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Stochastic Ground Water Flow Analysis, FY-81 Status Report

July 1983

Work Supported by Office of Nuclear Waste Isolation under Contract DE-AC06-76RLO 1830 with the U.S. Department of Energy

Pacific Northwest Laboratory
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STOCHASTIC GROUND WATER FLOW ANALYSIS FY-81 STATUS REPORT

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SUMMARY

The stochastic analysis of ground-water flow is a promising new method which can supply more comprehensive analyses of the ground-water environment. The work reported herein provided experience in the methodology while producing a research-oriented stochastic analysis capability.

Single-layer aquifers of horizontal extent were selected for this effort. Kriging has been employed to describe the uncertainty in field data. The resulting stochastic parameters enter the problem physics through boundary conditions and Darcy's equation. The mean and variance of the piezometric head are estimated by the stochastic analysis.

Stochastic analyses provide the engineer and decision maker with access to the mean solution and a measure of the sensitivity of the solution to uncertainties in the aquifer's parameters and boundary conditions. Preliminary results show that the statistical correlation between physical parameters and boundary conditions can have an affect on the stochastic response. This implies that Monte Carlo simulation, where independence of parameter values is assumed, may not be a satisfactory tool when statistical correlation is strong.

Important questions which remain to be answered include:

- What will be the groundwater system's stochastic response when non-zero random components are employed in held head or Dirichlet boundary conditions?
- What will be the groundwater system's stochastic reponse when non-stationary covariance functions are employed for both the transmissivity and boundary flux?
- What size of perturbation can the method of Keller-Gibbs tolerate?

Answers to the first two questions are important for the interpretation of results from either the Monte Carlo and perturbation approaches to stochastic groundwater flow analysis. An answer to the last question is essential prior

to the further development of application oriented computational packages based upon the perturbation method.

An important research tool has been created. The utility of this modeling approach is in supplying users with a confidence band about the mean solution. Once the size of perturbation question is resolved, two work efforts are suggested: 1) application of the method to the two-dimensional analysis of multi-layered systems to provide a stochastic analysis to the vertical path often taken by contaminants, and 2) the development and publication of baselined computational packages for both the horizontal and vertical analyses. Baselined codes would provide the necessary quality assured tracability for performance assessment simulations.

ABSTRACT

Research was conducted at Pacific Northwest Laboratory to develop a research computational package for the stochastic analysis of ground-water flow. Both unsteady and steady-state analysis were examined, and a steady-state research code was developed for the study of stochastic processes. This report describes the theoretical development of both unsteady and steady analyses, and presents the preliminary studies undertaken to verify and exercise the encoded algorithm.

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INTRODUCTION

A stochastic interpretation of ground-water flow has been studied to provide the ONWI program and the AEGIS staff with first-hand knowledge of the potential uses and incumbent difficulties of this relatively new analysis. Present flow analysis capabilities provide deterministic results and one must judgmentally evaluate results or undertake sensitivity studies to determine the effect of parameter uncertainty. The stochastic approach provides a variance envelope or band about the expected results giving the user direct information on the reliance that may be placed upon the solution.

Within the literature, the concept of uncertainty holds two distinct meanings. They are associated with the scale of variability which one is addressing. This report addresses parameter uncertainty on a large scale arising from sampling and interpolation error. The covariance structure employed in this analysis is on such a large scale that it effectively ignores the inherent variability of the media and its parameters on the small scale.

Uncertainty on the small scale involves the study of an aquifer's detailed morphology and the resulting variability in the path taken by fluids. This inherent uncertainty in the media's composition and its implications for both fluid and mass transport are presently under intense investigation. The study of uncertainty in this context is of great interest in that it provides a more comprehensive physics to describe fluid and mass transport. However, in the present work, the sampling of the aquifer will be at a significantly larger scale, and therefore, the detailed resolution of media parameters is lost. While the inherent uncertainty in the media's parameters does become a factor in our interpretation of the sample values and their interpolation, the covariance expressions we employ do not seek to resolve these small scale variabilities.

SELECTED LITERATURE

On the scale and in the generality in which we chose to solve the uncertainty problem, there are two methods of solution. The Monte-Carlo method involves the passing of a significant number of random parameter simulations through a deterministic model to obtain the stochastic solution of the ground-water flow problem. Freeze (1975) first published in this area, and more recently Delhomme (1979) has coupled kriged transmissivities, and deterministic ground-water simulations to form a conditional simulation of an aquifer. The Monte-Carlo method of stochastic analysis suffers from the expense of producing a representative number of deterministic solutions.

The method of moments provides a more direct analysis of the uncertainty problem. Two approaches to this analysis have appeared in the literature. Tang and Pinder (1977, 1979) have employed a matrix perturbation technique originally proposed by Keller (1964) to address wave propagation in random media. Gibbs (1980) applied the Keller method to mass transport within the ground-water environment. This latter, more elegant interpretation of the Keller method is applied herein.

A term by term perturbation approach was published by Sagar (1978). This technique has the distinct advantage of isolating the solution for expectation, variance, and/or covariance for any point of interest. Thus, only values at points of interest need be computed. However, in the general case where a great many or all points are of interest, the technique suffers from the expense of repeated computations.

Within the method of moments, all third and higher order terms are truncated. A variety of criteria have been advanced to describe the applicability of the method. While these criteria have not been addressed within the present study, it should be noted that the ground-water flow equations have a tremendous ability to smooth or filter the input data. With the caveat that inputs be reasonably well behaved, the method of moments has been found to be a fairly robust technique.

The present effort is unique in that kriging is used to stochastically describe inputs to the method of moments solution. Kriging was employed by Delhomme (1979) in the Monte-Carlo approach of conditional simulations. Its coupling to the Keller method of analysis yields a direct solution to the uncertainty problem.

OBJECTIVES AND SCOPE

The original charter of this research focused on the uncertainty in dynamic or transient ground-water flow analysis. Upon completion of the initial phase of the unsteady analysis, the matrix manipulations were revealed to be both many in number and significant in difficulty. While aspects of these manipulations have since been mastered, it was felt that to solve the dynamic case prior to addressing the steady-state case involved an element of folly. To disregard the gradualism ethic of scientific method invited simulations that one could not comprehend. Thus, the objective of the present work is the development of a research computational tool for the analysis of steady-state stochastic ground-water flows. In achieving this objective, considerable experience has been gained in the computation of covariance expressions similar to those of the dynamic problem. Thus, if a dynamic solution is deemed necessary, the experience necessary to develop an efficient simulation capability exists. The rapid response of aquifer systems and the relatively long time periods of interest in the waste isolation problem combine to imply the adequacy of steady-state flow analysis.

In this initial effort toward a stochastic analysis of ground water, the problem domain of interest is two-dimensional. Specifically, a vertically uniform aquifer of horizontal extent is modeled. Distinct material differences which would arise due to either vertical layering or horizontal discontinuities are not handled by the covariance relationships employed. This stochastic analysis package is at such an early stage in its development that a quality assured tool suitable for immediate use as a performance assessment methodology is beyond the scope of this work. However, the computational package is designed for field application and analysis. It is anticipated that this technology will be applied to both generic and more complex real domains in subsequent studies.

Chapters that follow include discussions of the ground-water flow equation and its weighted residual analogue. In the interest of completeness, the presentation of perturbation methods includes sections on dynamic analysis, steady-state analysis, the equivalence of the two method of moments solutions, and geostatistical estimation methods. Finally, the application of this methodology is discussed for two problems employed in verifying and exercising the resulting research code.

CONCLUSIONS AND RECOMMENDATIONS

Completion of this research effort demonstrates the viability of steady-state stochastic ground-water flow modeling. Available data can be stochastically characterized for use as input to the code. Multiple matrix/vector manipulations involving random components can be computed. The great number of these products required for the dynamic flow analysis may pose significant computational problems. However, the steady-state analysis can be applied to representative domains and the product evaluations can be efficiently performed. The inherent utility of a solution which directly supplies both the mean solution and its variance can be appreciated by anyone who has employed engineering judgement. The vast number of such judgements that combine to yield a deterministic solution are testimony to the need for stochastic analysis.

CONCLUSIONS

Preliminary results show the statistical correlation between physical parameters and boundary conditions can have an effect on the stochastic response of the aquifer. This implies that Monte Carlo simulations, where independence is assumed, may not be a satisfactory tool. Results of the stochastic steady-state analysis reveal that:

- The location of Dirichlet (held piezometric head) boundary conditions can alter both the probabilistic mean and variance of the stochastic analysis.
- The uncertainty in piezometric head reflects its dependence on transmissivity and boundary flux by decreasing continuously near Dirichlet boundary conditions.
- The transmissivity and boundary flux uncertainties with short correlation lengths can create stochastic head fields with much longer correlation lengths.

The research oriented computational package is operational and has been verified against a one-dimensional analytical solution and tested on a synthetic two-dimensional Hanford Site data set. Use of the code to examine the synthetic problem of the Hanford Site subregion has raised several questions giving rise to recommendations for the future study of the stochastic response of aquifer systems.

RECOMMENDATIONS

Use of the code to examine the synthetic problem of the Hanford Site subregion has raised several questions giving rise to recommendations for the future study of the stochastic response of aquifer systems. In the present analysis, held head boundary conditions are employed which fix the head at a deterministic value and its random component at zero. Held non-zero random components need to be examined for their impact upon the aquifer's stochastic response. In addition, non-stationary covariance functions need to be studied to determine their influence upon the aquifer's response since kriging estimation variances are commonly non-stationary. Of upmost importance is the determination of the size of perturbation which the method of Keller-Gibbs can tolerate. Use of the stochastic flux boundary condition has raised a question concerning the meaning of mass conservation with respect to stochastics. It is unclear how a mass conservation constraint can be applied when stochastic hydraulic conductivity and head gradient data are combined to produce the flux boundary condition. Finally, a generic problem which eliminates or controls the combined effects of transmissivity and flux boundary condition stochastics should be studied to determine the proper covariance relationship for morphologies of interest. A continued study of steady-state stochastic analysis should address each of these topics.

Upon completion of the efforts described above, the stochastic code should be packaged to provide a user oriented tool for performance assessment and design analysis. Such a package would include codes to determine the covariance parameters of the input data, the steady-state stochastic groundwater analysis code, and the geostatistical estimation of Darcian velocity from piezometric head and transmissivity data.

Application of stochastic theory to modeling of vertical ground-water flow is another area of interest. The multi-layer aspect and their interfaces could require some modification of the theory employed herein. Covariance relationships for a multi-layer problem would have to recognize the independence of stratigraphic units. Both the horizontal and vertical problem domains must be analyzed prior to extending the analysis to three dimensions. Coupling steady-state stochastic flow with dynamic transport capability should precede development of dynamic stochastic flow analysis.

GROUND-WATER FLOW EQUATIONS

Recognizing that the computational package to be developed would be relatively expensive, a physical domain was selected which was interesting from the applications viewpoint and attractive from the economical one. We begin by presenting the three-dimensional ground-water flow equation. The three-dimensional equations are integrated vertically to describe an aquifer as a two-dimensional, vertically uniform environment. Liebnitz's Rule and the kinematic relationship are used to simplify the resulting expression. Both the steady and unsteady-state form of the equation are presented.

The partial differential equation describing three-dimensional ground-water flow is presented as it appears in Pinder and Gray (1977).

$$\rho S_s h_{,t} - \nabla \cdot (\rho \overline{K}\, \nabla h) + \rho q = 0 \qquad (1)$$

where

g = acceleration of gravity (m/sec^2)

h = piezometric head = Hubbert's potential/g = ϕ^*/g (m)

$\overline{k}$ = intrinsic permeability (m^2)

$\overline{K}$ = hydraulic conductivity = $\rho g \overline{k}/\mu$ (m/sec)

p = pressure (newton (m^2)

q = volumetric discharge (m^3/sec/m^3)

S_s = specific storage = $\rho_0 g(\alpha + \theta\beta)$ (1/m)

v = discharge velocity (m^3/sec/m^2)

α = aquifer compressibility (m^2/newton)

β = fluid compressiblity (m^2/newton)

θ = porosity (dimensionless)

μ = absolute or dynamic viscosity (kg/m/sec)(newton sec/m^2)

ρ = density (kg/m^3)

ρ_0 = reference density (kg/m^3)

ϕ^* = Hubbert's potential = $gz + \int_{P_0}^{P} 1/[\rho(p)]\, dp + \frac{1}{2} v^2$

$\nabla()$ = grad operator = $\overline{i}()_{,x} + \overline{j}()_{,y} + \overline{k}()_{,z}$ and $\overline{i},\overline{j},\overline{k}$ are unit vectors in the positive x,y,z directions.

The first term in Equation (1) represents the time rate of change of mass storage. The second is the spatial rate of change in fluid mass flux, and the third is the rate at which fluid is lost to a mass sink. To arrive at this equation one has simply combined the momentum balance of Darcy's equation with the mass balance of the continuity equation. To produce a more tractable form of Equation (1) we assume the coordinate axes of our problem are collinear with the major and minor principle axes of the intrinsic permeability. The off-diagonal entries of the permeability tensor vanish and reduce Equation (1) to the following form:

$$\rho S_s h,_t - (\rho K_{11} h,_x),_x - (\rho K_{22} h,_y),_y - (\rho K_{33} h,_z),_z + \rho q = 0 \tag{2}$$

where the K_{ij} are the diagonal entries of the hydraulic conductivity tensor.

We wish to consider an aquifer as a horizontal, vertically homogeneous domain. Towards that end, Equation (2) is vertically integrated. Liebnitz's Rule and the kinematic relationship yield the following expressions:

Liebnitz's Rule

$$\left[\int_{g_1(x)}^{g_2(x)} f(x,t)\, dt\right],_x = f(x,g_2(x))\, g_2(x),_x - f(x,g_1(x))\, g_1(x),_x + \int_{g_1(x)}^{g_2(x)} [f(x,t)],_x\, dt \tag{3}$$

Kinematic Relationship at Cap Rock

$$-K_{11} h,_x z_t,_x - K_{22} h,_y z_t,_y + K_{33} h,_z + z_t,_t = 0 \tag{4}$$

where z_t = bottom of cap rock.

Substituting these expressions into the vertically integrated equation yields,

$$[\int_{z_b}^{z_t} \rho S_s h dz]_{,t} - [\int_{z_b}^{z_t} \rho K_{11} h_{,x} dz]_{,x} - [\int_{z_b}^{z_t} \rho K_{22} h_{,y} dz]_{,y}$$

$$+ \int \rho q dz - \rho S_s h\big|_{z_t} z_{t,t} + \rho S_s h\big|_{z_b} z_{b,t} + \rho z_{t,t} - \rho z_{b,t} = 0 \qquad (5)$$

Assuming that deformation is negligible, and that vertical variations in the head, storativity, hydraulic conductivity, and mass sink rate are similarly negligible we find,

$$\rho S_s h_{,t} \Delta z - (\rho \Delta z K_{11} h_{,x})_{,x} - (\rho \Delta z K_{22} h_{,y})_{,y} + \rho \Delta z q = 0 \qquad (6)$$

This equation will be our starting point in the prediction of flow within an aquifer of horizontal extent having vertically homogeneous properties and non-uniform thickness. The steady-state form of this equation simply omits the first term containing the time derivative of piezometric head.

GALERKIN WEIGHTED RESIDUAL METHOD AND TIME DISCRETIZATION

In either a deterministic or stochastic setting the partial differential equation must be reduced to an algebraic system of equations. We chose to employ a weighted residuals method, namely the Galerkin technique. The details of this numerical technique can be found in a number of recent treatises including Pinder and Gray (1977), Finlayson (1972), and Zienkiewicz (1977).

The essential aspect of the finite element technique is the selection of a set of basis functions to interpolate the dependent variable. In the Galerkin weighted residuals method one forms the inner product of the approximated partial differential equation and the basis functions. Setting this product to zero and solving for the dependent variable provides a "best" answer in the sense that the error is made orthogonal to the selected basis functions. The resulting algebraic system is given by

$$Ah + Bh_{,t} = f \qquad (7)$$

where

$$A = \sum_e \left[\int_{\Omega(e)} \rho \Delta z K_{11} W_{i,x} N_{j,x} d\bar{x} + \int_{\Omega(e)} \rho \Delta z K_{22} W_{i,y} N_{j,y} d\bar{x} \right] \qquad (8)$$

$$B = \sum_e \int_{\Omega(e)} \rho \Delta z S_s W_i N_j d\bar{x} \qquad (9)$$

$$f = \sum_e \left[\int_{\partial\Omega(e)} \rho \Delta z W_i (K_{11} N_{j,x} h_j \ell_x + K_{22} N_{j,y} h_j \ell_y) ds - \int_{\Omega(e)} W_i \rho \Delta z q d\bar{x} \right] \qquad (10)$$

and

$\Omega(e)$ = domain (element)

$\partial\Omega(e)$ = exterior boundary (element)

$\bar{x}$ = $x_1, x_2, x_3, \ldots$ or x, y, z

S = counterclockwise path around $\partial\Omega$

$\sum_e$ = summation over all elements.

The time derivative term remains to be discretized. A weighted finite difference approximation is used to produce the following general equation:

$$A\{\varepsilon h^{n+1} + (1 - \varepsilon)\ h^{n}\} + B\{h^{n+1} - h^{n}\}/\Delta t = \varepsilon f^{n+1} + (1 - \varepsilon)\ f^{n} \qquad (11)$$

where

$n+1$ = the advanced time step i.e., $(n+1) * \Delta t$

n = the current time step

$0 \leq \varepsilon \leq 1$

and

$\varepsilon = 0$: explicit method, conditionally stable, first order,

$\varepsilon = 0.5$: Crank-Nicholson, neutrally stable, second order,

$\varepsilon = 1.0$: fully implicit method, unconditionally stable, first order.

Rewritten to collect the n+1 and n terms yields,

$$[\varepsilon A + B/\Delta t]\ h^{n+1} = [(\varepsilon - 1)\ A + B/\Delta t]\ h^{n} + \varepsilon f^{n+1} + (1 - \varepsilon)\ f^{n} \qquad (12)$$

We are now in a position to introduce stochastic parameters into the A and B matrices and the vector f. Stochastic partial differential equations and more difficult subsequently solved than the more familiar deterministic systems.

PERTURBATION METHODS

Within the preceding formulation there are coefficient and parameter values which are imprecisely known and hence uncertain. Specifically, we are concerned with uncertainty due to errors in measurement and interpolation. The parameters of interest include hydraulic conductivity, storativity, and thickness. Boundary and initial conditions also introduce uncertainty in the problem. Expressing each of these quantities as random variables leads to matrices with deterministic and random components.

We chose to solve the stochastic ground-water flow problem by the moments method, specifically via perturbation techniques rather than Monte Carlo (Delhomme 1979, Freeze 1975). Two perturbation techniques have been advanced. One method perturbs on a term by term basis and employs a Taylor series expansion (Sagar 1978, Dettinger and Wilson 1981). The other includes all perturbations within a matrix formulation and employs a Neumann series approximation (Keller 1964, Tang and Pinder 1977, Gibbs 1980). Our objective is to apply the method of Keller-Gibbs to the ground-water flow equations. Both unsteady and steady treatments will be developed and a comparison will be made between the Taylor and Neumann series approaches for the steady-state case.

UNSTEADY ANALYSIS

The notation employed by Gibbs (1980) will in large part be followed. We first simplify our notation by rewriting Equation (12), i.e.,

$$Lh^{n+1} = Mh^{n} + \varepsilon f^{n+1} + (1 - \varepsilon)\, f^{n} \tag{13}$$

where

$$L = \varepsilon A + B/\Delta t$$

and

$$M = (\varepsilon - 1)\, A + B/\Delta t. \tag{14}$$

We define the probabilistic expectation operator, $< \cdot >$, to act upon both matrices and vectors. The expectation effectively removes the random component. Thus, we write,

$$L = L_0 + \eta L_1 \text{ and } f^i = f_0^i + \eta f_1^i \tag{15}$$

where

$$L_0 = \langle L \rangle; \quad \langle L_1 \rangle = 0; \quad f_0^i = \langle f^i \rangle; \quad \langle f_1^i \rangle = 0 \tag{16}$$

Similar expressions hold for the M matrix and the solution vector, h. Substituting the mean and random components (Equation 15) for L, M, and f^i into Equation (13) yields,

$$(L_0 + \eta L_1)\, h^{n+1} = (M_0 + \eta M_1)\, h^n + \varepsilon\{f_0^{n+1} + \eta f_1^{n+1}\} + (1 - \varepsilon)\,\{f_0^n + \eta f_1^n\} \tag{17}$$

By letting N vary from the initial condition (0) to the final time step (N) we write a time history of equations, i.e.,

$$\left.\begin{array}{ll}
n = 0 & L_0 h^1 + \eta L_1 h^1 = M_0 h^0 + \eta M_1 h^0 + \varepsilon\{f_0^1 + \eta f_1^1\} + (1 - \varepsilon)\,\{f_0^0 + \eta f_1^0\} \\
n = 1 & L_0 h^2 + \eta L_1 h^2 - M_0 h^1 - \eta M_1 h^1 = \varepsilon\{f_0^2 + \eta f_1^2\} + (1 - \varepsilon)\,\{f_0^1 + \eta f_1^1\} \\
n = 2 & L_0 h^3 + \eta L_1 h^3 - M_0 h^2 - \eta M_1 h^2 = \varepsilon\{f_0^3 + \eta f_1^3\} + (1 - \varepsilon)\,\{f_0^2 + \eta f_1^2\} \\
\vdots & \\
n = N & L_0 h^N + \eta L_1 h^N - M_0 h^{N-1} - \eta M_1 h^{N-1} \\
 & \quad = \varepsilon\{f_0^N + \eta f_1^N\} + (1 - \varepsilon)\,\{f_0^{N-1} + \eta f_1^{N-1}\}
\end{array}\right\} \tag{18}$$

One should realize that in the first equation the initial conditions are assumed known and therefore appear on the right-hand side. The equations shown above can be written in a compact matrix of matrices, vector of vectors form, but first we must separate the right-hand side (load vector) into its mean and random components. This is accomplished via the expectation operator, i.e.,

$$\mathcal{B} = \mathcal{B}_0 + \eta\mathcal{B}_1 \tag{19}$$

where

$$\mathcal{B}_0 = \langle\mathcal{B}\rangle, \qquad \langle\mathcal{B}_1\rangle = 0.$$

Thus,

$$\mathcal{B}_0 = \begin{Bmatrix} M_0h_0^0 + \eta^2 \langle M_1h_1^0\rangle + \varepsilon f_0^1 + (1 - \varepsilon)\ f_0^0 \\ \varepsilon f_0^2 + (1 - \varepsilon)\ f_0^1 \\ \varepsilon f_0^3 + (1 - \varepsilon)\ f_0^2 \\ \vdots \\ \varepsilon f_0^N + (1 - \varepsilon)\ f_0^{N-1} \end{Bmatrix} \tag{20}$$

and

$$\mathcal{B}_1 = \begin{Bmatrix} M_0h_1^0 + M_1h_0^0 + \varepsilon f_1^1 + (1 - \varepsilon)\ f_1^0 \\ \varepsilon f_1^2 + (1 - \varepsilon)\ f_1^1 \\ \varepsilon f_1^3 + (1 - \varepsilon)\ f_1^2 \\ \vdots \\ \varepsilon f_1^N + (1 - \varepsilon)\ f_1^{N-1} \end{Bmatrix} \tag{21}$$

It remains to define the two matrices of matrices, they are

$$\mathcal{L}_0 = \begin{bmatrix} L_0 & & & & & 0 \\ -M_0 & L_0 & & & & \\ & -M_0 & L_0 & & & \\ & & -M_0 & L_0 & & \\ 0 & & & \ddots & \ddots & \\ & & & & -M_0 & L_0 \end{bmatrix} \tag{22}$$

and

$$\mathcal{L}_1 = \begin{bmatrix} L_1 & & & & & 0 \\ -M_1 & L_1 & & & & \\ & -M_1 & L_1 & & & \\ & & -M_1 & L_1 & & \\ 0 & & & \ddots & \ddots & \\ & & & & -M_1 & L_1 \end{bmatrix} \tag{23}$$

We can now rewrite Equation (18) as:

$$(\mathcal{L}_0 + \eta \mathcal{L}_1)\, \mathcal{H} = \mathcal{B}_0 + \eta \mathcal{B}_1 \tag{24}$$

where the solution vector of vectors is

$$\mathcal{H} = \{h^1\ h^2\ h^3\ \dots\ h^i\ \dots\ h^N\}^T \tag{25}$$

and T implies transpose.

The formal solution to Equation (24) can be written as

$$\mathcal{H} = (\mathcal{L}_0 + \eta \mathcal{L}_1)^{-1}\, (\mathcal{B}_0 + \eta \mathcal{B}_1) \tag{26}$$

where

$$(L_0 + \eta L_1)^{-1} = [(I + \eta L_1 L_0{}^{-1})\ L_0]^{-1} = L_0^{-1}\ (I + \eta L_1 L_0^{-1})^{-1} \tag{27}$$

Provided the perturbations on the system are sufficiently small, we can expand the inverse matrix above in a Newmann series, i.e.,

$$(I + \eta L_1 L_0^{-1})^{-1} \approx I - \eta L_1 L_0^{-1} + \eta^2 (L_1 L_0^{-1})^2\ .\ .\ . \tag{28}$$

Substituting Equation (28) into Equation (26) and truncating all terms of third and higher order we find,

$$H = L_0^{-1}\ (I - \eta L_1 L_0^{-1})\ (B_0 + \eta B_1) + \eta^2 L_0^{-1}\ (L_1 L_0^{-1})^2\ B_0 + O(\eta^3) \tag{29}$$

Taking the expectation of H we find,

$$\langle H \rangle = H_0 = L_0^{-1}\{(I + \eta^2 \langle L_1 L_0^{-1} L_1 \rangle\ L_0^{-1})\ B_0 - \eta^2 \langle L_1 L_0^{-1} B_1 \rangle\} + O(\eta^3) \tag{30}$$

Applying L_0 to both sides of the equation,

$$L_0 H_0 = B_0 + \eta^2 \langle L_1 L_0^{-1} L_1 \rangle\ L_0^{-1}\ B_0 - \eta^2 \langle L_1 L_0^{-1} B_1 \rangle + O(\eta^3) \tag{31}$$

One must note that

$$L_0 H_0 = B_0 + O(\eta^2) \tag{32}$$

Thus, the expectation differs from the deterministic solution by second order effects. Substituting Equation (32) into the third term of Equation (31) and making the obvious rearrangements we find,

$$(L_0 - \eta^2 \langle L_1 L_0^{-1} L_1 \rangle)\ H_0 = B_0 - \eta^2 \langle L_1 L_0^{-1}\ B_1 \rangle + O(\eta^3) \tag{33}$$

In this form one can readily see the influence of the covariance functions. Transmissivity, storativity and their combination will directly influence the stiffness matrix. Covariance combinations of transmissivity, storativity, source/sink, boundary and initial conditions affect the load vector.

To obtain the expectation from Equation (33) we must accomplish two tasks. First, the inverse of $\mathcal{L}_0$ must be formed. Second, the triple matrix products must be evaluated. The first task is readily achieved. We recall Equation (22)

$$\mathcal{L}_0 = \begin{bmatrix} L_0 & & & & 0 \\ -M_0 & L_0 & & & \\ & -M_0 & L_0 & & \\ 0 & & \ddots & \ddots & \\ & & & -M_0 & L_0 \end{bmatrix} \tag{22}$$

Its inverse is simply

$$(\mathcal{L}_0^{-1})_{ij} = \begin{cases} 0, & i < j \\ L_0^{-1}, & i = j \\ L_0^{-2}(M_0 L_0^{-1})^{i-j}, & i > j \end{cases} \tag{34}$$

where i,j = 1, 2, ..., N

The triple products are evaluated by first forming the intermediate result $(\mathcal{L}_1 \mathcal{L}_0^{-1})$ and then post multiplying by either $\mathcal{L}_1$ or $\mathcal{B}_1$. In the first case we find

$$(\mathcal{L}_1 \mathcal{L}_0^{-1} \mathcal{L}_1)_{ij} = \begin{cases} 0, & i < j \\ L_1 L_0^{-1} L_1, & i = j \\ \left.\begin{array}{l} [L_1 L_0^{-1}(M_0 L_0^{-1})^{i-j} - M_1 L_0^{-1}(M_0 L_0^{-1})^{i-j-1}] L_1 \\ + [M_1 L_0^{-1}(M_0 L_0^{-1})^{i-j-2} - L_1 L_0^{-1}(M_0 L_0^{-1})^{i-j-1}] M_1 \end{array}\right\} & , i > j \end{cases} \tag{35}$$

Note that negative powers of these matrices are not admitted. Thus, for the case of $i = j + 1$,

$$(M_0L_0^{-1})^{i-j-2} = 0$$

Now, for the latter triple product,

$$(L_1L_0^{-1}B_1)_i = \begin{cases} L_1L_0^{-1}\{M_0h_1^0 + M_1h_0^0 + \varepsilon f_1^1 + (1 - \varepsilon)\ f_1^0\}, \quad i = 1 \\ L_1L_0^{-1}\{\varepsilon f_1^2 + (1 - \varepsilon)\ f_1^1\} \\ + [L_1L_0^{-1}\ (M_0L_0^{-1})]\ \{M_0h_1^0 + M_1h_0^0 + \varepsilon f_1^1 + (1 - \varepsilon)\ f_1^0\}, \quad i = 2 \\ L_1L_0^{-1}\{\varepsilon f_1^i + (1 - \varepsilon)\ f_1^{i-1}\} \\ + \sum_{k=1}^{i-1} [L_1L_0^{-1}(M_0L_0^{-1})^{i-k} - M_1L_0^{-1}(M_0L_0^{-1})^{i-k-1}] \\ \quad *\{\varepsilon f_1^k + (1 - \varepsilon)\ f_1^{k-1}\} \\ + [L_1L_0^{-1}(M_0L_0^{-1})i-1 - M_1L_0^{-1}(M_0L_0^{-1})^{i-k-1}] \\ \quad *\{M_0h_1^0 + M_1h_0^0 + \varepsilon f_1^1 + (1 - \varepsilon)\ f_1^0\}, \quad i \geq 3 \end{cases} \tag{36}$$

Recall that we are working with a matrix of matrices and a vector of vectors. Having obtained expressions for the triple products we can return to Equation (33) and begin to examine the system of equations describing the expectation as time progresses. Three systems of equations will be developed. The first and second for the first and second time steps. The third will be a general expression for the third and all subsequent time steps.

First Δt, i = 1

$$\left.\begin{aligned}[L_0 - \eta^2 \langle L_1 L_0^{-1} L_1 \rangle]\, h_0^1 = M_0 h_0^0 + \eta^2 \langle M_1 h_1^0 \rangle + \varepsilon f_0^1 + (1-\varepsilon)\, f_0^0 \\ - \eta^2 \langle L_1 L_0^{-1} \{ M_0 h_1^0 + M_1 h_0^0 + \varepsilon f_1^1 + (1-\varepsilon)\, f_1^0 \} \rangle \end{aligned}\right\} \quad (37)$$

Second Δt, i = 2

$$\left.\begin{aligned}[L_0 - \eta^2 \langle L_1 L_0^{-1} L_1 \rangle]\, h_0^2 = M_0 h_0^1 + \eta^2 \langle L_1 L_0^{-1} (M_0 L_0^{-1}) L_1 - L_1 L_0^{-1} M_1 \rangle\, h_0^1 \\ + \varepsilon f_0^2 + (1-\varepsilon) f_0^1 - \eta^2 \langle L_1 L_0^{-1} \{ \varepsilon f_1^2 + (1-\varepsilon) f_1^1 \} \rangle \\ - \eta^2 \langle L_1 L_0^{-1} (M_0 L_0^{-1}) \{ M_0 h_1^0 + M_1 h_0^0 + \varepsilon f_1^1 + (1-\varepsilon) f_1^0 \} \rangle \\ + \eta^2 \langle M_1 h_1^1 \rangle \end{aligned}\right\} \quad (38)$$

where

$$M_1 h_1^1 = - M_1 L_0^{-1} L_1 h_0^1 + M_1 L_0^{-1} \{ M_0 h_1^0 + M_1 h_0^0 + \varepsilon f_1^1 + (1-\varepsilon)\, f_1^0 \} \quad (39)$$

All Subsequent Δt, $i \geq 3$

$$\left.\begin{aligned}[L_0 - \eta^2 \langle L_1 L_0^{-1} L_1 \rangle]\, h_0^i = M_0 h_0^{i-1} + \eta^2 \sum_{k=1}^{i-1} \langle [L_1 L_0^{-1} (M_0 L_0^{-1})^{i-k} L_1 \\ - L_1 L_0^{-1} (M_0 L_0^{-1})^{i-k-1} M_1] \rangle\, h_0^k \\ + \varepsilon f_0^i + (1-\varepsilon)\, f_0^{i-1} \\ - \eta^2 \langle L_1 L_0^{-1} \{ \varepsilon f_1^i + (1-\varepsilon)\, f_1^{i-1} \} \rangle \\ - \eta^2 \sum_{k=2}^{i-1} \langle L_1 L_0^{-1} (M_0 L_0^{-1})^{i-k} \{ \varepsilon f_1^k + (1-\varepsilon)\, f_1^{k-1} \} \rangle \\ - \eta^2 \langle L_1 L_0^{-1} (M_0 L_0^{-1})^{i-1} \{ M_0 h_1^0 + M_1 h_0^0 + \varepsilon f_1^i \\ + (1-\varepsilon)\, f_1^0 \} \rangle + \eta^2 \langle M_1 h_1^{\,i-1} \rangle \end{aligned}\right\} \quad (40)$$

where

$$
\left.
\begin{aligned}
<M_1 h_1^{i-1}> = {} & <M_1 L_0^{-1} \{\varepsilon f_i^{i-1} + (1 - \varepsilon)\ f_1^{i-2}\}> + \sum_{k=2}^{i-2} <M_1 L_0^{-1} (M_0 L_0^{-1})^{i-k-1} \\
& * \{\varepsilon f_1^{k-1} + (1 - \varepsilon) f_1^{k-2}\}> + <M_1 L_0^{-1} (M_0 L_0^{-1})^{i-2} \{M_0 h_1^0 + M_1 h_0^0 \\
& + \varepsilon f_1^1 + (1 - \varepsilon)\ f_1^0\}> - <M_1 L_0{}^{-1} L_1> h_0^{i-1} \\
& - \sum_{k=1}^{i-2} [<M_1 L_0^{-1} (M_0 L_0^{-1})^{i-k-1} L_1> - <M_1 L_0^{-1}\ (M_0 L_0^{-1})^{i-k-2} M_1>] h_0^k
\end{aligned}
\right\} \quad (41)
$$

Note that the summations in Equations (40) and (41) involve the product $(M_0 L_0^{-1})$ raised to a power. As the information, either h^i or f^i, becomes further removed in time, the product is raised to a higher power. How quickly this information is made small by $(M_0 L_0^{-1})$ will dictate the number of terms carried in a computation.

The reader should be aware of the incomplete nature of this analysis. Having achieved an expectation solution there remains to develop the covariance solution. Once this is achieved, one could chose to obtain the variance/covariance after each time step, and effectively restart the problem for each Δt. Thus, one could use Equation (37) to obtain all expectation solutions. As one may well guess, obtaining the variance/covariance will not be easy.

While being incomplete, we have established the relationships of the unsteady state analysis of expectation. Having studied the matrix/vector manipulations required of this solution, it was decided to defer further efforts toward obtaining a solution until the steady-state problem was posed, solved, and studied.

STEADY-STATE (Keller-Gibbs)

The motivation for addressing the steady-state stochastic analysis of ground-water flow arises from the spirit of gradualism in the scientific method and the historical perspective of waste isolation studies. One proceeds a step at a time, each step more difficult than its predecessor, until the comprehensive solution is obtained. A steady-state analysis of stochastic ground-water flow is a reasonable first step and will provide many of the tools necessary to perform and understand an unsteady analysis. Historically, the flow and contaminant transport models of waste isolation in the far-field have been uncoupled. Due to the large time periods of interest and the relatively quick response of aquifer systems, the flow analyses have been steady-state. Contaminant transport associated with the flow is then run as unsteady (dynamic) to yield the desired breakthrough and contaminant level information sought. For these reasons we will proceed with the steady-state analysis of stochastic ground-water flow.

Much of the steady-state analysis can be taken directly from the unsteady analysis. We will go a step further by discussing the implementation of these equations to obtain a solution. Both the Newmann series (Keller 1964, Gibbs 1980) and the Taylor series (Sagar 1978) techniques of perturbation analysis will be presented and compared.

We begin with the ground-water flow equation and its Galerkin technique analogue. Omitting the storage term in Equation (6) we obtain the steady-state formulation for flow in a variably thick, horizontal aquifer. This equation is,

$$- (\rho\Delta z K_{11} h,_{x}),_{x} - (\rho\Delta z K_{22} h,_{y}),_{y} + \rho\Delta z q = 0 \tag{42}$$

The Galerkin technique analogue to this PDE in a deterministic setting is

$$A\ h = f \tag{43}$$

where A and f are defined by Equations (8) and (10). As in the unsteady analysis the basis functions of the weighted residuals method remain deterministic while the parameters and constraints of the aquifer system are recognized as stochastic. Stochastic inputs to this problem include hydraulic conductivity and thickness (transmissivity), volumetric discharge rate, Neumann boundary conditions, and Dirichlet boundary conditions. These give rise to a stochastic partial differential equation with a stochastic solution for the the piezometric head.

The Neumann series technique of perturbation analysis advanced by Keller (1964) and Gibbs (1980) is applied to Equation (43). The matrix and vectors are broken into an expectation and random component as before, i.e.,

$$
\begin{aligned}
A &= A_0 + \eta A_1 \\
f &= f_0 + \eta f_1 \\
h &= h_0 + \eta h_1
\end{aligned}
\tag{44}
$$

Using a completely analogous approach as in the unsteady-state analysis we find,

$$h = A_0^{-1} [I - \eta A_1 A_0^{-1}]\{f_0 + \eta f_1\} + \eta^2 A_0^{-1}[A_1 A_0^{-1}]^2 f_0 + O(\eta^3) \tag{45}$$

The expectation of h, h_0, is simply

$$h_0 = A_0^{-1}\{f_0 + \eta^2 \langle A_1 A_0^{-1} A_1 \rangle A_0^{-1} f_0 - \eta^2 \langle A_1 A_0^{-1} f_1 \rangle + O(\eta^3)\} \tag{46}$$

We note that

$$A_0 h_0 = f_0 + O(\eta^2) \tag{47}$$

This allows us to write

$$[A_0 - \eta^2 \langle A_1 A_0^{-1} A_1 \rangle]\, h_0 = f_0 - \eta^2 \langle A_1 A_0^{-1} f_1 \rangle + O(\eta^3) \tag{48}$$

Equation (46) or (48) could be used to calculate the expectation of the piezometric head. The latter relationship does reveal that uncertainty in A_0 (i.e., A_1) serves to modify A_0 while covariance information involving uncertainty in A_0 and f_0 serve to modify f_0. Either equation employed in solutions of h_0 requires that A_0 inverse be formed. Thus, if two matrix-vector products are cheaper than a Guass elimination, Equation (46) is preferred. However, the economy of this computation will not be very important in light of the triple matrix products.

We now seek the second half of our solution, the variance/covariance of the piezometric head. The tedious details are omitted; one is simply manipulating Equations (45) and (46) to obtain

$$\eta^2 \langle h_1 h_1^T \rangle = \langle \{h_0 + \eta h_1\}\{h_0 + \eta h_1\}^T \rangle - h_0 h_0^T \tag{49}$$

The resulting variance/covariance matrix is given by

$$\langle h_1 h_1^T \rangle = A_0^{-1}[\langle f_1 f_1^T \rangle - \langle f_1 h_d^T A_1 \rangle - \langle A_1 h_d f_1^T \rangle + \langle A_1 h_d h_d^T A_1 \rangle] A_0^{-1} \tag{50}$$

where h_d = deterministic solution = $A_0^{-1} f_0$. Equation (50) yields the covariance of the piezometric heads over the entire domain. Entries of $\langle h_1 h_1^T \rangle$ yield the values of the variance/covariance matrix.

In obtaining the variance/covariance matrix and in the work that follows we have made a simplifying assumption. We assume the transmissivity is homogeneous and isotropic within any element of the weighted residual discretization. This assumption enables one to extract the transmissivity (k_{11}, k_{22}) from the integrands of Equations (8), (9), and (10). The matrices are now symmetric and the evaluation of Equation (49) is greatly simplified. Thus, the reader should be cautious in transferring our resulting expressions to non-symmetric problems. The evaluation of variance/covariance could be far more difficult.

Implementation - Dirichlet Boundary Conditions

In the course of the preceding analysis we have assumed that the coefficient matrix A_0 was nonsingular. For this to be valid using the weighted residual method, we must set a Dirichlet boundary condition.

The matrix representation of the steady-state problem was given by

$$Ah = f \tag{43}$$

Expanding the matrix and vectors into their expectation and random components we write,

$$(A_0 + \eta A_1)\{h_0 + \eta h_1\} = \{f_0 + \eta f_1\} \tag{51}$$

Inserting the Dirichlet conditions and employing a partition method in the matrix format we write,

$$\left[\begin{bmatrix} A_0' & A_0'' \\ 0 & I \end{bmatrix} + \eta \begin{bmatrix} A_1' & A_1'' \\ 0 & 0 \end{bmatrix}\right] \begin{Bmatrix} h_0' + \eta h_1' \\ h_0'' + \eta h_1'' \end{Bmatrix} = \begin{Bmatrix} f_0' + \eta f_1' \\ h_0'' + \eta h_1'' \end{Bmatrix} \tag{52}$$

where single and double prime notation is employed to trace the different portions of the partitioned system. The resulting solution for the piezometric head is

$$\left.\begin{aligned} h_0' + \eta h_1' = {} & A_0'^{-1}f_0' - \eta A_0'^{-1}A_1'A_0'^{-1}f_0' + \eta^2 A_0'^{-1}(A_1'A_0'^{-1})^2 f_0' \\ & - A_0'^{-1}A_0''f_0'' + \eta A_0'^{-1}A_1'A_0'^{-1}A_0''f_0'' - \eta^2 A_0'^{-1}(A_1'A_0'^{-1})^2 A_0''f_0'' \\ & + \eta A_0'^{-1}f_1' - \eta A_0'^{-1}A_1''h_0'' - \eta A_0'^{-1}A_0''h_1'' + \eta^2 A_0'^{-1}A_1'A_0'^{-1}A_1''h_0'' \\ & - \eta^2 A_0'^{-1}A_1'A_0'^{-1}f_1' + \eta^2 A_0'^{-1}A_1'A_0'^{-1}A_0''h_1'' - \eta^2 A_0'^{-1}A_1''h_1'' \end{aligned}\right\} \tag{53}$$

Taking the expectation of Equation (53) we find

$$
\left.
\begin{aligned}
h'_0 = {} & A_0'^{-1} \{f'_0 - A''_0 h''_0 + \eta^2 <A'_1 A_0'^{-1} A'_1> A_0'^{-1} \{f'_0 - A''_0 h''_0\} \\
& + \eta^2 <A'_1 A_0'^{-1} A''_1> h''_0 - \eta^2 <A'_1 A_0'^{-1} b'_1> + \eta^2 <A'_1 A_0'^{-1} A''_0 h''_1> \\
& - \eta^2 <A''_1 h''_1>\}
\end{aligned}
\right\} \quad (54)
$$

Finally, we form the variance/covariance matrix, i.e.,

$$
\eta^2 <h'_1 h_1'^T> = <\{h'_0 + \eta h'_1\}\{h'_0 + \eta h'_1\}^T> - h'_0 h_0'^T \qquad (55)
$$

Making the substitutions and performing the various manipulations we find,

$$
\left.
\begin{aligned}
<h'_1 h_1'^T> = {} & A_0'^{-1} [<A'_1 A_0'^{-1} f'_0 f_0'^T A_0'^{-1} A'_1> - <A'_1 A_0'^{-1} f'_0 h_0''^T A_0''^T A_0'^{-1} A'_1> - <A'_1 A_0'^{-1} f'_0 f_1'^T> \\
& + <A'_1 A_0'^{-1} f'_0 h_0''^T A_1''^T> + <A'_1 A_0'^{-1} f'_0 h_1''^T> A_0''^T - <A'_1 A_0'^{-1} A''_0 h''_0 f_0'^T A_0'^{-1} A'_1> \\
& + <A'_1 A_0'^{-1} A''_0 h''_0 h_0''^T A_0''^T A_0''^T A_0'^{-1} A'_1> + <A'_1 A_0'^{-1} A''_0 h''_0 f_1'^T> - <A'_1 A_0'^{-1} A''_0 h''_0 h_0''^T A_1''^T> \\
& - <A'_1 A_0'^{-1} A''_0 h''_0 h_1''^T> A_0''^T - <f'_1 f_0'^T A_0'^{-1} A'_1> + <f'_1 h_0''^T A_0''^T A_0'^{-1} A'_1> + <f'_1 f_1'^T> \\
& - <f'_1 h_0''^T A_1''^T> - <f'_1 h_1''^T> A_0''^T + <A''_1 h''_0 f_0'^T A_0'^{-1} A'_1> - <A''_1 h''_0 h_0''^T A_0''^T A_0'^{-1} A'_1> \\
& - <A''_1 h''_0 f_1'^T> + <A''_1 h''_0 h_0''^T A_1''^T> + <A''_1 h''_0 h_1''^T> A_0''^T + A''_0 <h''_1 f_0'^T A_0'^{-1} A'_1> \\
& - A''_0 <h''_1 h_0''^T A_0'^{-1} A'_1> - A''_0 <h''_1 f_1'^T> + A''_0 <h''_1 h_0''^T A_1''^T> + A''_0 <h''_1 h_1''^T> A_0''^T] A_0'^{-1}
\end{aligned}
\right\} \quad (56)
$$

In a standard deterministic solution procedure one would simply modify the load vector, f'_0, and employ Guass elimination. However, the above development is necessary since in a stochastic formulation the simple modification can not be made. The pairs of information which become the covariance must be carried through the computation. Only when they have been paired can they be evaluated in a deterministic sense, and their impact upon the expectation and random component ascertained.

Implementation - The Triple Matrix Product

Since the variance/covariance calculations consume so much of the execution time, we would be remiss to omit a brief discussion of them. From the previous section it is obvious that there are a considerable number of covariance evaluations to be completed. To make matters worse, these evaluations can not be explicitly written until the pairs of random components are identified. Thus, in the triple matrix product, $(A_1 A_0^{-1} A_1)$, the initial multiplication of $(A_1 A_0{}^{-1})$ does not produce a simple matrix. Rather, one is forced to save the value and identify each contribution to the matrix product. When the post product with A_1 is completed, the identities of the covariance pairs are revealed, and the evaluations can be made. Thus, one can readily see that considerable core storage must be employed and a considerable amount of bookkeeping done if one choses to form A_1 and then complete the triple product.

An element by element generation of the triple product has been utilized in the present work. A trade-off is made between core requirements and computation time. One forms the individual entries through an element contribution summation procedure, i.e.,

$$\langle A_1 A_0{}^{-1} A_1 \rangle = \left[\sum_{e=1}^{N_e} A_1^e \right] A_0^{-1} \left[\sum_{e=1}^{N_e} A_1^e \right] \tag{57}$$

where

N_e = number of elements

A_1^e = element contributions to the A_1 matrix.

The computer algorithm is designed to sum the contributions of all elements (Figure 1). This algorithm can be made more efficient if one selects to include only contributing elements on the inner loop.

Outer Loop on "i"

Create A_e^i

Product A_e^i with A_0^{-1}

Inner Loop on "j"

Create A_e^j

Product $A_e^i A_0^{-1}$ with A_e^j

Accumulate these products to obtain $\langle A_1 A_0 A_1 \rangle$

Finish Inner Loop

Finish Outer Loop

FIGURE 1. An Algorithm to Evaluate the Triple Product

STEADY-STATE (Sagar)

There are two perturbation techniques advanced in the open literature. We have applied the Neumann series approach advanced by Keller (1964), Tang and Pinder (1977), and Gibbs (1980). The second technique employs a Taylor series approach and was applied to stochastic ground-water flow by Sagar (1978). The two methods would appear to have different criteria with regard to the size of perturbation and the stability of computation. In this section we will develop the Taylor series approach to steady-state stochastic ground-water flow, and show the equivalence of the two techniques.

We begin with the deterministic equation for steady-state ground-water flow

$$A\ h = f \tag{43}$$

Assuming A and f are stochastic produces a stochastic partial differential equation with a stochastic solution vector, h. As before, the expectation is defined by

$$\langle A \rangle = A_0;\ \langle f \rangle = f_0 \tag{58}$$

Employing only the expectations of the stochastic input (transmissivity, etc.), we would obtain the deterministic solution, h_d, i.e.,

$$A_0\, h_d = f_0 \tag{59}$$

Solving for h_d by inverting A_0 yields,

$$f_d = A_0^{-1} f_0 = R_0 f_0$$

where R_0 equals A_0^{-1}. Perturbing the i, k (row, column) entry of A_0 by a quantity, δ, the R_0 matrix would be perturbed in the following way

$$R_\delta - R_0 = -\frac{\delta}{1 + r_{ki}\delta} \begin{Bmatrix} r_{1i} \\ r_{2i} \\ \vdots \\ r_{Ni} \end{Bmatrix} \{r_{k1} r_{k2} \cdots r_{kN}\} \tag{60}$$

where R_δ is the perturbed inverse and r_{ik} are entries in the R_0 matrix. Employing Einstein notation

$$R_\delta - R_0 = -\frac{\delta}{1 + r_{ki}\delta}\, r_{ji}\, r_{k\ell}^T \qquad j,\ell = 1, 2, \ldots, N \tag{61}$$

Hence, the change in the solution due to a perturbation upon a_{ik} (the perturbed A_0 entry) can be written as

$$h(a_{ik} + \delta) - h(a_{ik}) = \frac{-\delta}{1 + r_{ki}\delta}\; r_{ji}\, r_{k\ell}^T\, f_\ell;\ j,\ \ell = 1, 2, \ldots N \tag{62}$$

Thus we have an expression for the impact of perturbations in A_0 upon the solution.

Recognizing that perturbations upon the load vector, f, will directly influence the solution, we can write a Taylor series expansion for the solution about the deterministic quantities a°_{ik} and f°_i. A superscript zero denotes the mean or deterministic component. The Taylor series expansion is given by

$$h(a_{ik}, f_i) = h_d + (a_{ik} - a^\circ_{ik})\, h,_{a_{ik}} + (f_i - f^\circ_i)\, h,_{f_i}$$

$$+ \frac{1}{2} [(a_{ik} - a^\circ_{ik})(a_{sq} - a^\circ_{sq})\, h,_{a_{ik} a_{sq}}$$

$$+ (f_i - f^\circ_i)(f_s - f^\circ_s)\, h,_{f_i f_s}$$

$$+ (a_{ik} - a^\circ_{ik})(f_s - f^\circ_s)\, h,_{a_{ik} f_s}$$

$$+ (f_i - f^\circ_i)(a_{sq} - a^\circ_{sq})\, h,_{f_i a_{sq}}]$$

$$+ \text{third and higher order terms} \qquad (63)$$

From Sagar (1978), we take the following notation,

$$a_{ik} - a^\circ_{ik} = \xi_{ik}$$

$$f_i - f^\circ_i = \beta i \qquad (64)$$

$$u_k = r^T_{k\ell} f_\ell$$

The partial derivatives within Equation (63) are given by,

$$\text{i)}\ h,_{a_{ik}} = \lim_{\delta \to 0} \frac{1}{\delta} \cdot \frac{-\delta}{1 + r_{ki}\delta}\, r_{ji}\, r_{k\ell} f_\ell\ ;\ j, \ell = 1, 2, \ldots N$$

$$= -\, r_{ji}\, r_{k\ell} f_\ell\ ;\ j, \ell = 1, 2, \ldots N \qquad (65)$$

ii) $h,_{\alpha_{ik}\alpha_{sq}} = (-\ r_{ji}r_{k\ell}f_\ell),_{\alpha_{sq}}\ ;\ j,\ell\ = 1,\ 2,\ \ldots N$

$$= -\ [r_{ji},_{\alpha_{sq}}\ r_{k\ell} + r_{ji}r_{k\ell},_{\alpha_{sq}}]f_\ell;\ j,\ \ell = 1,\ 2,\ \ldots N$$

where

$$r_{ji},_{\alpha_{sq}} = \underset{\delta\to 0}{\text{limit}}\ \frac{1}{\delta}\cdot\frac{-\delta}{1 + r_{qs}\delta}\ r_{js}r_{qi} = -\ r_{js}r_{qi}$$

Similarly

$$r_{k\ell},_{\alpha_{sq}} = -\ r_{ks}r_{q\ell}$$

Thus,

$$h,_{\alpha_{ik}\alpha_{sq}} = r_{js}r_{qi}r_{k\ell}f_\ell + r_{ji}r_{ks}r_{q\ell}f_\ell\ ;\ j,\ell = 1,\ 2,\ \ldots N \tag{66}$$

iii) $$h,_{f_j} = \underset{\delta\to 0}{\text{limit}}\ \frac{1}{\delta}\cdot r_{ij}\delta = r_{ij};\ i = 1,\ 2,\ \ldots N \tag{67}$$

iv) $$h,_{f_if_s} = 0 \tag{68}$$

v) $h,_{\alpha_{ik}f_\ell} = -\ (r_{ji}r_{k\ell}f_\ell),_{f_\ell}$

$$= -\ r_{ji}r_{k\ell};\ j = 1,\ 2,\ \ldots N \tag{69}$$

Substituting Equations (65) through (69) into (63) yields,

$$h(\alpha_{ik},f_i) = h_d - \xi_{ik}r_{ji}r_{k\ell}f_\ell + \beta_i r_{ij} + \tfrac{1}{2}[\xi_{ik}\xi_{sq}(r_{js}r_{qi}r_{k\ell}f_\ell + r_{ji}r_{ks}r_{q\ell}f_\ell)$$

$$= \xi_{ik}\beta_s(-\ r_{ji}r_{ks}) + \xi_{sq}\beta_i(-r_{js}r_{qi})] \tag{70}$$

where repeated indices imply summation and i, j, k, s, q = 1, 2, ...N. Note that if one interchanges s and q for i and k respectively in the second order terms we have:

$$\xi_{ik}\xi_{sq}(r_{js}r_{qi}r_{k\ell}f_{\ell}) \rightarrow \xi_{sq}\xi_{ik}(r_{ji}r_{ks}r_{q\ell}f_{\ell})$$

and (71)

$$\xi_{ik}\beta_{s}(r_{ji}r_{ks}) \rightarrow \xi_{sq}\beta_{i}(r_{js}r_{qi})$$

Since we sum over all i, k, s, and q from 1 to N, we may simply combine terms and rewrite Equation (70) in the following form:

$$h(a_{ik},f_{i}) = h_{d} - r_{ji}\xi_{ik}r_{k\ell}f_{\ell} + r_{ij}\beta_{j} + \frac{1}{2}[r_{js}\xi_{sq}r_{qi}\xi_{ik}r_{k\ell}f_{\ell} - r_{ji}\xi_{ik}r_{ks}\beta_{s}] \quad (72)$$

where i, j, k, s, and q = 1, 2, ...N.

Equation (72) is an expansion in terms of random components for the stochastic piezometric head. Using Neumann series notation,

$$r_{ji} = A_0^{-1};\quad r_{k\ell}r_{\ell} = A_0^{-1}f_0;\quad r_{ij}\beta_j = A_0^{-1}f_1;\quad \xi_{sq} = A_1;\quad \xi_{ik} = A_1$$

We have

$$r_{ji}\xi_{ik}r_{k\ell}f_{\ell} = A_0^{-1}A_1A_0^{-1}f_0;\qquad r_{ij}\beta_J = A_0^{-1}f_1$$

$$r_{js}\xi_{sq}r_{qi}\xi_{ik}r_{k\ell}f_{\ell} = A_0^{-1}(A_1A_0^{-1})^2f_0$$

$$r_{ji}\xi_{ik}r_{ks}\beta_s = A_0^{-1}A_1A_0^{-1}f_1$$

Finally, Equation (72) can be rewritten as

$$h(a_{ik}, f_i) = [A_0^{-1} - A_0^{-1}A_1A_0^{-1}]\{f_0 + f_1\} + A_0^{-1}\ (A_1A_0^{-1})^2\ f_0$$

This is identical to Equation (45) which resulted from the Keller-Gibbs approach with a Neumann expansion of the matrix inverse. The two techniques yield identical expectations and variance/covariances for the perturbation analysis of stochastic steady-state ground-water flow. The size of random perturbation permitted by the application of the Keller-Gibbs or Sagar approach to stochastic ground-water problems is yet to be resolved.

GEOSTATISTICAL ESTIMATION OF HYDROLOGIC PARAMETERS

The fact that field data are subject to spatial variability as well as measurement error has made ground-water modelers realize that hydrologic parameters are stochastic (Bakr et al. 1978; Delhomme 1978, 1979; Gelhar, Gutjahr and Naff 1979). Hydrologic parameter uncertainty may be stochastically characterized in terms of its variance and correlation structure using geostatistical techniques. Small scale variability due to heterogeneities in media properties generally cannot be estimated from measurements taken on a typical field scale (e.g., one mile intervals). Small scale variability may be specified (perhaps inaccurately) by considering the general morphology of the aquifer (e.g., sandstone or limestone layers) and using predetermined variance and correlation structure. For the applications discussed in this report, only hydrologic parameter uncertainties corresponding to large-scale field measurements will be considered.

OVERVIEW OF GEOSTATISTICAL TECHNIQUES

Geostatistics and kriging are statistical techniques that can be used to estimate a surface from spatially distributed data. They were developed in the early 1960's, primarily by the French mathematician Georges Matheron, to solve mining estimation problems (Agterberg 1974, Akima 1975; Chiles 1975; Davis 1973; Delfiner and Delhomme 1975; Krige 1966; Matheron 1963; 1971; Olea 1974). Geostatistics is the more general term, but kriging, which refers to the estimation method itself, is often used in a more general sense.

Let $Z(x)$ be the value of a continuous surface at location $x = (x^1, x^2)$ in the plane. $Z(x)$ is assumed to be the realization of a stochastic process. Given that Z is observed at discrete locations $x_1, \ldots, x_n$, the kriging estimate of a random variable W is the linear combination of the observed data

$$W^* = \sum_i \lambda_i Z(x_i)$$

such that:

(i) $E(W - W^*) = 0$

(ii) $E(W - W^*)^2$ is minimal

(E denotes the probabilistic expectation operator.) Typically W is one of the following random variables:

(i) $Z(x_0)$ - punctual value

(ii) $\nabla Z(x_0) = (Z_{x^1}(x_0), Z_{x^2}(x_0))$ - gradient value

(iii) $\int_A Z(x)dx$ - integrated value over a set A in the plan

(iv) $\nabla^2 Z(x_0) = Z_{x^1x^1}(x_0) + Z_{x^2x^2}(x_0)$ - Laplacian value

We shall be concerned only with kriging punctual and integrated values for transmissivity, and gradient values for the piezometric head.

Traditional least squares regression analysis is not appropriate for estimating W because the observed Z data is not necessarily statistically independent. Least squares regression estimates ignore any stochastic continuity or correlation present in the Z surface.

Assume that Z(x) is the realization of a stochastic process that locally has a polynomial first moment and finite second moment. Specifically, for any point x_0 in the plane there exists a neighborhood N of x_0 such that for x and y within N:

(i) $E[Z(x)] = m(x) = \sum_\ell a_\ell f^\ell(x)$ where $\{a_\ell\}$ are unknown constants and $\{f^\ell(x)\}$ are monomial functions of some finite order

(ii) $E[(Z(x) - m(x))(Z(y) - m(y))] = c(x,y)$ is a known covariance function.

The monomial functions of order one are for $x = (x^1, x^2)$; $1, x^1, x^2$. The monomial functions of order two are $1, x^1, x^2, (x^1)^2, x^1x^2, (x^2)^2$.

The kriging estimate of a random variable involves calculating the optimal set of kriging weights $\lambda_1, \ldots, \lambda_n$ such that

$$E[W - W^*]^2 = Var(W) + \sum_i \sum_j \lambda_i\lambda_j c(x_i,x_j) - 2\sum_i \lambda_i Cov(W,Z(x_i))$$

is minimized subject to the constraint $E[W - W^*] = 0$. Var and Cov, respectively denote the variance and covariance operators. The determination of the kriging weights depends only upon the covariance and mean structure of W and Z. The kriging weights do not depend upon the observed Z data.

For example, if $W = Z(x_0)$, the quantity

$$E[Z(x_0) - Z^*(x_0)]^2 = \mathrm{Var}(Z(x_0)) + \sum_i \sum_j \lambda_i \lambda_j c(x_i,x_j) - 2 \sum_i \lambda_i c(x_0,x_i) \qquad (73)$$

is minimized subject to the constraints

$$\sum_i \lambda_i f^\ell(x_i) = f^\ell(x_0), \text{ all } \ell$$

The covariance of the kriging error is given by

$$\mathrm{Cov}(Z(x_0) - Z^*(x_0), Z(y_0) - Z^*(y_0)) = c(x_0,y_0)$$
$$+ \sum_i \sum_j \lambda_i(x_0)\lambda_j(y_0)c(x_i,x_j) - \sum_i \lambda_i(x_0)c(x_i,y_0) - \sum_j \lambda_j(y_0)c(x_j,x_0) \qquad (74)$$

where x_0, y_0, x_1, ..., x_n, ... are all within the neighborhood N.

For kriging block average transmissivities or hydraulic gradients, similar equations to (73) and (74) may be derived by replacing $Z(x_0)$ with $W = \int_A Z(x)dx$ or $W = Z_{x^i}(x)$.

For gradient kriging the underlying stochastic process (for which Z(x) is a realization) is assumed to be differentiable in each of its coordinates with probability equal to one. We shall further assume that the covariance function $c(x,y) = c(x^1,x^2,y^1,y^2)$ has continuous second order partial derivatives in all four coordinates which ensures (Parzen1962, p. 83) that:

(i) $\mathrm{Cov}(Z_{x^k}(x_0), Z(y_0)) = c_{x^k}(x_0,y_0)$

(ii) $\mathrm{Cov}(Z_{x^k}(x_0), Z_{x^k}(y_0)) = c_{x^k y^k}(x_0,y_0)$

Furthermore, if c(x,y) is stationary, i.e., $c(x,y) = g(x^1 - y^1, x^2 - y^2)$ $= g(h^1, h^2)$ then

(i) $\mathrm{Cov}(Z_{x^k}(x_0), Z(y_0)) = g_{h^k}(x^1 - y^1, x^2 - y^2)$

(ii) $\mathrm{Cov}(Z_{x^k}(x_0), Z_{x^k}(y_0)) = - g_{h^k h^k}(x^1 - y^1, x^2 - y^2)$

In order to calculate W* we must know the order of the monomials used in Equations (73) and (74) and the covariance function c(x,y). In practice, these parameters are never known at the outset and must be estimated from the available Z data. Parameter estimation procedures are described in an essay on geostatisical methods applied to pore velocity modeling (Devary and Doctor 1981).

PRODUCT ESTIMATION UNCERTAINTIES

The estimation of Darcian velocity involves the estimation of the hydrologic parameter surfaces

(i) T(x) transmissivity

(ii) $\nabla\Phi(x)$ gradient of the potentiometric head

which are related by Darcy's Law

$$q(x) = (q_1(x), q_2(x)) = - T(x)\ \nabla\Phi(x)$$

Assuming that T(x), and $\nabla\Phi(x)$ are realizations of stochastic processes and unbiased estimators T*(x), and $\nabla\Phi^*(x)$ exist for these hydrologic parameters (e.g., from kriging), then we must consider the estimator

$$q^*(x) = - T^*(x)\nabla\Phi^*(x)$$

Specifically, we must examine the bias and the estimation error of q*(x).

Assume that the spatial correlation between the T, Φ surface values was entirely attributed to the spatial correlation between the mean values E[T(x)], and $E[\Phi(x)]$. This implies that T(x), and $\Phi(x)$ may be modeled as mutually independent stochastic processes. The estimation bias,

$$E[q^*(x) - q(x)] = 0$$

since $T^*(x)$ and $\nabla\Phi^*(x)$ are unbiased, mutually independent estimators of $T(x)$ and $\nabla\Phi(x)$. The estimation error variance may be written using a first order linear expansion

$$\mathrm{Var}[q_i^*(x) - q_i(x)] = (\Phi^*_{x^i}(x))^2\, \mathrm{Var}(T^*(x) - T(x)) + (T^*(x))^2\, \mathrm{Var}(\Phi^*_{x_i}(x) - \Phi_{x_i}(x)) \quad (75)$$

where $i = 1$ or 2 and $\nabla\Phi(x) = (\Phi_{x^1}(x), \Phi_{x^2}(x))$. The estimation error cross covariance is given by

$$E[q^*_i(x) - q_i(x)][q^*_j(y) - q_j(y)]$$

$$= (\Phi^*_{x_i}(x)\Phi^*_{x_j}(y))\, \mathrm{Cov}(T^*(x) - T(x), T^*(y) - T(y)) \quad (76)$$

$$+ (T^*(x)T^*(y))\, \mathrm{Cov}(\Phi^*_{x_i}(x) - \Phi_{x_i}(x), \Phi^*_{x_j}(y) - \Phi_{x_j}(y))$$

where $i = 1$ or 2, $j = 1$ or 2, and x and y are values in the plane.

APPLICATION OF STEADY-STATE STOCHASTIC ANALYSIS

The development and use of computer-based algorithms will be discussed in this chapter. Our goal is to produce a steady-state analysis package, and to provide insight into the computational aspects of the unsteady problem. Research codes have been developed for both the Neumann and Taylor series methods of analysis. The implementation of the methods differ markedly. Solution of the stochastic problem via a Neumann series method results in a system of algebraic equations. One obtains the expectation, variance and covariance for all points from this calculation. The Taylor series approach yields the same result for individual points via a summation sequence. Thus the latter is more flexible in that only points of interest need be calculated. The trade-off lies in the repeated computations and bookkeeping of the Taylor series approach when all or a majority of points are of interest.

Two problems have been designed for verifying and testing the analysis. While the codes that have been developed are two-dimensional, they can be reduced to examine a one-dimensional problem. An analytical solution has been developed in one dimension. This problem has been useful in determining that the algorithms have been properly coded. A second problem dealing with a subregion of the Hanford Site is used to provide two-dimensional aspects of the stochastic calculations.

ANALYTICAL SOLUTION - ONE-DIMENSIONAL CASE

The stochastic Galerkin technique was applied to a one-dimensional steady-state flow problem. Exact analytical solutions for one-dimensional flow permit verification of the deterministic and stochastic aspects of the technique.

Let T(x) denote the transmissivity on the one-dimensional domain, $1 \le x \le 7$. Assume that T(x) is a log-normal process with mean value (E[T(x)]) given by

$$E[T(x)] = x/10$$

and covariance ($C(x_1,x_2)$) given by

$$C(x_1,x_2) = (0.01)x_1x_2[\exp(0.00995\ \exp(-(x_1 - x_2)^2/2)) - 1]$$

Assume that the piezometric head evaluated at x = 7, h(7), and the flow evaluated at x = 1, q(1), are both deterministic or non-random quantities and are given by

$$h(7) = E[h(7)] = 400$$

$$q(1) = E[q(1)] = -1$$

(The flow is from left-to-right in the interval $1 \leq x \leq 7$.)

Since the flow is constant in one dimension, the head may be written as the closed-form solution

$$h(x) = h(7) + \int_x^7 \frac{1}{T(s)}\, ds \qquad (77)$$

Thus the expected value of h(x) is given by

$$E[h(x)] = 400 + \int_x^7 E\left[\frac{1}{T(s)}\right]ds$$

$$= 400 + 10.1\ \ell n(7/x)$$

The variance of h(x), denoted by $\sigma^2[h(x)]$, is given by

$$\sigma^2[h(x)] = 102.01 \int_x^7\int_x^7 \frac{1}{s_1 s_2}[\exp(0.00995\ \exp(-(s_1 - s_2)^2/2)) - 1]ds_1 ds_2$$

For x = 1,

$$E[h(1)] = 419.65$$

$$\sigma^2[h(1)] = 1.54$$

and the deterministic solution of h(1), which is calculated from Equation (77) letting T(s) = s/10, equals 419.46.

The stochastic Galerkin technique was applied to this one-dimensional problem using the following discretization

$$T(s) = (k - 0.5)/10, \quad (k - 1) \leq s \leq k, \; k = 2, \ldots, 7 \qquad (78)$$

A comparison of analytical and computed solutions is given in Table 1.

TABLE 1. Comparison of Analytical and Computed Solutions for One-Dimensional Case

	Deterministic Head at s = 1	Expectation of Head at s = 1	Variance of Head at s = 1
Analytical	419.5	419.7	1.54
Neumann	419.1	419.3	1.52
Taylor	419.1	419.3	1.51

Notice the excellent agreement between the analytical and the two stochastic numerical solution values. The difference in calculated mean values is entirely due to the discretization of Equation (78). Both the Neumann and Taylor series solutions produced excellent results. Thus, we conclude that the algorithm has been correctly encoded.

HANFORD SITE SUBREGION

The study area employed in this application of the stochastic methodology resembles in large part a subregion of the Hanford Site located between the 200 areas. This subregion, surrounded by dotted lines in Figure 1, was employed in an earlier study involving the geostatistical estimation of pore water velocities (Devary and Doctor 1981). Since kriged values of potentiometric head, hydraulic gradient, and transmissivity were readily available for this domain, it was selected for preliminary tests of the stochastic flow computation package.

The values of piezometric head and transmissivity associated with this subregion and employed in kriging both transmissivity and boundary conditions

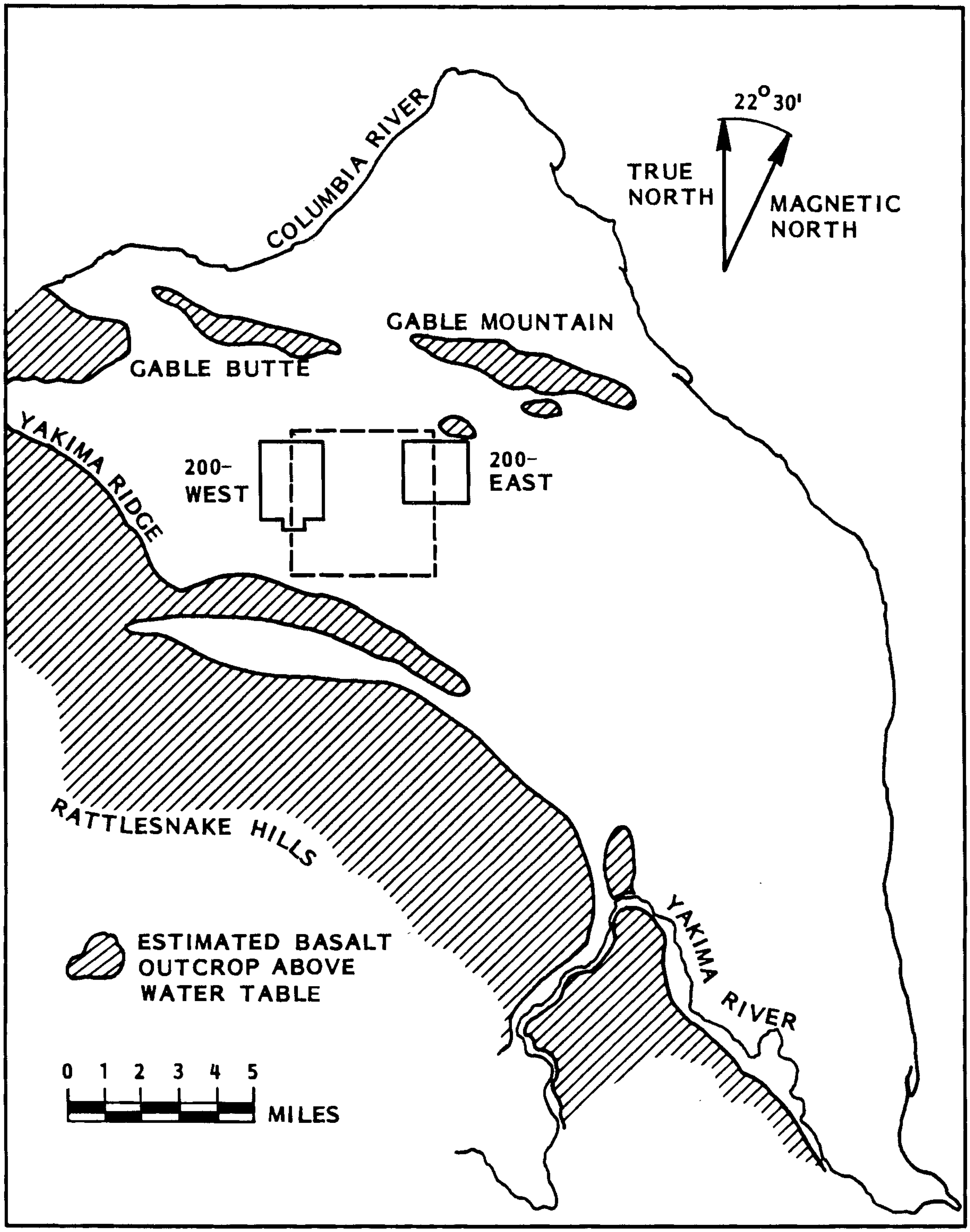


FIGURE 1. Map of the Hanford Site Displaying the Study Area as a Dashed Square

are synthetic. The head data shown in Figure 2 and reported in Appendix A were created on uniform 2000-foot intervals by the VTT model of the Hanford Site's unconfined aquifer system (Kipp et al. 1972). The bottom topography and hydraulic conductivity displayed in Figure 2 were also taken from VTT model files. Thus, the head data is a deterministic solution for head, and it is consistent with the point values of transmissivity used by the VTT code.

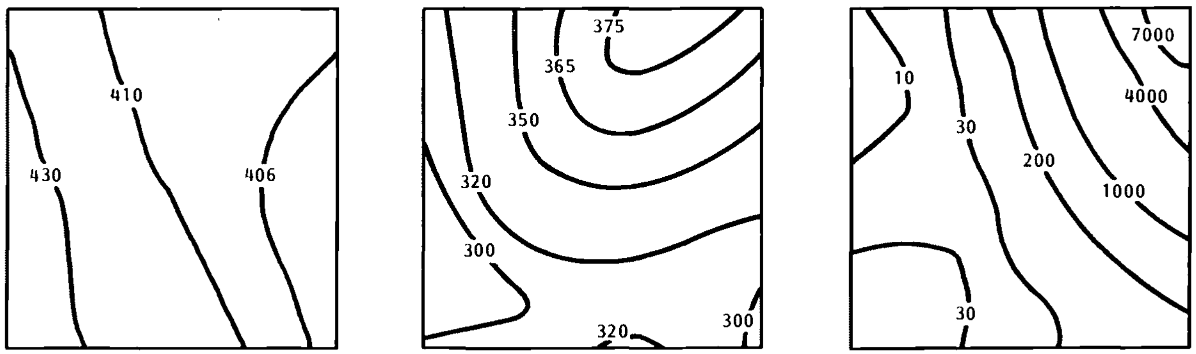
Our statement of the deterministic ground-water flow problem differs in two ways from the VTT model of the basin. First, element average values of transmissivity are employed rather than point values (see Appendix A). Second, the boundary conditions on the VTT problem domain are applied at the aquifer's boundaries (i.e. Rattlesnake Hills, Columbia River, etc.) while our problem is driven by boundary conditions on the perimeter of the study area (Figure 3). No direct method exists for extracting boundary conditions on a subregion from the VTT results. Therefore, kriged head gradients and transmissivities were combined to define the stochastic flux boundary conditions for our problem. Since kriged fluxes are not constrained to conserve mass, no guarantee exists that the resulting mean flux values are absolutely consistent with the VTT steady-state solution. Results of the deterministic analysis within the stochastic code are very close to the VTT results. However, no strict comparison can or will be made since the interior parameters and driving forces are not identically defined in the two analyses.

Stochastic Parameters and Boundary Conditions

Uncertainty enters the steady-state formulation through the transmissivity and boundary flux terms. The mean values for both quantities are shown in Figure 3.

Transmissivity

Point values of transmissivity were developed from the hydraulic conductivity and bathymetry data for the aquifer. The transmissivity data were represented as a log-normal stochastic process, specifically, log(T) is a Gaussian process with a biquadratic mean value and stationary covariance function given by



a) VTT COMPUTED PIEZOMETRIC HEAD (ft)

b) BOTTOM TOPOGRAPHY EMPLOYED IN VTT MODEL OF HANFORD (ft)

c) HYDRAULIC CONDUCTIVITY (ft/day)

FIGURE 2. Contour Plots of Piezometric Head, Bottom Topography, and Hydraulic Conductivity Taken from the VTT Model of the Hanford Site

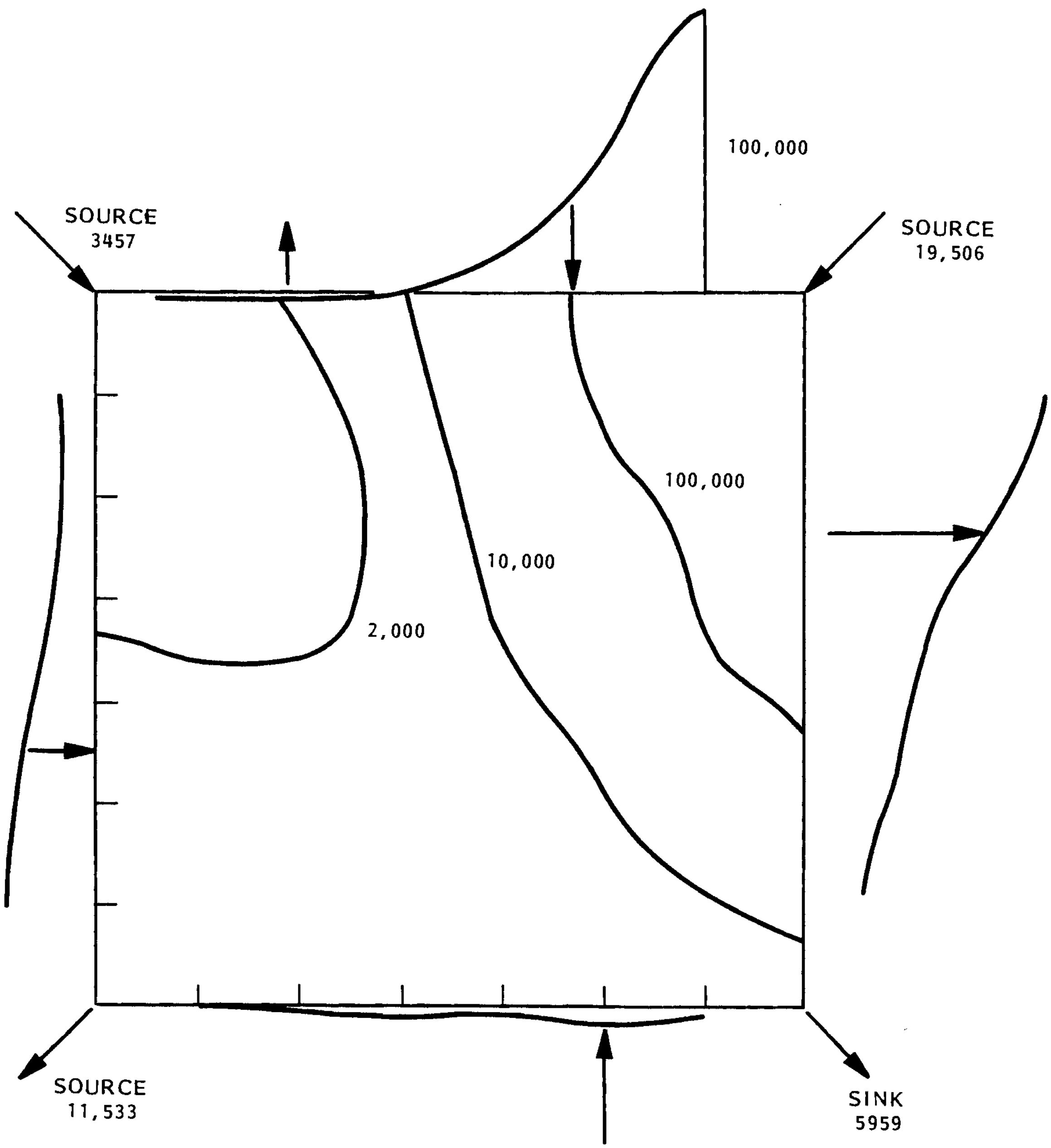


FIGURE 3. Mean Values of Transmissivity (ft^2/day) and Boundary Flux (ft^3/day)

$$\mathrm{Cov}(\log(T(x_i)), \log(T(x_j)) = 0.4334 \exp(-0.294 |x_i - x_j|^2) \quad (79)$$

From the kriged surface of log (T), the mean values and covariance functions of the following quantities were calculated using the log-normal techniques described in Devary and Doctor (1981):

(i) $T_2(x) = \frac{1}{A_{\Omega(e)}} \int T(x)\,dx$ • two-dimensional elemental average (A denotes area of $\Omega(e)$)

(ii) $T_1(x) = \frac{1}{\ell_{\partial\Omega(e)}} \int (T(x)\,dx$ • one-dimensional average over the boundary of an element (ℓ denotes length of $\partial\Omega(e)$)

Letting $T^*(x)$ denote the mean (estimated) elemental average of T over an element centered at x, i.e., $T_2(x)$, the covariance of the estimation error was found to be:

$$\mathrm{Cov}(T_2(x) - T^*(x), T_2(y) - T^*(y))$$
$$= T^*(x)\, T^*(y)[\exp(0.01446 \exp(-0.10778 |x - y|^2)) - 1] \quad (80)$$

This is equivalent to assuming log $(T_2(x) - T^*(x))$ is a stationary Gaussian process.

Boundary Flux

The potential values were represented as a Gaussian process with biquadratic mean and stationary covariance given by

$$\mathrm{Cov}(\phi(x_i), \phi(x_j)) = 10.70 \exp(-0.194 |x_i - x_j|^2) \quad (81)$$

From the kriged surfaces of the potential gradient and log (T) the mean values and covariance functions of the Darcian flux were calculated using the error propagation techniques described in Devary and Doctor (1981). Letting $V^*(x)$ denote the mean (estimated) value of the average value of the flux (V) over the boundary of an element centered at node point x, i.e.

$$V_1(x) = \frac{1}{\ell_{\partial\Omega(e)}} \int V \, ds$$

the covariance of the estimation error is given by:

$$\mathrm{Cov}(V_1(x) - V^*(x), V_1(y) - V^*(y))$$

$$= V_1^*(x)V_1^*(y)[\exp(0.00375 \exp(-2.72109 \ |x - y|^2)) - 1] \qquad (82)$$

This is equivalent to assuming $\log(v_1(x) - v^*(x))$ is a stationary Gaussian process. In this case and also in Equation (80) the underlying lognormal distribution for the transmissivities (Equation (79)') is the dominant factor in determining the distribution of the transmissivity and Darcian flux estimation error distributions.

The cross-covariance between the estimation errors of $V_1(x)$ and $T_2(x)$ was estimated to be a neglibible quantity and was therefore assumed to be zero in the analysis.

RESULTS OF THE STOCHASTIC ANALYSIS

A steady-state stochastic analysis of the Hanford Site subregion was conducted using the parameters and boundary conditions described in the preceding section. The stochastic response of the aquifer is characterized by the mean, variance, and correlations of the piezometric head. The mean stochastic solution differs from the deterministic solution by second and higher order moments. The stochastic contribution to the mean, i.e., these second and higher order moments, will be displayed. Variance is reported here as the measure of the random component; however, the square root of the variance, the standard deviation, could have been used. The correlation coefficient is a dimensionless parameter displaying the correlation existing between head values fixed distances apart.

In the results that follow, a Dirichlet boundary condition for piezometric head is located in the northeast corner of the Hanford Site subregion. This location corresponds to the upper-right corner of the plots.

The Dirichlet boundary condition provides a point of reference for the solution. In the solution presented herein the mean component of the Dirichlet head boundary condition is set to the aquifer's water level while the random component is set to zero.

The deterministic solution obtained by the code is shown in Figure 4, and the stochastic contribution to the mean is displayed in Figure 5. The stochastic contribution has a zero value in the upper-right corner and gradually increases with increasing distance from the boundary condition location. Transmissivity and boundary condition influences are seen in the slightly irregular contours. Figure 6 shows the variance of the piezometric head. Once again, the upper-right corner contains a zero value with the variance gradually increasing with increasing distance from the boundary condition location. It can be readily seen from both the theory and these results that the location of the Dirichlet boundary condition readily influences both the stochastic contribution to the mean and the variance. In actual field studies the Dirichlet condition would correspond to a head value having a measurement error. This introduces random Dirichlet boundary conditions. The influence of such a non-zero random component is unknown at this time and deserves further study.

Figure 7 shows the covariance of piezometric head with a reference point taken to be the southwest or lower-left corner of the Hanford Site subregion. Again, the covariance is tied to zero at the upper-right corner due to the prescribed Dirichlet condition.

The correlation coefficient is a nondimensional parameter useful in evaluating the sphere of influence of a point in the system. By definition the correlation coefficient is:

$$\rho_{u,v} = \frac{\mathrm{Cov}(u,v)}{\sigma_u \, \sigma_v}$$

where

$\rho_{u,v}$ = correlation coefficient between u and v

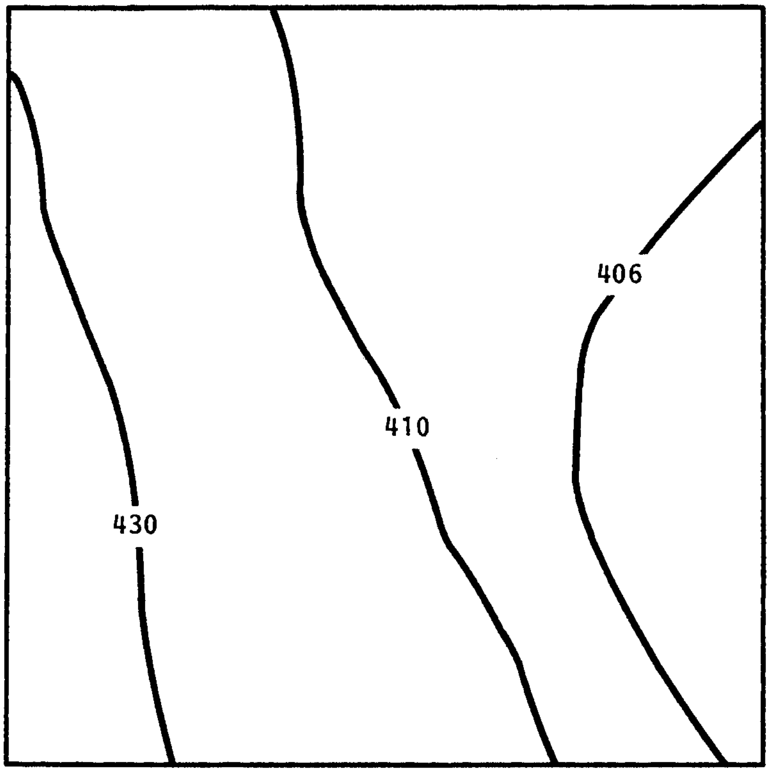


FIGURE 4. Deterministic Solution Corresponding to the Mean Stochastic Dirichlet Boundary Condition in the Upper-Right Corner

Cov(u,v) = covariance of u about v, and

σ_i = standard deviation at the point i (i.e., u or v).

Since,

$$\mathrm{Cov}(u,u) = \mathrm{Var}(u)$$

and,

$$\mathrm{Var}(u) = \sigma_u^2$$

it follows that $\rho_{u,u} = 1.0$. The absolute value of the correlation function is always less than or equal to one.

A contour plot of correlation coefficient about the lower-left node is shown in Figure 8. This information corresponds to the covariance data displayed in Figure 7 and is more readily interpreted to determine the sphere

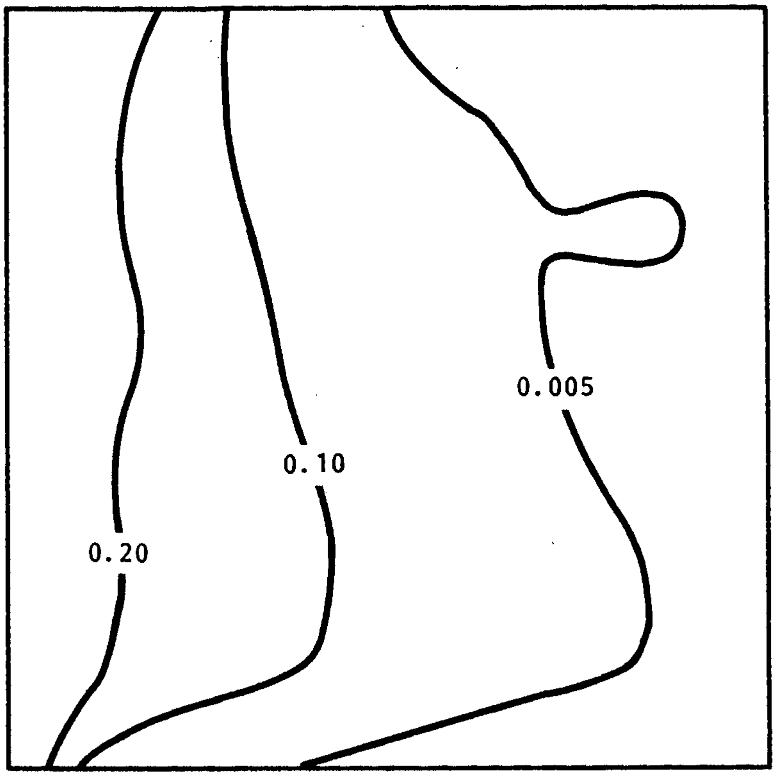


FIGURE 5. Stochastic Contribution to Mean Piezometric Head When Upper-Right Corner is Fixed

of influence of the piezometric head at the lower-left corner. Notice that the correlation coefficient is equal to 0.5 at approximately 10,000 ft for the piezometric head while the distance corresponding to the log-transmissivity correlation coefficient equalling 0.5 is approximately 4,000 ft. This is attributed to the smoothing of the transmissivity and flux input that occurs in the ground-water flow equation. Thus, uncertain transmissivities and boundary fluxes with relatively short correlation legnths can create stochastic head fields with much longer correlation lengths. This is physically realistic since transmissivity and boundary flux influences are local in nature while perturbations in the piezometric head surface tend to influence larger regions. These interpretations to the stochastic response of an aquifer are not new; Bakr, et al. (1978) have reported similar results.

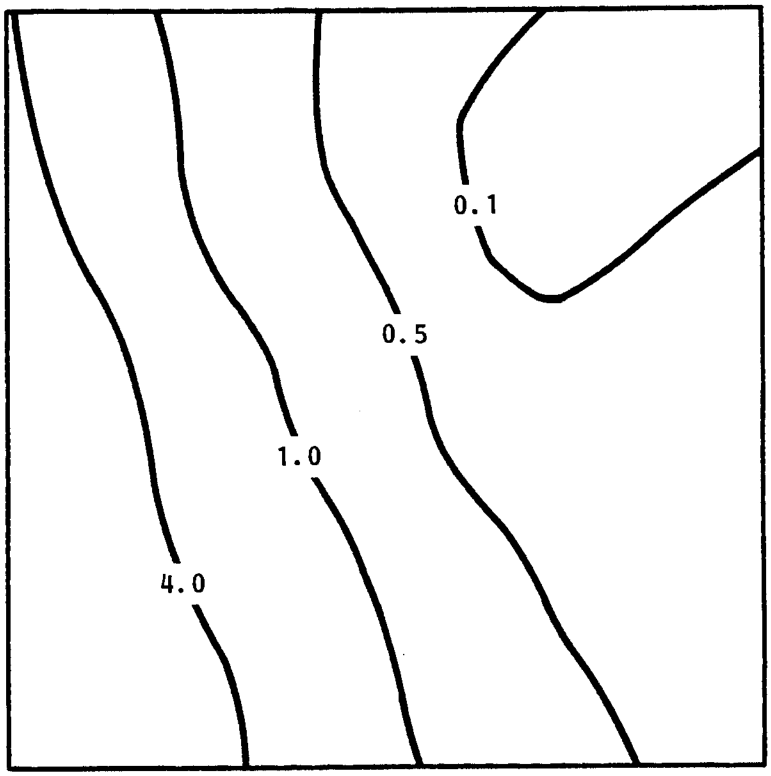


FIGURE 6. Variance (ft^2) of Piezometric Head When Upper Right Corner is Fixed

One must also be cognizant of the wealth of questions that remain to be addressed and answered. Study of a generic problem that exhibits controlled transmissivity and boundary condition situations is needed to determine the size of perturbation which this technique can sustain. The independent stochastic impacts of transmissivity and boundary conditions, the influence of non-stationary covariance functions, and the impact of boundary conditions which specify a non-zero random component must also be studied. As in the case of purely deterministic solutions, the stochastic solution depends continuously upon the boundary conditions and hydrologic parameters. However, the nature of this continuous dependence for the stochastic analysis is far more complex and will require a sustained research effort before the power of this analysis method can be fully comprehended and implemented.

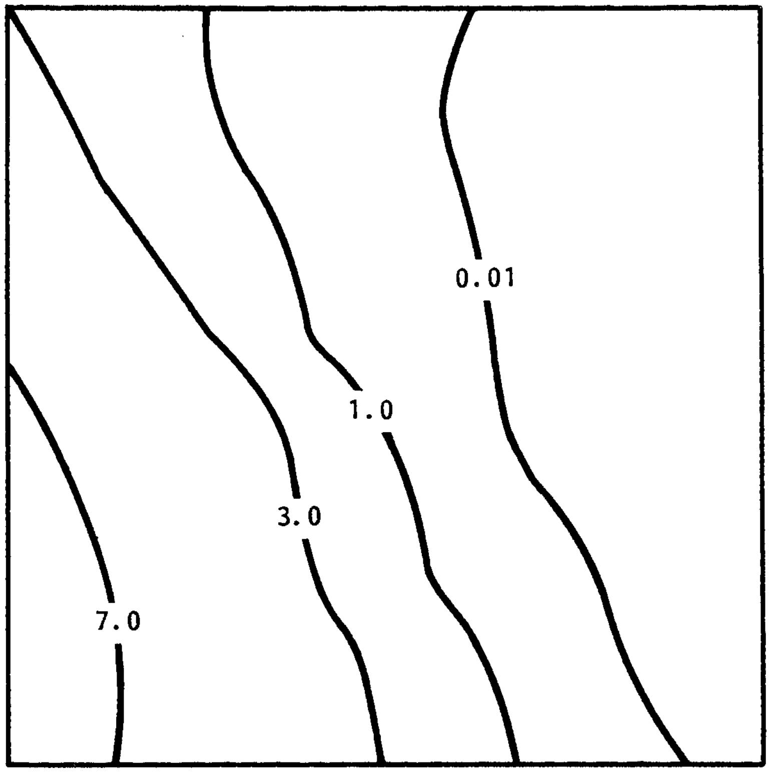


FIGURE 7. Covariances of Piezometric Head About the Lower-Left Node

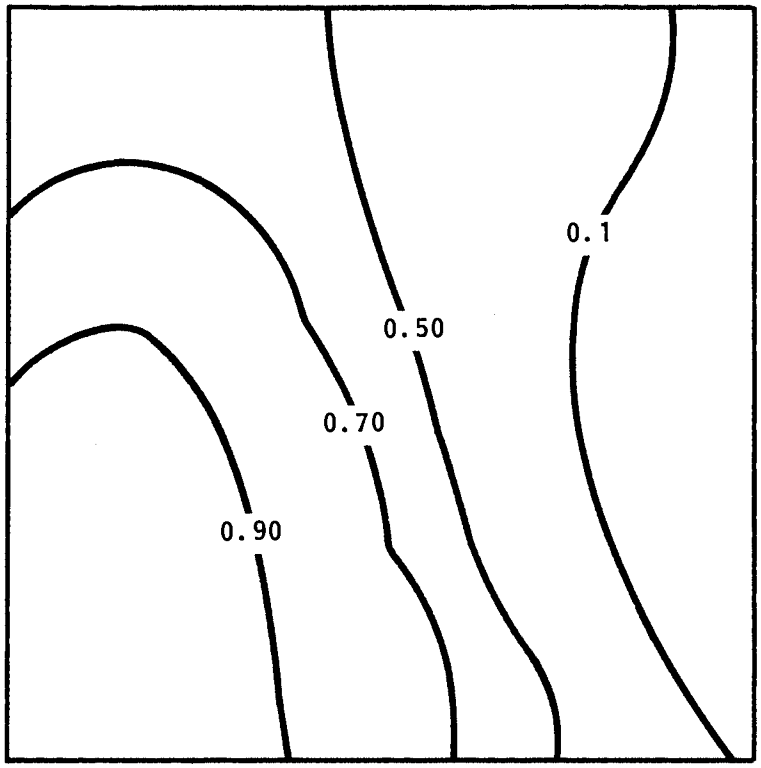


FIGURE 8. Correlation of Piezometric Head About the Lower-Left Node

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APPENDIX A

APPENDIX A

This appendix contains the raw data taken from the VTT model of the Hanford Site for the subregion shown in Figure 1. The values for potential, bottom of unconfined zone, and hydraulic conductivity are nodal values taken from the model's data files. They are recorded here in the interest of completeness since these files are periodically updated. The tabular values recorded left to right, top to bottom are the values west to east, south to north for the region shown in Figure 1.

TABLE A.1. Piezometric Head Data (feet)

0.0000E-01	4.4007E+02	4.3625E+02	4.3227E+02	4.2765E+02	4.2262E+02	4.1733E+02	4.1252E+02
4.0875E+02	4.0613E+02	4.0470E+02	0.0000E-01				
4.4548E+02	4.4125E+02	4.3715E+02	4.3288E+02	4.2807E+02	4.2258E+02	4.1678E+02	4.1168E+02
4.0794E+02	4.0569E+02	4.0466E+02	4.0415E+02				
4.4670E+02	4.4221E+02	4.3776E+02	4.3312E+02	4.2791E+02	4.2182E+02	4.1541E+02	4.1022E+02
4.0692E+02	4.0537E+02	4.0469E+02	4.0428E+02				
4.4824E+02	4.4318E+02	4.3814E+02	4.3286E+02	4.2706E+02	4.2039E+02	4.1334E+02	4.0831E+02
4.0608E+02	4.0523E+02	4.0478E+02	4.0443E+02				
4.4944E+02	4.4399E+02	4.3831E+02	4.3224E+02	4.2551E+02	4.1777E+02	4.1028E+02	4.0684E+02
4.0575E+02	4.0524E+02	4.0490E+02	4.0462E+02				
4.5071E+02	4.4462E+02	4.3812E+02	4.3098E+02	4.2291E+02	4.1378E+02	4.0788E+02	4.0628E+02
4.0569E+02	4.0532E+02	4.0504E+02	4.0481E+02				
4.5252E+02	4.4486E+02	4.3711E+02	4.2853E+02	4.1875E+02	4.0993E+02	4.0701E+02	4.0619E+02
4.0579E+02	4.0548E+02	4.0523E+02	4.0503E+02				
4.5266E+02	4.4404E+02	4.3497E+02	4.2504E+02	4.1426E+02	4.0827E+02	4.0682E+02	4.0633E+02
4.0600E+02	4.0571E+02	4.0547E+02	4.0527E+02				
4.5028E+02	4.4136E+02	4.3178E+02	4.2135E+02	4.1158E+02	4.0788E+02	4.0699E+02	4.0663E+02
4.0633E+02	4.0603E+02	4.0575E+02	4.0552E+02				
4.4634E+02	4.3777E+02	4.2833E+02	4.1810E+02	4.1024E+02	4.0793E+02	4.0732E+02	4.0705E+02
4.0679E+02	4.0646E+02	4.0611E+02	4.0580E+02				
4.4219E+02	4.3392E+02	4.2532E+02	4.1626E+02	4.0989E+02	4.0808E+02	4.0766E+02	4.0750E+02
4.0732E+02	4.0701E+02	4.0662E+02	4.0617E+02				
0.0000E-01	4.3027E+02	4.2302E+02	4.1535E+02	4.0999E+02	4.0838E+02	4.0802E+02	4.0795E+02
4.0790E+02	4.0774E+02	4.0745E+02	0.0000E-01				

TABLE A.2. Hydraulic Conductivity (gal/day)

0.0000E-01	3.3936E+02	3.9351E+02	4.0217E+02	3.5986E+02	2.9917E+02	2.5422E+02	2.2502E+02
2.0550E+02	2.1109E+02	3.1039E+02	0.0000E-01				
2.4934E+02	3.2021E+02	3.6750E+02	3.5078E+02	2.8541E+02	2.2284E+02	1.9916E+02	2.0159E+0
2.2830E+02	3.1156E+02	5.8597E+02	1.1152E+03				
2.4496E+02	2.9612E+02	3.1804E+02	2.9261E+02	2.3398E+02	1.9567E+02	2.1232E+02	2.5685E+01
3.3788E+02	6.0777E+02	1.2694E+03	2.2155E+03				
2.4171E+02	2.6213E+02	2.7141E+02	2.6431E+02	2.3588E+02	2.0666E+02	2.1384E+02	3.3284E+02
6.9968E+02	1.6104E+03	3.0848E+03	5.1016E+03				
2.1104E+02	2.1156E+02	2.1870E+02	2.2787E+02	2.2955E+02	2.1422E+02	2.5783E+02	7.7293E+02
2.4125E+03	4.9759E+03	9.1631E+03	1.5074E+04				
1.4871E+02	1.4381E+02	1.4881E+02	1.6848E+02	1.8882E+02	2.1646E+02	6.1175E+02	2.6861E+03
7.4613E+03	1.4535E+04	2.5995E+04	4.2204E+04				
6.6826E+01	6.9910E+01	7.3489E+01	9.1476E+01	1.2737E+02	2.9349E+02	1.6898E+03	7.0046E+03
1.6598E+04	2.6990E+04	4.0613E+04	6.8365E+04				
5.8168E+01	5.6024E+01	5.5361E+01	6.8080E+01	1.0720E+01	5.1041E+01	3.4783E+03	1.3189E+04
2.5753E+04	3.8262E+04	5.8364E+04	7.3707E+04				
5.9201E+01	5.9051E+01	6.1453E+01	7.4152E+01	1.5033E+02	9.1683E+02	5.8333E+03	2.0615E+04
3.4153E+04	4.9939E+04	7.2298E+04	7.0529E+04				
6.0656E+01	6.1113E+01	6.8562E+01	8.7766E+01	2.6206E+02	1.7734E+03	9.2650E+03	2.8450E+04
5.2326E+04	7.7009E+04	7.6299E+04	6.5895E+04				
5.5118E+01	6.0186E+01	7.1709E+01	9.8483E+01	3.0185E+02	1.8277E+03	1.1003E+04	3.6536E+04
8.3402E+04	9.4603E+04	7.1938E+04	6.0937E+04				
0.0000E-01	6.4745E+01	7.6003E+01	1.1091E+02	3.5855E+02	2.0748E+03	1.1047E+04	4.6170E+04
1.0980E+05	1.0148E+05	6.9520E+04	0.0000E-01				

TABLE A.3. Bottom of Unconfined Zone (ft)

0.0000E-01	3.8738E+02	3.8646E+02	3.8296E+02	3.7745E+02	3.7103E+02	3.6246E+02	3.5205E+02
3.3922E+02	3.2746E+02	3.1032E+02	0.0000E-01				
3.3204E+02	3.3938E+02	3.4608E+02	3.4851E+02	3.4523E+02	3.3984E+02	3.3430E+02	3.2929E+02
3.2153E+02	3.0919E+02	2.8967E+02	2.6730E+02				
2.8899E+02	2.9686E+02	3.0400E+02	3.0928E+02	3.1161E+02	3.1843E+02	3.2128E+02	3.1990E+02
3.1374E+02	2.9815E+02	2.8179E+02	2.6715E+02				
2.6093E+02	2.7107E+02	2.8306E+02	2.9107E+02	2.9646E+02	3.1057E+02	3.1739E+02	3.1712E+02
3.1241E+02	2.9891E+02	2.8698E+02	2.7706E+02				
2.4472E+02	2.5560E+02	2.7637E+02	2.9557E+02	3.1340E+02	3.2056E+02	3.2119E+02	3.1933E+02
3.1595E+02	3.1060E+02	3.0050E+02	2.8987E+02				
2.3670E+02	2.5375E+02	2.8338E+02	3.1334E+02	3.3316E+02	3.4143E+02	3.4426E+02	3.3519E+02
3.2457E+02	3.2208E+02	3.2082E+02	2.9864E+02				
2.3988E+02	2.6633E+02	2.9485E+02	3.2153E+02	3.4402E+02	3.5530E+02	3.5925E+02	3.5734E+02
3.5192E+02	3.4212E+02	3.3313E+02	3.1341E+02				
2.5184E+02	2.8202E+02	3.0381E+02	3.2648E+02	3.5070E+02	3.6369E+02	3.6995E+02	3.6793E+02
3.6201E+02	3.5426E+02	3.4178E+02	3.2364E+02				
2.7508E+02	2.9142E+02	3.0889E+02	3.2788E+02	3.5305E+02	3.6929E+02	3.7639E+02	3.7589E+02
3.7112E+02	3.6278E+02	3.5381E+02	3.3826E+02				
2.8492E+02	2.9745E+02	3.1213E+02	3.2916E+02	3.5301E+02	3.6745E+02	3.7612E+02	3.7852E+02
3.7757E+02	3.7320E+02	3.6786E+02	3.6033E+02				
2.9002E+02	3.0043E+02	3.1305E+02	3.3135E+02	3.5311E+02	3.6389E+02	3.7061E+02	3.7507E+02
3.8138E+02	3.8389E=02	3.8360E+02	3.8351E+02				
0.0000E-01	2.9567E+02	3.1008E+02	3.3211E+02	3.5421E+02	3.6449E+02	3.7054E+02	3.7452E+02
3.8492E+02	3.9231E+02	3.9342E+02	0.0000E-01				

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