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13. ABSTRACT (Maximum 200 words)

Our project aimed at developing theoretical and computational methods to predict unsaturated flow in randomly heterogeneous soils and to assess the corresponding prediction errors. Our objective was to avoid the need for either Monte Carlo simulation or upscaling, by developing ways to render predictions and uncertainty assessments directly, in a computationally efficient and accurate manner. This final technical report describes our accomplishments, which consist of developing two novel approaches, one based on the Kirchhoff transformation and the other on a Gaussian method of approximation. Both methods have been implemented in two spatial dimensions using the finite element method, and applied to superimposed mean uniform and convergent flows with and without conditioning on measured values of hydraulic conductivity. Methods have been examined to extend the applicability of both methods to transient flows in soils having arbitrary constitutive characteristics. The report cites several papers published, submitted for publication or under preparation based on our work. The project has contributed toward three doctoral dissertations at the University of Arizona.

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Final Technical Report
ARO Project 39124-EV
Conditional Analysis of Unsaturated Flow in Randomly Heterogeneous Soils
Without Monte Carlo Simulation or Upscaling
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Start Date: July 15, 1999; End Date: July 14, 2002

ABSTRACT

This study focused on flow in the unsaturated or vadose zone, which forms a major hydrologic link between the ground surface and underlying groundwater aquifers. To properly understand its role in protecting groundwater from surface and near surface sources of contamination, one must be able to analyze quantitatively fluid flow in unsaturated soils. The difficulty is that such soils are ubiquitously heterogeneous, with hydraulic properties that fluctuate from point to point in a seemingly erratic manner. The common approach has been to delineate this variation, and analyze unsaturated flow in randomly heterogeneous soils, deterministically. Yet with increasing frequency, the popular deterministic approach is proving to be inadequate. Our project aimed at developing theoretical and computational methods to predict, in an optimum fashion, unsaturated flow in randomly heterogeneous soils under the action of uncertain forcing terms and to assess the corresponding prediction errors. Previously, such predictions and assessments required the conduct of numerous Monte Carlo simulations on a fine grid, which is computationally demanding and therefore seldom used in practice. An alternative is to conduct Monte Carlo simulations on a coarse grid, which is still computationally intensive (due to the need for many repetitions) and leads to a loss of accuracy due to the need to average (upscale) the flow equations over relatively large grid cells. Our objective was to avoid the need for either Monte Carlo simulation or upscaling by developing ways to render predictions and uncertainty assessments directly, in a computationally efficient and accurate manner. This final technical report describes our accomplishment in the development of two novel approaches, one based on the Kirchhoff transformation and the other on a Gaussian method of approximation. The report also describes some initial ideas about how to extend the applicability of these two approaches to multidimensional and transient flows in a broader class of soils than we have considered previously. The report cites publications based on research supported in part by this ARO grant.

INTRODUCTION

Our project dealt with the effect of measuring randomly varying soil hydraulic properties on one's ability to predict unsaturated flow subject to random sources and/or initial and boundary conditions. Our aim was to develop theoretical and computational methods for the optimum prediction of unsaturated flow (in terms of pressure head, water content, flux and velocity) in randomly heterogeneous soils under the action of uncertain forcing terms (boundary conditions, initial conditions, sources and sinks), and assessment of the associated prediction errors. In the past, such predictions and assessments required the conduct of numerous (hundreds or thousands) Monte Carlo simulations on a fine computational grid, which is computationally demanding and therefore seldom used in practice. An alternative is to conduct Monte Carlo

simulations on a coarse grid, which is still computationally intensive (due to the need for many repetitions) and leads to a loss of accuracy due to the need to average (upscale) the flow equations over relatively large grid cells. Our objective was to avoid the need for either Monte Carlo simulation or upscaling by developing ways to render predictions and uncertainty assessments directly (in a finite number of computational steps) in a computationally efficient and accurate manner. Whereas the Monte Carlo method requires specifying the probability distribution of soil parameters (which, for convenience, are typically assumed to be multivariate Gaussian or log-Gaussian, mostly without direct evidence), one of the two approaches we are pursuing (that based on the Kirchhoff transformation) is free of such distributional requirements.

Our study focused on flow in the unsaturated or vadose zone. This zone forms a major hydrologic link between the ground surface and underlying groundwater aquifers. To properly understand its role in protecting groundwater from surface and near surface sources of contamination, one must be able to analyze quantitatively fluid flow in unsaturated soils. The difficulty is that such soils are ubiquitously heterogeneous, with hydraulic properties (saturated conductivity, porosity, parameters of constitutive functional relationships between relative conductivity, pressure head and saturation) that fluctuate from point to point in a seemingly erratic manner. This erratic spatial variability, together with random errors of measurement and interpretation, renders the soil parameters uncertain and the corresponding flow equations stochastic. In practice, the random spatial variability of soil hydraulic properties, and the stochastic nature of unsaturated flow variables (pressure head, saturation, flux, velocity), are often ignored. Instead, the common approach is to delineate the spatial variation of soil properties deterministically and express the unsaturated flow equations in a similar fashion. Another popular assumption is that flow through the vadose zone is largely vertical and one is justified ignoring lateral variations in soil hydraulic properties and flow variables. Yet with increasing frequency, such attitudes are proving to be counter productive. Consider for illustration, the case of leaking underground tanks at Hanford.

A recent report to Congress by the US General Accounting Office (GAO/RCED-98-80, March 1998) suggests that the common practice of ignoring lateral flow might have misled the DOE to believe, for many years, that the vadose zone at Hanford constitutes an effective barrier for contaminant migration between tank wastes and underlying groundwater. The DOE had assumed that wastes would move slowly, if at all, through the vadose zone, thereby obviating the need for detailed studies of flow conditions in the thick unsaturated zone at Hanford. The GAO report cites evidence that may indicate otherwise. Indeed, in December 1997 the DOE had announced publicly that highly radioactive wastes from previously leaking underground storage tanks had migrated all the way down to groundwater. Current understanding of how wastes move through the vadose zone to the groundwater has proven to be inadequate for key technical decisions on how to clean up the wastes at Hanford in an environmentally sound and cost-effective manner. To better understand fluid flow and contaminant transport processes in the vadose zone, one must recognize that unsaturated soils and rocks form part of a complex three-dimensional, multiphase, multiscale heterogeneous and anisotropic hydrogeologic system. This system does not constitute a perfect sequence of horizontal layers; if it did, flow and transport rates would be controlled by the least permeable layer and would therefore be correspondingly low. In reality, unsaturated medium properties vary spatially in a complex manner, which often allows fluids

and contaminants to move around low-permeability obstacles much faster than would be possible in the perfectly stratified case. Preferential flow through high-permeability channels and/or the formation of unstable fingers could further enhance the rate of contaminant migration from a source in the vadose zone to the water table. A panel of four vadose zone experts concluded (DOE/RL-97-49, April 1997) that characterization of the vadose zone at Hanford is an essential step toward understanding contamination of the groundwater, assessing the resulting health risks, and defining the concomitant groundwater monitoring program needed to verify risk assessments. As flow and transport in the heterogeneous vadose zone at Hanford are poorly understood, previous and ongoing computer modeling efforts are inadequate and based on unrealistic and sometimes optimistic assumptions, which render their output unreliable.

A recent study of groundwater and soil cleanup by the U.S. National Academy (National Research Council, 1999) recognizes that the geologic and geochemical characteristics of a site have a major influence on the performance of subsurface cleanup systems. According to this study, the subsurface is usually highly heterogeneous and characterizing this variability is extremely difficult. This heterogeneity and difficulty in characterization complicate the design of subsurface cleanup systems because predicting system performance under such uncertain conditions is difficult. Further, many types of cleanup systems, including not only pump-and-treat systems but also systems using in situ chemical oxidation, biodegradation, and other processes, require the circulation of water, aqueous solutions, or other fluids underground. The physical heterogeneity of the subsurface interferes with uniform delivery of fluids to contaminated locations. As a result, some contaminated zones will receive little or no treatment if a fluid is pumped in or out of the zone. Technologies for treating DNAPL source zones, and dissolved plumes emanating from DNAPL sources, are limited primarily by geological heterogeneities, which can interfere with circulation of treatment fluid and water or can limit access to the subsurface. Soil heterogeneity affects soil vapor extraction performance as air flows most easily through coarse-grained soils and very little if at all through predominantly clayey soils. Frequently, volatile organic compounds will accumulate preferentially on the surface of and within clay lenses and layers, and airflow will be minimal in the most highly contaminated soils. An accurate knowledge of geological heterogeneities is vital for evaluating the hydrogeological limits on subsurface contaminant remediation.

In a January 2000 Editorial titled "It's the Heterogeneity!" the Editor of the most widely read groundwater journal (Wood, 2000) reminds his readers that the heterogeneity of chemical, biological, and flow conditions should be a major concern in any remediation scenario. In his view, many in the groundwater community either failed to "get" the message or were forced by political considerations to provide rapid, untested, site-specific active remediation technology. It was their lack of appreciation of heterogeneity that led them to the belief that they could remediate aquifers by simply pumping out and treating offending solute. "It's the heterogeneity," and it is the Editor's guess that the natural system is so complex that it will be many years before one can effectively deal with heterogeneity on societally important scales.

The purpose of our work under this ARO grant was to help accelerate the process. Though the complex and uncertain nature of subsurface flow conditions is now widely recognized, there does not yet appear to be a satisfactory way to characterize and quantify them mathematically

and computationally. Our goal was to develop a mathematical framework, and computational algorithms that help materially advance the corresponding state of science and technology. We pursued this goal through (a) the development of stochastically-derived deterministic "conditional moment equations" that allow optimum unbiased prediction of flow in randomly heterogeneous unsaturated soils on a multiplicity of spatial scales, under the action of uncertain forcing terms, as well as assessment of the corresponding prediction errors, and (b) the development of associated analytical and computational methods of solution. Rather than requiring repeated Monte Carlo simulations on a fine grid, our computational methods are designed to yield a solution in one single simulation on a relatively coarse grid. Rather than working with upscaled quantities which are often difficult to justify theoretically, or compare with measurements, all quantities that enter into our equations are defined on a scale compatible with potentially available field data (their support scale).

ACCOMPLISHMENTS

The grant funded a doctoral student, Mr. Donghai Wang, who plans to complete his Ph.D. dissertation in spring 2003. The grant also provided partial funds for the Co-PI, Dr. Daniel M. Tartakovsky, of the Scientific Computing Group within the Theoretical Division at Los Alamos National Laboratory. In addition to the Principal Investigator, persons not funded by the grant in any major way, who however have collaborated with us, include Dr. Orna Amir and Dr. Zhiming Lu. The latter two have been funded primarily by a National Science Foundation grant that expired on January 31, 2001. Dr. Amir has completed her doctorate in December 1999 and Dr. Lu in May 2000. Both the PI and Dr. Tartakovsky have served as members of Dr. Amir's and Dr. Lu's doctoral committees. We describe briefly the research and relevant work products completed by members of this team to date.

Laying the Groundwork

Our research was founded on two papers that have appeared in the fall of 1999. In the paper by _Neuman et al._ (1999) we lay the foundations of a new conditional moment approach for the solution of stochastic unsaturated flow equations with random parameters and uncertain forcing terms. The paper shows that the approach leads to deterministic equations for the conditional moments, which can be solved by standard numerical methods, thereby obviating the need for Monte Carlo simulations. The parameters in these equations may be local (depending on one point in space-time) or nonlocal (depending on two such points). As they are conditional on measurements, the parameters are not unique properties of the soil but vary with the underlying database. The conditional mean solution constitutes an optimum unbiased predictor of the otherwise unknown state of the system, and conditional second moments provide a measure of the corresponding prediction uncertainty. Since all moments are defined on the same consistent measurement (support) scale ω as the data, there is no need for upscaling, though one can easily integrate the conditional mean solution in space-time, if one so desires. As the conditional mean solution is smooth relative to its random counterpart, it can in principle be resolved on a numerical grid which is coarser than that typically required for the Monte Carlo simulation of random fields.

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The paper of *Neuman et al.* (1999) describes two methods for the development of conditional moment equations and their solution. One method is based on the Kirchhoff transformation and the other on a Gaussian closure approximation. The method using Kirchhoff transformation is described more fully in a paper by <u>*Tartakovsky et al.* (1999)</u>. There we demonstrate that the Kirchhoff transformation fully linearizes the stochastic steady state unsaturated flow equation in the absence of gravity, and does the same for flow with gravity when the Gardner model, $K = K_s \exp(\alpha\psi)$, applies; here K is unsaturated hydraulic conductivity, K_s is saturated hydraulic conductivity, α is a positive exponent, and ψ is (negative) pressure head. Consequently, the method yields exact conditional mean flow equations for both situations, as well as exact equations for the conditional variance-covariance of pressure head and flux. Both sets of equations are nonlocal (integro-differential) in that they contain parameters depending on more than one point in space. Both the local (depending on one point in space) and nonlocal parameters in our moment equations are conditional on data and therefore nonunique. The conditional mean solution constitutes an optimum unbiased predictor of the otherwise unknown state of the system, and conditional second moments provide a measure of the corresponding prediction uncertainty.

The linear Kirchhoff-transformed stochastic flow equations yield exact conditional moment equations which, however, cannot be solved without a closure approximation. The closure approximation we use is based on perturbation analysis. As such, it is nominally limited either to mildly heterogeneous soils, or to strongly heterogeneous soils in which hydraulic properties have been measured with sufficient accuracy, at a sufficiently large number of points, to allow estimating them everywhere else in the soil with a relatively low degree of uncertainty. We shall see later that, in reality, our perturbation approach works well even in strongly heterogeneous soils in the absence of such conditioning.

The paper of *Tartakovsky et al.* (1999) demonstrates rigorously that the concept of effective hydraulic conductivity does not generally apply to statistically averaged unsaturated flow equations except when they are unconditional and flow is driven solely by gravity. It points out that all conditional parameters and moments in our equations are smooth relative to their random counterpart and can therefore be resolved, in principle, on a numerical grid which is coarser than that typically required for the Monte Carlo simulation of random fields. The paper proceeds to develop analytical solutions for the Kirchhoff potential, pressure head and their variances under vertical infiltration, without conditioning, to second order of approximation in the standard deviation (first order in the variance) of natural log saturated hydraulic conductivity. It then compares these with Monte Carlo results obtained by solving the stochastic Richards equation numerically. Our second order approximations are generally far superior to zero order approximations, and the variance of pressure heads compares much better with Monte Carlo values than does the variance of Kirchhoff potentials. Both the analytical pressure head and its variance compare well with Monte Carlo results for natural log conductivity variances at least as large as 1. This accords well with theoretical analysis (presented in the paper) which shows that our analytical solution remains asymptotic for input variances as large as 2.

The Gaussian method of approximation, introduced by *Neuman et al.* (1999), is more general than the method based on Kirchhoff transformation in that it imposes fewer restrictions on the functional form of constitutive relationships between unsaturated hydraulic conductivity, pressure head and saturation. It however requires assuming that the reference pressure head is multivariate Gaussian (or log-Gaussian) about its conditional mean.

The Kirchhoff method of solution has been developed and explored further by Drs. Lu and Tartakovsky. The Gaussian method has been the research focus of Dr. Amir and Mr. Wang. We present a brief description of their accomplishments and findings.

Numerical Analysis Based on Kirchhoff Transformation

In May 2000, Zhiming Lu completed his doctoral dissertation (*Lu, 2000*) on nonlocal finite element analysis of conditional steady state unsaturated flow in bounded, randomly heterogeneous soils using the Kirchhoff transformation. The highlights of his work are described in a paper by *Lu et al.* (2002) published earlier this year in the archival journal *Water Resources Research*.

Dr. Lu's work consists of the development, and computer implementation, of a finite element algorithm for the prediction of steady state unsaturated flow in the vertical plane. He considers flow in a bounded, randomly heterogeneous soil profile under the influence of random forcing terms. His aim is to predict pressure head and flux at each point in the two-dimensional vertical profile without resorting to Monte Carlo simulation, upscaling or linearization of the constitutive relationship between unsaturated hydraulic conductivity and pressure head. To achieve this, he represents the latter relationship through Gardner's exponential model (described earlier), treating its exponent α as a random constant and saturated hydraulic conductivity, K_s, as a spatially correlated random field. This allows him to linearize the steady state unsaturated flow equations by means of the Kirchhoff transformation, integrate them in probability space, and obtain exact integro-differential equations for the conditional mean and variance-covariance of transformed pressure head and flux, in the manner of *Tartakovsky et al.* (1999). Expansion of the nonlocal conditional moment equations in powers of σ_Y and σ_α, which represent measures of the standard estimation errors of saturated natural log hydraulic conductivity $Y = \ln K_s$ and $\beta = \ln \alpha$, respectively, leads to a set of recursive closure approximations. Zhiming solves these approximate moment equations by finite elements, to second-order of approximation, for superimposed mean uniform and divergent flow regimes.

As the conditional mean quantities are generally smoother than their random counterparts, the recursive moment equations can be solved (in principle) on a relatively coarse grid without upscaling. Dr. Lu, however, uses a fine grid to compare his nonlocal finite element solution with conditional and unconditional Monte Carlo simulations, conducted on the same grid by standard finite elements. Dr. Lu's comparison demonstrates that his direct finite element solution of the moment equations is highly accurate for mildly heterogeneous soils and works well for soils that are moderately to strongly heterogeneous.

Extension of Approach Based on Kirchhoff Transformation to Soils with Spatially Varying Exponent α

Our analytical and numerical approaches based on the Kirchhoff transformation treat the exponent α in the *Gardner* (1958) constitutive relation $K = K_s \exp(\alpha\psi)$ as a random constant that does not vary in space. In a recent *Journal of Hydrology* article (*Tartakovsky et al., 2002*) we describe a way to relax this requirement by allowing α to be a statistically homogeneous random field. Our approach utilizes the "partial mean-field" concept, according to which the random field $\alpha(x)$ is replaced by its spatially varying conditional ensemble mean while saturated hydraulic conductivity remains a random field. The Kirchhoff transformation can then be applied to the resulting (nonlinear) stochastic partial differential equation in a manner similar to that of our earlier analyses. The accuracy of this approach depends on a complex interplay between the statistical parameters of $\alpha(x)$ (mean, variance and correlation scale), an issue explored in the above paper.

Analysis Based on Gaussian Approximation

In December 1999 Orna Amir completed her doctoral dissertation, titled "Gaussian Analysis of Unsaturated Flow in Randomly Heterogeneous Porous Media" (*Amir, 1999*). Based on the assumption that pressure head ψ is multivariate Gaussian about its conditional mean, Dr. Amir was able to derive governing equations for the mean and variance of ψ without linearizing either the constitutive relation between unsaturated hydraulic conductivity and pressure head, or the governing unsaturated flow equations (so that the governing moment equations remain nonlinear, as is the underlying stochastic Richards' equation). Contrary to all other known solutions of the stochastic unsaturated flow problem, our Gaussian approach places no obvious restrictions on the variance of the corresponding constitutive parameters. This is evident from Dr. Amir's computational results.

Dr. Amir illustrated the application and effectiveness of the Gaussian closure approximation by developing a closed system of coupled nonlinear, ordinary differential equations for the first and second moments of pressure head under one-dimensional steady state unsaturated flow through a randomly stratified soil. Her equations are written (by choice, not necessity) for unsaturated hydraulic conductivity that varies exponentially with pressure head, where now the exponent α is not a random constant (as it was in the case of the Kirchhoff transformation) but a spatially varying random field. Rather than treating the soil as a continuum, Dr. Amir found it helpful to represent it by a discrete assembly of layers, each of which has uniform but random properties $Y = \ln K_s$ and $\beta = \ln \alpha$, which however are auto- and cross-correlated between the layers.

Dr. Amir solved her one-dimensional, steady state nonlinear moment equations numerically and compared the results with those obtained by Monte Carlo simulation, based on an existing analytical solution of Richards' equation for this case. The comparison shows excellent agreement between the two sets of results over a remarkably broad range of constitutive parameters. A paper that describes this part of Dr. Amir's work has appeared in the journal

Transport in Porous Media (*Amir and Neuman*, 2001a). An earlier, less complete version has appeared in a book published as a *Geological Society of America Special Paper* (*Amir and Neuman*, 2000).

Extension of Gaussian Approach to Transient Flow

In her dissertation, Dr. Amir extended her one-dimensional Gaussian solution to the case of transient flow with an exponential constitutive relationship between saturation and pressure head. Upon comparing her mean solution with that obtained by the Monte Carlo method (this time through numerical solution of the one-dimensional Richards' equation), Dr. Amir found that the two agree very well for a wide range of constitutive parameters. However, she found a less satisfactory agreement between the variances and covariances of pressure head obtained by the two methods.

Though Dr. Amir is now in Israel, she continues to collaborate with us on this project. During the last year, Dr. Amir was able to improve substantially the quality of pressure head variance and covariance assessments based on her one-dimensional Gaussian approach. A paper summarizing her most recent work on this topic has been submitted for publication in the journal *Transport in Porous Media* (*Amir and* Neuman, 2002b).

Extension of Gaussian Approach to Multidimensional Flow

To lay the groundwork for a multi-dimensional application of our Gaussian approach, *Amir* (1999) proposed solving steady state flow in a two-dimensional domain by finite elements by representing the soil as a checkerboard of square elements, each having uniform random constitutive properties $Y = \ln K_s$ and $\beta = \ln \alpha$, which however are auto- and cross-correlated between the elements. The computational implementation of this finite element algorithm has become the domain of a doctoral student supported by this grant, Mr. Donghai Wang.

Donghai has formulated, developed and implemented a finite element algorithm based on the above idea. He has applied his algorithm to two-dimensional flow in a bounded vertical domain under coupled mean uniform and convergent flows, and compared his results with those of standard Monte Carlo simulations. His excellent results are summarized in a paper presented at (and included in the Proceedings of) the Fourteenth International Conference on Computational Methods in Water Resources that took place in Delft, The Netherlands, in June 2002 (*Wang et al.*, 2002). Mr. Wang is presently completing his doctoral dissertation, which he plans to defend in spring 2003. We plan to prepare one or more journal articles based on his dissertation in spring and summer 2003.

Following is a brief technical description of Mr. Wang's work.

Consider steady state unsaturated flow in a bounded domain Ω governed by mass continuity and Darcy's law,

$$-\breve{\nabla}\cdot\mathbf{q}(\breve{x})+f(\breve{x})=0 \qquad \mathbf{q}(\breve{x})=-K(\breve{x},\breve{\psi})\breve{\nabla}(\breve{\psi}+\breve{x}_3) \tag{1}$$

subject to boundary conditions

$$\breve{\psi}(\breve{x})=\breve{\Psi}(\breve{x}) \qquad\qquad \text{on } \Gamma_D$$
$$-\mathbf{q}(\breve{x})\cdot\mathbf{n}(\breve{x})=Q(\breve{x}) \qquad \text{on } \Gamma_N \tag{2}$$

Here $\breve{\nabla}$ is gradient operator with respect to the spatial position vector $\breve{x}$, $\mathbf{q}$ is flux, f is a source term, K is a spatially correlated random hydraulic conductivity field, $\breve{\psi}$ is pressure head, $\breve{x}_3$ is the vertical, Γ_D is Dirichlet boundary, Γ_N is Neumann boundary, and $\mathbf{n}$ is a unit outer normal to the boundary. The forcing terms f, $\breve{\Psi}$, Q are random and mutually uncorrelated. All quantities are defined, and measurable, on a bulk support volume ω that is small compared to the flow domain Ω. Flow takes place under strictly unsaturated conditions such that $\breve{\psi}<0$. The random nature of K and the forcing terms render (1) – (2) stochastic.

We represent hydraulic conductivity using the Gardner (1958) constitutive model

$$K(x,\psi)=K_s(x)K_r(x,\psi) \qquad K_r(x,\psi)=e^{\alpha(x)\psi(x)} \tag{3}$$

where K_s is saturated hydraulic conductivity, K_r is relative conductivity, and α is a positive exponent. The flux in (1) and (2) then becomes

$$\mathbf{q}(x)=-K_s e^{\alpha\breve{\psi}}\nabla(\breve{\psi}+\breve{x}_3) \tag{4}$$

We treat $Y(x)=\ln K_s(x)$ as a correlated Gaussian random field and $A=-\ln\alpha$ as a normally distributed random variable. Using (4), we rewrite (1) - (2) in dimensionless form as

$$0=\frac{1}{\langle\alpha\rangle}\nabla\cdot\left\{\frac{K_s(x)}{\langle\alpha\rangle}e^{\psi(x)}\nabla\left[\alpha\psi(x)+\langle\alpha\rangle x_3\right]\right\} \tag{5}$$

$$\psi(x)=\Psi(x) \qquad\qquad\qquad\qquad \text{on } \Gamma_D$$
$$-\frac{K_s(x)}{\langle\alpha\rangle}e^{\psi(x)}\nabla\left[\alpha\psi(x)+\langle\alpha\rangle x_3\right]\cdot\mathbf{n}(x)=Q(x) \quad \text{on } \Gamma_N \tag{6}$$

where $\langle\alpha\rangle$ is ensemble mean of α, ∇ is gradient operator with respect to dimensionless x, and ψ and x are dimensionless variables defined as

$$\psi=\breve{\psi}/\alpha \qquad\qquad x=\breve{x}/\langle\alpha\rangle \tag{7}$$

Considering that $\langle \alpha \rangle = e^{-\langle A \rangle + \sigma_A^2/2}$ where $\langle A \rangle$ is the mean of A and σ_A^2 is its variance, we can rewrite $(5) - (6)$ as

$$0 = e^{\langle A \rangle - \sigma_A^2/2} \nabla \cdot \left[e^{Y + \langle A \rangle - \sigma_A^2/2} e^{\psi} \nabla \left(e^{-A} \psi + e^{-\langle A \rangle + \sigma_A^2/2} x_3 \right) \right] \tag{8}$$

$$\psi(\boldsymbol{x}) = \Psi(\boldsymbol{x}) \qquad\qquad \text{on } \Gamma_D$$
$$-e^{Y + \langle A \rangle - \sigma_A^2/2} e^{\psi} \nabla \left(e^{-A} \psi + e^{-\langle A \rangle + \sigma_A^2/2} x_3 \right) \cdot \mathbf{n}(\boldsymbol{x}) = Q(\boldsymbol{x}) \qquad \text{on } \Gamma_N \tag{9}$$

We take the flow domain to be a checkerboard of R densely spaced, nonoverlapping subdomains Ω_r, $r = 1, 2, \ldots R$, within each of which Y and A are random constants, Y_r and A_r:

$$Y(\boldsymbol{x}) = \{Y_r, \boldsymbol{x} \in \Omega_r \forall \mathrm{r}\} \qquad\qquad A(\boldsymbol{x}) = \{A_r, \boldsymbol{x} \in \Omega_r \forall \mathrm{r}\} \tag{10}$$

Multiplying (8) by a deterministic weight function ϕ_n, integrating over the global domain Ω, rewriting as the sum of integrals over R sub-domains Ω_r, and taking ensemble mean yields

$$0 = \sum_{r=1}^{R} e^{\langle A_r \rangle - \sigma_{A_r}^2/2} \int_{\Omega_r} \nabla \cdot \left\langle e^{Y + \langle A \rangle - \sigma_{A_r}^2/2} e^{\psi} \nabla \left(e^{-A} \psi + e^{-\langle A \rangle + \sigma_{A_r}^2/2} x_3 \right) \right\rangle \phi_n \, d\Omega \tag{11}$$

Applying Green's identity, then rewriting ψ as $\langle \psi \rangle + \psi'$ and Y as $\langle Y \rangle + Y'$, (11) becomes

$$0 = -\sum_{r=1}^{R} e^{\langle Y_r \rangle + \langle A_r \rangle - \sigma_{A_r}^2} \int_{\Omega_r} e^{\langle \psi \rangle} \left\langle e^{\psi' + Y'} \nabla \left(e^{-A'} \langle \psi \rangle + e^{-A'} \psi' + e^{\sigma_{A_r}^2/2} x_3 \right) \right\rangle \cdot \nabla \phi_n \, d\Omega$$
$$+ \sum_{r=1}^{R} e^{\langle Y_r \rangle + \langle A_r \rangle - \sigma_{A_r}^2} \int_{\Gamma \cap \Omega_r} \phi_n e^{\langle \psi \rangle} \left\langle e^{\psi' + Y'} \nabla \left(e^{-A'} \langle \psi \rangle + e^{-A'} \psi' + e^{\sigma_{A_r}^2/2} x_3 \right) \right\rangle \cdot \mathbf{n} \, d\Gamma \tag{12}$$

Treating ψ, Y and A as Gaussian and defining

$$p = e^{\langle \psi \rangle} \left\langle e^{\psi' + Y' - A'} \right\rangle \qquad\qquad \zeta = \langle \psi' A' \rangle + \langle Y' A' \rangle \tag{13}$$

allows simplifying (12) as

$$0 = -\sum_{r=1}^{R} e^{\langle Y \rangle_r + \langle A_r \rangle - \sigma_{A_r}^2} \int_{\Omega_r} \left(\nabla p + p e^{\zeta} i_3 \right) \cdot \nabla \phi_n \, d\Omega + \sum_{r=1}^{R} e^{\langle Y_r \rangle + \langle A_r \rangle - \sigma_{A_r}^2} \int_{\Gamma \cap \Omega_r} \phi_n \left(\nabla p + p e^{\zeta} i_3 \right) \cdot \mathbf{n} \, d\Gamma \tag{14}$$

where $i_3 = (0,0,1)^T$. Approximating p and ζ by

$$p^n = \sum_{m=1}^{N} p_m \phi_m, \quad \zeta^n = \sum_{m=1}^{N} \zeta_m \phi_m \tag{15}$$

where p_m and ζ_m are values of p and ζ at nodes $m = 1, 2, \ldots N$ and ϕ_n now serve as Lagrange interpolation functions, then using (9), yields the Galerkin finite element scheme

$$0 = -\sum_{r=1}^{R} e^{\langle Y_r \rangle + \langle A_r \rangle - \sigma_{A_r}^2} \sum_{m=1}^{N} p_m \int_{\Omega_r} \left(\nabla \phi_m \cdot \nabla \phi_n + \phi_m e^{\sum_{m=1}^{N} \zeta_m \phi_m} i_3 \cdot \nabla \phi_n \right) d\Omega + \sum_{r=1}^{R} e^{\langle Y_r \rangle + \langle A_r \rangle - \sigma_{A_r}^2} \sum_{m=1}^{N} p_m \int_{\Gamma_D \cap \Omega_r} \phi_n \nabla \phi_m \cdot n \, d\Gamma$$

$$+ \sum_{r=1}^{R} e^{\langle Y_r \rangle + \langle A_r \rangle - \sigma_{A_r}^2} \int_{\Gamma_D \cap \Omega_r} \phi_n P e^{\langle Y'\Psi' \rangle + \langle Y'A' \rangle} i_3 \cdot \mathbf{n} \, d\Gamma - \sum_{r=1}^{R} e^{\langle A_r \rangle - \frac{\sigma_{A_r}^2}{2}} \int_{\Gamma_N \cap \Omega_r} \phi_n Q \, d\Gamma \tag{16}$$

where P is p at the $\Gamma_D \cap \Omega_r$. Setting $n = 1, 2, \ldots N$ yields a system of N equations in N unknown values of p_n. However, the equations are nonlinear due to their dependence on ζ.

To derive a complementary system of equations for ζ_m we multiply (11) by A' and ϕ_n, integrate over Ω, rewrite as a sum of integrals over Ω_r, take ensemble mean, apply Green's identity and account for (9) to obtain

$$0 = -\sum_{r=1}^{R} e^{\langle Y_r \rangle + \langle A_r \rangle - \sigma_{A_r}^2} \left(\sum_{i,j=1}^{N} p_i \zeta_j \int_{\Omega_r} \nabla(\phi_i \phi_j) \cdot \nabla \phi_n \, d\Omega - \sigma_A^2 \sum_{i=1}^{N} p_i \int_{\Omega_r} \nabla \phi_i \cdot \nabla \phi_n \, d\Omega + \sum_{i,j=1}^{N} p_i \zeta_j \int_{\Omega_r} \phi_i \phi_j e^{\sum_{j=1}^{N} \zeta_j \phi_j} i_3 \cdot \nabla \phi_n \, d\Omega \right)$$

$$+ \sum_{r=1}^{R} e^{\langle Y_r \rangle + \langle A_r \rangle - \sigma_{A_r}^2} \left(\sum_{i,j=1}^{N} p_i \zeta_j \int_{\Gamma_D \cap \Omega_r} \phi_n \nabla(\phi_i \phi_j) \cdot \mathbf{n} \, d\Gamma - \sigma_A^2 \sum_{i=1}^{N} p_i \int_{\Gamma_D \cap \Omega_r} \phi_n \nabla \phi_i \cdot \mathbf{n} \, d\Gamma \right)$$

$$+ \sum_{r=1}^{R} e^{\langle Y_r \rangle + \langle A_r \rangle - \sigma_{A_r}^2} \int_{\Gamma_D \cap \Omega_r} \phi_n P \left(\langle A'\Psi' \rangle + \langle Y'A' \rangle \right) e^{\langle A'\Psi' \rangle + \langle Y'A' \rangle} i_3 \cdot \mathbf{n} \, d\Gamma - \sum_{r=1}^{S} e^{\langle A_r \rangle - \frac{\sigma_{A_r}^2}{2}} \int_{\Gamma_N \cap \Omega_r} \phi_n \langle A'Q \rangle d\Gamma \tag{17}$$

Setting $n = 1, 2, \ldots N$ yields a system of N equations in N unknown values of ζ_n. The coupled nonlinear equations (16) – (17) are solved simultaneously by (in our case Picard) iteration for p and ζ.

To compute the covariance function $C_\psi(\mathbf{x}, \tilde{\mathbf{x}}) \equiv \langle \psi'(\mathbf{x}) \psi'(\tilde{\mathbf{x}}) \rangle$ of dimensionless pressure head ($\mathbf{x}$ and $\tilde{\mathbf{x}}$ being two arbitrary points in space), we first require an equation for the mixed moment $\varphi(\mathbf{x}) \equiv \langle Y'(\mathbf{x}) \psi'(\mathbf{x}) \rangle$. Multiplying (8) by Y' and following the same procedure as before yields a system of N linear equations for nodal values of φ,

$$0 = -\sum_{r=1}^{R} e^{\langle Y_r \rangle + \langle A_r \rangle - \sigma_{A_r}^2} \sum_{m=1}^{N} \varphi_m \left(-\int_{\Omega_r} \left(\phi_m \nabla p + p \nabla \phi_m + p \phi_m e^\zeta i_3 \right) \cdot \nabla \phi_n \, d\Omega + \int_{\Gamma \cap \Omega_r} \phi_n \left(\phi_m \nabla p + p \nabla \phi_m + p \phi_m e^\zeta i_3 \right) \cdot \mathbf{n} \, d\Gamma \right)$$

$$+ \sum_{r=1}^{R} e^{\langle Y_r \rangle + \langle A_r \rangle - \sigma_{A_r}^2} \left(-\int_{\Omega_r} \left[(\sigma_Y^2 - \langle Y'A' \rangle) \nabla p + \sigma_Y^2 p e^\zeta i_3 \right] \cdot \nabla \phi_n \, d\Omega + \int_{\Gamma \cap \Omega_r} \phi_n \left[(\sigma_Y^2 - \langle Y'A' \rangle) \nabla p + \sigma_Y^2 p e^\zeta i_3 \right] \cdot \mathbf{n} \, d\Gamma \right) \tag{18}$$

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Multiplying (8) by $\tilde{\psi}' = \psi'(\tilde{x})$ and following a similar procedure yields a system of $N \times N$ equations for $C_{m,\tilde{m}} = C_\psi(x_m, \tilde{x}_{\tilde{m}})$,

$$0 = -\sum_{r=1}^{R} e^{\langle Y_r \rangle + \langle A_r \rangle - \sigma_{A_r}^2} \sum_{m=1}^{N} C_{m\tilde{m}} \left(-\int_{\Omega_r} \left(\phi_m \nabla p + p \nabla \phi_m + p\phi_m e^\zeta i_3 \right) \cdot \nabla \phi_n \, d\Omega + \int_{\Gamma \cap \Omega_r} \phi_n \left(\phi_m \nabla p + p \nabla \phi_m + p\phi_m e^\zeta i_3 \right) \cdot \mathbf{n} \, d\Gamma \right)$$

$$+ \sum_{r=1}^{R} e^{\langle Y_r \rangle + \langle A_r \rangle - \sigma_{A_r}^2} \left(-\int_{\Omega_r} \left[\nabla \left(p(\tilde{\varphi} - \tilde{\eta}) \right) + \tilde{\varphi} p e^\zeta i_3 \right] \cdot \nabla \phi_n \, d\Omega + \int_{\Gamma \cap \Omega_r} \phi_n \left[\nabla \left(p(\tilde{\varphi} - \tilde{\eta}) \right) + \tilde{\varphi} p e^\zeta i_3 \right] \cdot \mathbf{n} \, d\Gamma \right)$$

(19)

Computation is facilitated by the fact that (18) and (19) contain identical coefficient matrices and the symmetric nature of the matrix $C_{m,\tilde{m}}$.

Additional details about these derivations can be found in Amir (1999).

The variance σ_ψ^2 is obtained from the covariance $C_\psi(x, \tilde{x})$ by setting $x = \tilde{x}$. Finally, the mean solution is obtained via

$$\langle \psi \rangle = \ln p - \left(\sigma_Y^2/2 + \sigma_A^2/2 + \sigma_\psi^2/2 + \varphi \right)$$

(20)

For illustration purposes we consider flow in a vertical plane of size 4×8 (all terms being given in arbitrary consistent units) having impermeable side boundaries (Figure 1). A constant deterministic flux $Q_b = 0.01$ is prescribed at the top and zero pressure head at the bottom. A point source of magnitude $Q_s = 1$ causes the otherwise near-uniform mean flow to become locally divergent in the domain interior. For simplicity, Y and A are taken to be spatially and mutually uncorrelated. We solve the problem using our finite element Gaussian closure algorithm, and (for comparison) by 5,000 Monte Carlo simulations using standard finite elements, on a grid of 20×40 square elements with bilinear weight and interpolation functions.
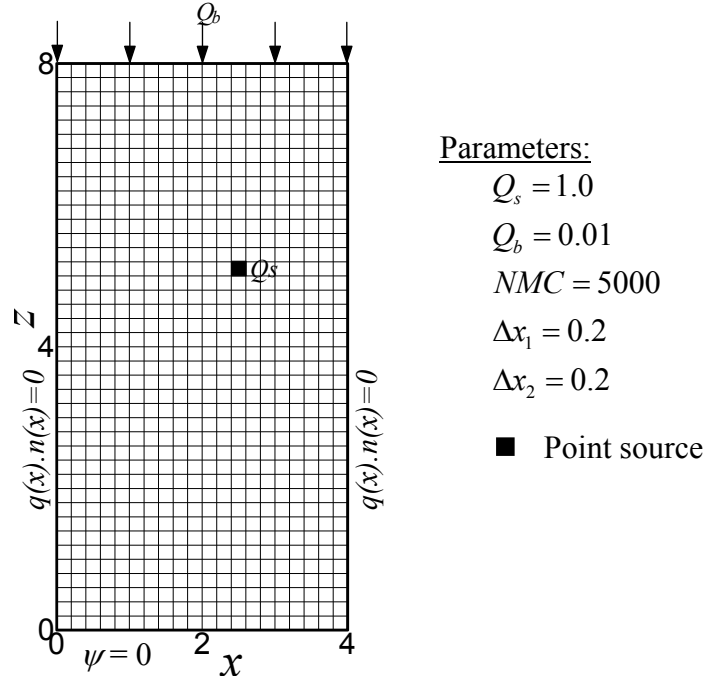
Figure 1. Problem definition and associated grid

Figure 2 depicts contours and profiles of mean dimensionless pressure head and its variance obtained by the two methods for a medium having uniform but random Y and A values characterized by $\langle Y \rangle = 3$, $\sigma_Y^2 = 2$, $\langle A \rangle = 0$, and $\sigma_A^2 = 0.02$. The two solutions are seen to agree very well despite the relatively large value of σ_Y^2.

Figure 3 shows how the mean and variance of Y and A vary spatially in two cases for which we present solutions in Figures 4 and 5. In both cases, the Gaussian Closure and Monte Carlo methods yield virtually identical dimensionless mean pressure head values but slightly different variances. Overall, we consider these results to be very good.

Our solution of (16) – (17) converges in 3 to 4 iterations. This, and the fact that we need to solve our Gaussian closure equations only once, helps explain why our solution has taken only about one fourth the time required for the completion of 5,000 standard Monte Carlo simulations
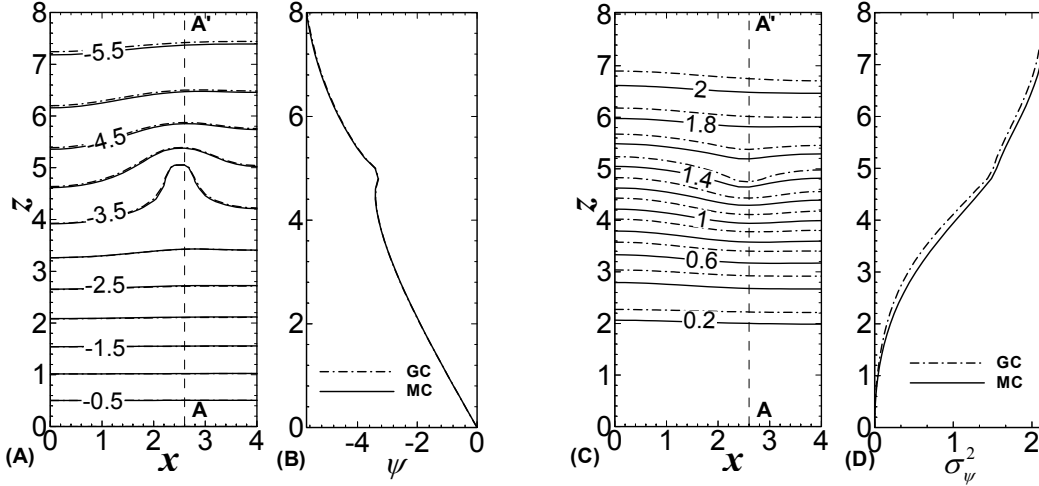
Figure 2. Contours and profiles of mean pressure head (A, B) and variance of pressure head (C, D) obtained by Monte Carlo (MC, solid) and Gaussian closure (GC, dash-dot) for homogeneous domain with $<Y> = 3$, $\sigma_Y^2 = 2$ and $<A> = 0$, $\sigma_A^2 = 0.02$
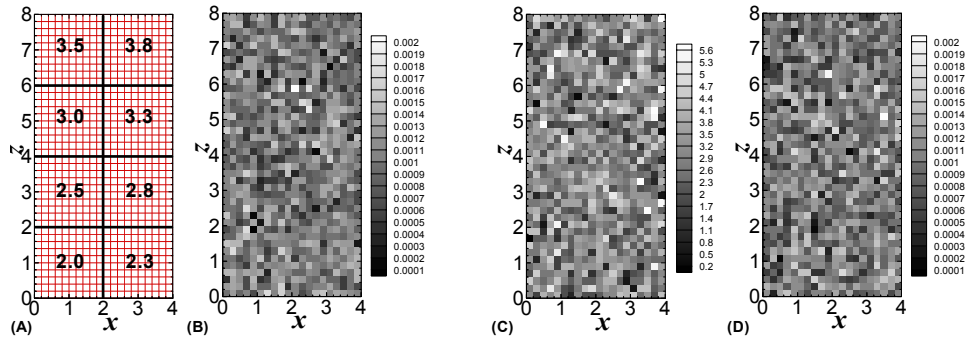

Figure 3. Variation of $\langle Y \rangle$ and σ_A^2 in cases of Figure 4 (A and B) and Figure 5 (C and D). In both cases $\sigma_Y^2 \equiv 1$ and $\langle A \rangle \equiv 0$.
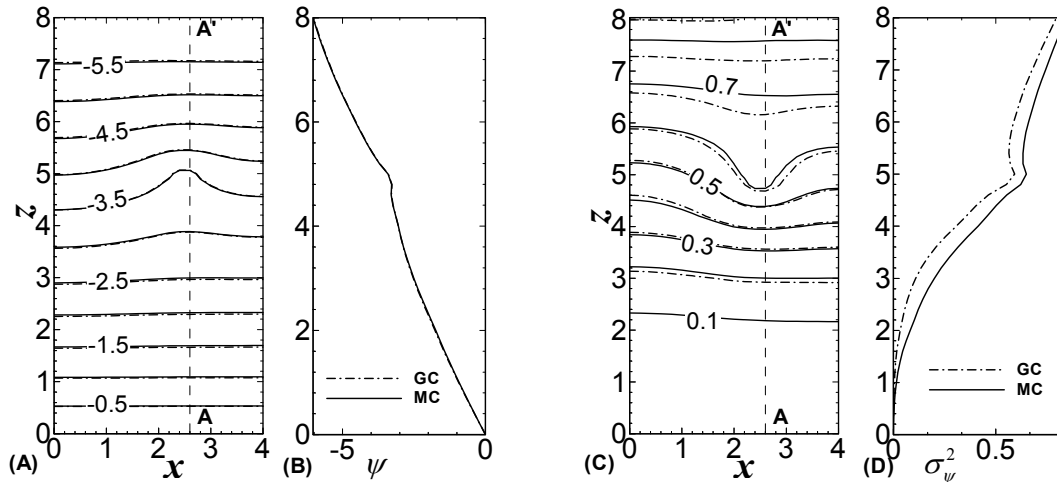
Figure 4. Contours and profiles of dimensionless mean pressure head (A-B) and variance of dimensionless pressure head (C-D) obtained by Monte Carlo (MC, solid) and Gaussian closure (GC, dash-dot) for parameters defined in Figure 3A-B.
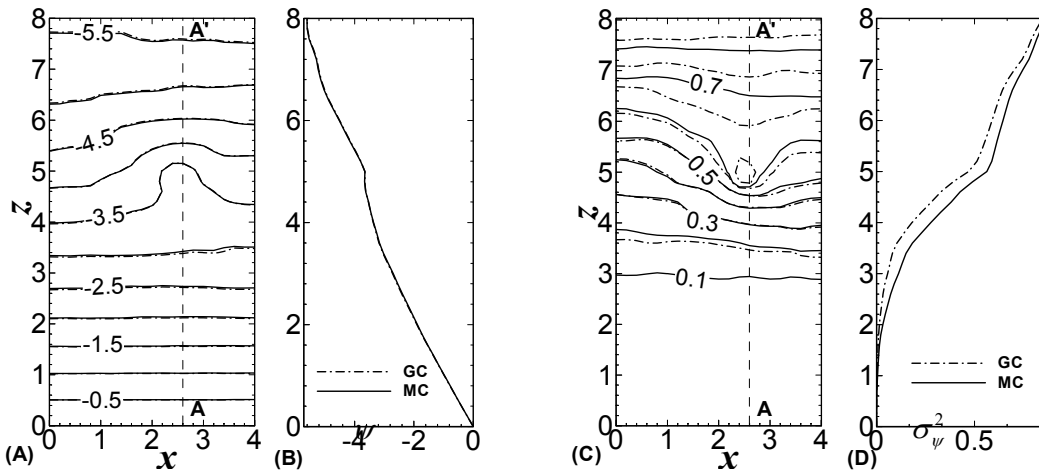
Figure 5. Contours and profiles of dimensionless mean pressure head (A-B) and variance of dimensionless pressure head (C-D) obtained by Monte Carlo (MC, solid) and Gaussian closure (GC, dash-dot) for parameters defined in Figure 3C-D.

Advances in Modeling Soil Constitutive Relations

A paper by *Assouline and Tartakovsky* (2001) on this topic has recently been published in *Water Resources Research*. It describes the development of a new two-parameter expression for relative hydraulic conductivity of partially saturated soils. The new expression is based on a premise by *Assouline et al.* (1998) that the probability distribution of particle volumes in natural soils results from a series of sequential fragmentations. These fragmentations are caused by cyclical wetting and drying; physical, chemical and biological processes; and cultivation

practices. Assouline assumes the fragmentation process to be uniform and random, and the probability of particle fragmentation to be proportional to its volume. This leads to a probability distribution of soil particles that is asymptotically exponential. The latter is a particular case of the Weibull distribution. *Assouline and Rouault* (1997) and *Rouault and Assouline* (1998) have established a power relationship between particle volume and pore volume. It implies that pore volume distribution is described by the general Weibull model. Coupling this with the capillary law has allowed *Assouline et al.* (1998) to express the relationship between effective saturation and pressure head in terms of pressure head at the wilting point and two empirical parameters, which are determined by fitting the function to experimental data. Assouline and Tartakovsky extended the approach by deriving a corresponding relationship between relative hydraulic conductivity, effective saturation and pressure head. Upon fitting their relative conductivity model to data representing various soil types, the authors found that it fits these data better than do the widely used models of *Brooks and Corey* (1964) and *van Genuchten* (1980).

SUMMARY OF ACCOMPLISHMENTS

The goal of this work was to advance, as far as possible, our ability to render reliable predictions of flow in randomly heterogeneous soils under conditions of uncertainty in a computationally efficient manner, and to assess the uncertainty of these predictions. We have developed two major techniques to accomplish this goal, one based on the Kirchhoff transformation and the other on a Gaussian closure approximation. Both techniques presently utilize the finite element method to solve two-dimensional steady state unsaturated flow problems with gravity in the presence of arbitrary source and boundary terms. We have started working on methods to extend these techniques to transient flows in soils having arbitrary constitutive properties.

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