $C_{h\theta}$ is derived by taking the expectation of eqn (40)

$$\nabla.[K_g\nabla H]+K_g E\{(\nabla\theta)(\nabla h)\} = 0 \tag{41}$$

It is convenient to write the second term on the left hand side of (41) in the following manner

$$E\{(\nabla h)(\nabla\theta)\} = E\{\nabla(\nabla' h\theta')\}_{\mathbf{x}'=\mathbf{x}} = \{\nabla(\nabla' C_{h\theta'})\}_{\mathbf{x}'=\mathbf{x}} \tag{42}$$

In eqn (42), the argument $\mathbf{x}'$ is set equal to $\mathbf{x}$ after both operators are applied on the cross covariance moment. The substituting of eqn (42) into eqn (41) yields

$$\nabla.[K_g\nabla H]+K_g\{\nabla(\nabla' C_{h\theta'})\}_{\mathbf{x}'=\mathbf{x}} = 0 \tag{43}$$

Equation (43) is exact because we did not make an assumption about the magnitude of the random variables or the probabilistic distribution of h. Similarly, two equations involving the cross covariance moment and the covariance of h are derived by multiplying eqn (40) by h' and θ' to obtain

$$K_g(\nabla C_{\theta\theta'})(\nabla H)+K_g\{\nabla''(\nabla\overline{\theta''\theta' h})\}_{\mathbf{x}''=\mathbf{x}} + \nabla.(K_g\nabla C_{h\theta'}) = 0 \tag{44}$$

$$\nabla[K_g\nabla C_{hh'}]+K_g\{\nabla''(\nabla\overline{\theta'' h' h})\}_{\mathbf{x}''=\mathbf{x}} + K_g(\nabla C_{\theta h'})(\nabla H) = 0 \tag{45}$$

Equations (40), (44) and (45) involve more than three unknowns due to the second terms on the left side of eqns (44) and (45). In the perturbation method, one truncates the moment of the product of more than two random variables: accordingly the second terms on the left hand side of eqns (44) and (45) are neglected. Also, in the Gaussian method, i.e. if h and θ are assumed jointly normal, these same two terms are identical to zero as demonstrated in the Appendix in eqn (A.14). So we conclude, that for these strict flow conditions in the above formulation, both methods disregard the same terms and will be equivalent.

Gutjahr[8] used this equivalence to rationalize the good agreement between Monte Carlo simulations and the perturbation method, which yielded satisfactory results even when the input standard deviation is larger than four (Gutjahr & Gelhar[7]). As demonstrated by Gutjahr[8] and here, the equivalence between the two methods is restricted to the case of steady-state flow in infinite domains. However, the set of equations, that were derived in (30), (33) and (34) applies for the general case of transient ground water flow.

5 CONCLUSION

The Gaussian and the perturbation methods were compared to solve the ground water flow equation with random parameters. In the Gaussian method, the moment generating function was used to express high order moments in terms of low order moments to secure a solution to the closure problem. For transient flow, the two methods were different and the Gaussian method becomes a perturbation method if the magnitudes of the random variables are small. For steady-state flow, it is possible to derive a formulation under which the Gaussian and the perturbation methods are equivalents. The hydraulic head is more likely to be multivariate joint normally distributed with the hydraulic conductivity if the correlation length of the conductivity random field is short.

The Gaussian and perturbation methods involve the same number of unknowns and will require similar computations. The Gaussian method, which assumes that the first two moments of a frequency distribution exhausts the statistical properties of this distribution, is practical for field applications. In practice most ground water modelers limited their interest to the evaluation of the first two moments. Also, the Gaussian method can be suitable to calibrate the hydraulic conductivity (the inverse problem) when simultaneous observations of hydraulic head and conductivity are available. In this case, prior specification of a joint frequency distributions of hydraulic head and conductivity fields is needed to condition field statistics. Finally, the Gaussian method preserves the lognormal frequency distribution of hydraulic conductivity that is usually observed in the field.

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APPENDIX

The objective of this Appendix is to determine the high order moments of random variables. If both h and θ have an expectation of zero and are jointly normal, the moment generating function (MGF) is used to achieve this goal. By definition, the MGF, $M(u)$, for a single random variable z is given by the exponential transform (Haugen[9]):

$$M(u) = \int_{\Omega} [e^{(uz)}] f(z)\, dz \tag{A.1}$$

where $f(z)$ is the probability density function of the random variable z. The integration in eqn (A.1) is carried over the ensemble space Ω of the random variable z. Various moments of z can be obtained from eqns (A.1) by differentiation with respect to u. For example, the kth moment of z, $E(z^k)$ is

$$E(z^k) = \left.\frac{\partial^k M}{\partial u^k}\right|_{u=0} \tag{A.2}$$

For the case where $f(z)$ is the Gaussian frequency distribution function, the integration in eqn (A.1) yields the MGF for the normally distributed random variable z. Mathematically

$$M(u) = e^{\frac{\sigma_z^2 u^2}{2}} \tag{A.3}$$

This result is generalized to a vector $\mathbf{z}$ of order n, $\mathbf{z} = (z_1, z_2, \ldots, z_n)$, of joint multivariate normal random variables. Haugen[9] provides the following expression for the MGF, M_n

$$M_n(u_1, u_2, \ldots, u_n) = e^{\left[\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\sigma_{ij}u_i u_j\right]} \tag{A.4}$$

where $\{\sigma_{ij}\}$ is the covariance matrix, a square matrix whose elements are the second moments of the variables. Symbolically $\{\sigma_{ij}\}$ has the form,

$$\sigma_{ij} = E(z_i z_j\} \tag{A.5}$$

$$\sigma_{ij} = \sigma_i^2 = E(z_i z_i)$$

In what follows, we demonstrate the applications of the MGF that are relevant to this manuscript.

Case of univariate normal distribution: Evaluation of $E(e^z)$

If the higher order moment of interest is an exponential function of the random variable z (e.g. e^z or e^{-z}) then it follows from the exponential transformation in eqn (A.1), and the result in eqn (A.3) that

$$E(e^{-z}) = M(u=-1) = \{e^{\frac{1}{2}\sigma_{zz}u^2}\}_{u=-1} = e^{\frac{1}{2}\sigma_{zz}}$$

Using the definition in eqn (A.5), this last expression becomes

$$E(e^{-z}) = e^{\frac{\sigma_z^2}{2}} \tag{A.6}$$

Similarly, one has the result

$$E(e^{z}) = e^{\frac{\sigma_z^2}{2}} \tag{A.7}$$

Case of bivariate normal distribution: Evaluation of $E(\exp(z_1+z_2))$

The moment generating function for the case of the bivariate normally distributed random variables z_1 and z_2 is obtained from eqn (A.4) by setting n equal to 2. The result is

$$M_2(u_1, u_2) = e^{\{\frac{1}{2}\sigma_{1,1}u_1^2 + \frac{1}{2}\sigma_{2,2}u_2^2 + \sigma_{1,2}u_1u_2\}} \tag{A.8}$$

Then it follows from the definition of the MGF that the moment $E(z_1 \exp(-z_2))$ is obtained from the expression

$$E(z_1 e^{-z_2}) = \left.\frac{\partial M_2}{\partial u_1}\right|_{u_1=0, u_2=-1} \tag{A.9}$$

Substituting the expression in (A.8) into (A.9) yields

$$E(z_1 e^{-z_2}) = -\sigma_{1,2} e^{\frac{\sigma_2^2}{2}} \tag{A.10}$$

Case of trivariate normal distribution: Evaluation of $E(z_1z_2z_3)$

The MGF for three jointly distributed normal random variables is obtained from eqn (A.4) by setting $n = 3$

$$M_3(u_1, u_2, u_3) = e^{\{\frac{1}{2}(\sigma_1^2u_1^2 + \sigma_2^2u_2^2 + \sigma_3^2u_3^2) + \sigma_{1,2}u_1u_2 + \sigma_{1,3}u_1u_3 + \sigma_{2,3}u_2u_3\}} \tag{A.11}$$

The moment $E(z_1z_2z_3)$ is determined by the expression

$$E(z_1z_2z_3) = \left.\frac{\partial^3 M_3}{\partial u_1 \partial u_2 \partial u_3}\right|_{u_1=0, u_2=0, u_3=0} \tag{A.12}$$

This differentiation of eqn (A.11) yields the expression

$$\begin{aligned}\frac{\partial^3 M_3}{\partial u_1 \partial u_2 \partial u_3} &= \sigma_{1,2}(\sigma_{3,3}u_3 + \sigma_{1,3}u_1 + \sigma_{2,3}u_2)M_3 \\ &+ \sigma_{1,3}(\sigma_{2,2}u_2 + \sigma_{1,2}u_1 + \sigma_{2,3}u_3)M_3 \\ &+ \sigma_{2,3}(\sigma_{1,1}u_1 + \sigma_{1,2}u_2 + \sigma_{1,3}u_3)M_3 \\ &+ (\sigma_{1,1}u_1 + \sigma_{1,2}u_2 + \sigma_{1,3}u_3) \\ &\times (\sigma_{2,2}u_2 + \sigma_{1,2}u_1 + \sigma_{2,3}u_3) \\ &\times (\sigma_{3,3}u_3 + \sigma_{1,3}u_1 + \sigma_{2,3}u_2)M_3\end{aligned} \tag{A.13}$$

The substitution of eqn (A.13) into eqn (A.11) provides the result

$$E(z_1z_2z_3) = \left.\frac{\partial^3 M_3}{\partial u_1 \partial u_2 \partial u_3}\right|_{u_1=0, u_2=0, u_3=0} = 0 \tag{A.14}$$

Similarly, the moment $E(z_1z_2\exp(z_3))$ is derived from the MGF using the relation

$$E(z_1z_2 e^{z_3}) = \left.\frac{\partial^2 M_3}{\partial u_1 \partial u_2}\right|_{u_1=0, u_2=0, u_3=1} \tag{A.15}$$

The substitution of this last relation into eqn (A.11) yields

$$E(z_1z_2 e^{z_3}) = (\sigma_{1,2} + \sigma_{1,3}\sigma_{2,3}) e^{\frac{\sigma_3^2}{2}} \tag{A.16}$$