UNCERTAINTY AND SENSITIVITY ANALYSES OF GROUNDWATER TRAVEL TIME IN A TWO-DIMENSIONAL VARIABLY-SATURATED FRACTURED GEOLOGIC MEDIUM

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ABSTRACT

This paper presents a method for sensitivity and uncertainty analysis of a hypothetical nuclear waste repository located in a layered and fractured unconfined aquifer. Groundwater travel time (GWTT) has been selected as the performance measure. The repository is located in the unsaturated zone, and the source of aquifer recharge is due solely to steady infiltration impinging uniformly over the surface area that is to be modeled. The equivalent porous media concept is adopted to model the fractured zone in the flow field. The evaluation of pathlines and travel time of water particles in the flow domain is performed based on a Lagrangian concept. The Bubnov-Galerkin finite-element method is employed to solve the primary flow problem (non-linear), the equation of motion, and the adjoint sensitivity equations. The matrix equations are solved with a Gaussian elimination technique using sparse matrix solvers. The sensitivity measure corresponds to the first derivative of the performance measure (GWTT) with respect to the parameters of the system. The uncertainty in the computed GWTT is quantified by using the first-order second-moment (FOSM) approach, a probabilistic method that relies on the mean and variance of the system parameters and the sensitivity of the performance measure with respect to these parameters. A test case corresponding to a layered and fractured, unconfined aquifer is then presented to illustrate the various features of the method.

INTRODUCTION

Groundwater travel time (GWTT) is a subsystem performance measure established by the U.S. Nuclear Regulatory Commission for evaluating a potential high-level nuclear waste (HLW) repository in a geologic medium (10CFR60.113). The GWTT is defined to provide an estimate of water travel time associated with the fastest likely path of radionuclides that might be released from the repository horizon and transported to the accessible environment.

This paper presents a method for estimating the sensitivity and uncertainty of the GWTT, based on a deterministic method of analysis. The approach to our calculation proceeds in four steps, as follows:

(i) The hydrologic analysis consists of the steady-state calculation of the water pressure head and velocity distribution in the variably-saturated, fractured geologic medium, including an exact determination of the water-table height at the seepage face of the flow domain. Of the existing approaches in modeling groundwater flow through fractured media[1] the equivalent porous medium approach is the one adopted in this work.

(ii) The pore velocity distribution then is used to obtain the preferential flow paths and GWTTs for a set of particles released from the same repository location. While particle pathlines and travel times are Lagrangian quantities and velocities are computed through an Eulerian-based approach, the former behave like streamlines under steady-state flow conditions[2]. Consequently, the motion of a typical water particle remains solely a function of the system parameters where its mass bears no relevancy to the process.

(iii) The adjoint sensitivity theory developed by researchers at Oak Ridge National Laboratory[3] was our method of choice. In the field of geohydrology, this theory has been successfully used by several researchers[4,5] in conjunction with optimization work associated with aquifer parameter estimation. It has also been used in sensitivity studies to identify key system parameters and assumptions for a selected performance measure. This method is unequivocally the method of choice when first-order gradient evaluation of the performance measure with respect to the system parameters is required, particularly when, as in this paper, the primary equations are nonlinear differential equations. The adjoint method of analysis can considerably improve the numerical efficiency of codes, as well as provide significant savings in computational time.

(iv) The quantification of the prediction uncertainty is formulated by means of a deterministic method based on the FOSM technique[6], which has been used successfully in groundwater modeling by various investigators[5,7]. This method allows for a rapid evaluation of the first and second moment of the performance measure based on the knowledge of similar statistical data pertaining to the system parameters and the sensitivity coefficients of the performance measure to these parameters.

The application of the methodology outlined herein is illustrated by means of a numerical example focused on a conceptual model of a hypothetical nuclear waste disposal site, where we have attempted to duplicate to a reasonable degree many of the hydrogeologic features of the proposed site on a reduced scale. In the following section, we will report the fundamental governing equations required in this study.

GOVERNING EQUATIONS

The groundwater-flow regime in a saturated-unsaturated porous medium is assumed to be laminar[1], justifying the application of Darcy's law. The components of the equation of motion in the vertical plane of a variably saturated unconfined aquifer may be written as

$$q_{x_i} = - K_{ij} K_r \left(\frac{\partial h}{\partial x_j} + \frac{\partial z}{\partial x_j} \right) \quad , \quad i,j = 1,2 \tag{1}$$

where h is the pressure head defined as $p/\rho g$ (L), p is the fluid pressure ($ML^{-1}t^{-2}$), K_{ij} represents the components of the saturated hydraulic conductivity tensor, ($k_{ij}\rho g/\mu$) (Lt^{-1}), k_{ij} are the components of the saturated intrinsic permeability tensor (L^2), K_r is the dimensionless relative permeability, ρ is the fluid density (ML^{-3}), μ is the dynamic fluid viscosity ($ML^{-1}t^{-1}$), g is the acceleration of gravity (Lt^{-2}), z is the elevation from datum (L), and x_1 and x_2 are the horizontal and vertical (positive upward) Cartesian coordinates (L).

The components of the interstitial (or apparent) velocity, V_{x_i}, in the unsaturated portions of the flow region is given by the ratio of q_{xi} and θ ($h < 0$), where θ is the moisture content [i.e., $\theta = \phi\ (S - S_r)$], ϕ is the porosity, and S and S_r correspond to water saturation ($0 \leq S \leq 1$) and irreducible (or residual) water saturation of the porous medium, respectively. For a saturated region (i.e., $h \geq 0$), θ is substituted by the effective porosity, ϕ_e [i.e., $\phi_e = \phi(1 - S_r)$].

From mass conservation requirements and using Eq (1), the equation describing steady-state, single-phase flow of fluid in the reported flow domain, in the absence of sources or sinks and under isothermal conditions, may then be written as

$$\frac{\partial}{\partial x_i}\left[K_{ij}K_r\left(\frac{\partial h}{\partial x_j} + \frac{\partial z}{\partial x_j}\right)\right] = 0 \quad , \quad i,j = 1,2 \tag{2}$$

subject to boundary conditions corresponding to: (i) prescribed pressure head, h_1 (Dirichlet), on the portion, Γ_1, of the boundary, (ii) prescribed rate of flux, q_r (Neumann), on the portion, Γ_2, of the boundary.

The response function or performance measure, R, considered in this work is the GWTT of a typical water particle along its pathline, S, written as,

$$R = R(h,\alpha) = \sum_{i=1}^{n} dt_i = \sum_{i=1}^{n} \int_{S_i}^{S_{i+1}} \frac{dS}{V_{r_i}} \tag{3}$$

where h refers to the dependent variable to be solved, α's represent the parameters of the system, V_r is the resultant velocity, dS is the net displacement of the water particle within a time step, dt_i, and n is the time step number.

The evaluation of the sensitivity of the performance measure, R, to a typical parameter, α_k, is given by

$$\frac{dR}{d\alpha_k} = \frac{\partial R}{\partial \alpha_k} + \frac{\partial R}{\partial h_k{}^T}\frac{dh}{d\alpha_k} \tag{4}$$

where superscript T denotes the transposed state of vector, h, and $dh/d\alpha_k$ corresponds to the vector of state sensitivities.

The differential equation corresponding to the adjoint state variable, Ψ^*, is obtained through a differentiation of Eq (1) with respect to the system parameter, α, coupled with an orthogonalization procedure by weighting differentiable functions over the solution domain and successive application of Green's theorem[3]. The equation is written as,

$$\frac{\partial}{\partial x_j}\left[\left(K_{ji}K_r\right)\frac{\partial \psi^*}{\partial x_i}\right] - K_{ij}K_{r,h}\left[\frac{\partial h}{\partial x_j} + \frac{\partial z}{\partial x_j}\right]\frac{\partial \psi^*}{\partial x_i} + \frac{\partial R}{\partial h} = 0 \tag{5}$$

with associated boundary conditions, $\Psi^* = 0$ (on Γ_1) and $(K_{ij}\, K_r)\, \Psi^*_{,xi}\, n_j = 0$ (on Γ_2).

With $K_{ji} = K_{ij}$ by Onsager's principle, the performance measure marginal sensitivity may be shown to correspond to

$$\frac{dR}{d\alpha_k} = \int_A \left\{\frac{\partial R}{\partial \alpha_k} - \psi^* \frac{\partial}{\partial x_i}\left[\left(K_{ij}K_r\right)_{,\alpha_k}\left[\frac{\partial h}{\partial x_j} + \frac{\partial z}{\partial x_j}\right]\right]\right\} dA + \int_{\Gamma_2} \psi^* q_{,\alpha_k}\, d\Gamma_2 \tag{6}$$

where the first term represents the direct sensitivity effect, and the remaining terms represent the marginal sensitivity to the parameters of interest, α_k. A corresponds to any particular area of the flow domain. Note that the solution of Eq (6) requires, on the one hand, a knowledge of h and Ψ^* obtained through the solution of Eqs (1) and (5), and, on the other hand, the derivatives of

R with respect to h and the α_k. The normalized sensitivity coefficient, S, which represents the fractional or percentage change in R resulting from a fractional or percentage change in the value of α is defined as

$$S = \frac{dR/R}{d\alpha/\alpha} = \frac{d(\ln R)}{d(\ln \alpha)} \tag{7}$$

UNCERTAINTY ANALYSIS

The uncertainty analysis reported here highlights one of the attractive features of the adjoint sensitivity method of analysis. As available parameter statistical information was restricted to the first two statistical moments of α, that is, mean vector and covariance matrix, the FOSM method[6] is adopted to estimate the deterministic uncertainty of the performance measure around its mean, in terms of the uncertainty of the system parameters. It may be shown that the variance of R for a system of correlated variables, p, is given by

$$var\left(R\right) = \sigma_R^2 = \sum_{i=1}^{p} \sum_{j=1}^{p} \left[cov\left(\alpha_i, \alpha_j\right) \frac{dR}{d\alpha_i} \frac{dR}{d\alpha_j}\right] \tag{8}$$

where $cov\left(\alpha_i, \alpha_j\right)$ is the covariance of two parameters, α_i and α_j, commonly written, $cov\left(\alpha_i, \alpha_j\right) = \rho_{ij}\sigma_i\sigma_j$ with correlation ρ_{ij} .

MATERIAL PROPERTIES

Functional models of the saturation and permeability curves for both media (i.e., rock matrix and fracture) have been adopted in this work. The van Genuchten[8] relation between saturation and capillary pressure head is given by

$$S = S_r + \frac{(1 - S_r)}{(1 + (\alpha\,|h|)^{\beta})^{\lambda}} \tag{9}$$

where α and β are constants to be determined, and $\lambda = 1 - 1/\beta$.

The van Genuchten[8] and Mualem[9] models describing the relationship between relative intrinsic conductivity and capillary pressure head are given by

$$K_r = \frac{(1 - (\alpha|h|)^{\beta-1}\ [1 + (\alpha|h|)^{\beta}]^{-\lambda}\ )^2}{[1 + (\alpha|h|)^{\beta}]^{\lambda/2}} \tag{10}$$

and

$$K_r = [1 + (\alpha|h|)^{\beta}]^{-\lambda/2}\left(1 - \left[\frac{(\alpha|h|)^{\beta}}{1 + (\alpha|h|)^{\beta}}\right]^{\lambda}\right)^2 \tag{11}$$

MATHEMATICAL MODELS

The test problems were investigated using two deterministic, finite-element-based, computer codes: TRIPM[10] and PARTICLE[11]. TRIPM uses the Bubnov-Galerkin method to compute the steady-state solutions of the groundwater flow problem, and yields the nodal distribution of pressures, velocities, and the inverse of the coefficient matrix of the adjoint state vector including first-order derivatives of the velocity components and the primary equation with respect to the system parameters. All these outputs are required by PARTICLE, which in turn will compute the trajectory and travel time of a liquid particle based on a Lagrangian approach. PARTICLE also estimates the sensitivity coefficients of GWTT with respect to the various parameters of the system. In their turn these sensitivity coefficients are used to perform the uncertainty analysis of the mean groundwater travel time based on the FOSM approach.

ILLUSTRATIVE EXAMPLE

The hydrology of the potential nuclear waste repository at Yucca Mountain seems to suggest that the flow domain is closely analogous to a multilayered, unconfined aquifer. Furthermore, some of the units close to the surface exhibit the presence of fractures that dip at angles close to 90°. The sole source of aquifer recharge is attributed to precipitation.

The system geometry in the illustrative example is represented by a vertical cross section of a ditch-drained, vertically-stratified, unconfined aquifer, as illustrated in Figure 1. The height and width of the rectangular flow domain correspond to 100 m and 50 m, respectively. In this instance, the ditch is assumed to be water free (AG = 0). The upstream boundaries, BC, including the aquifer base, AB, are assumed to be impervious. An infiltration rate of 1 mm/yr was assumed to prevail on portion CD of the boundary at all times. The flow domain includes five distinct horizontal rock units of uniform thickness. The second layer from the top denotes the presence of a large set of orthogonal fractures. With the exception of their length which varies between 0.025 - 15 m, these are assumed to have constant material properties. The hypothetical repository horizon, H_1-H_2, which has a width of 50 m, is located in the uppermost layer at an elevation of 43 m and at a distance of 30 m from the seepage face. The rock matrix and fracture properties, including the constants in material characteristic curves, are given in Table I.

Table I. Material Properties for the Hydrogeologic Units and Fractures

Rock Layer	Thickness, m	ϕ	K_{11}, m/yr	K_{11}/K_{22}	Constants in Material Characteristic Curves: S_r	α, m^{-1}	β
1 (b)	8.0	0.17	3.09×10^{-4}	2	0.07	5.19×10^{-3}	1.78
2 (b)	10.0	0.12	7.41×10^{-4}	10	0.12	1.44×10^{-2}	1.47
3 (a)	7.0	0.37	1.55	10	0.31	1.37	2.345
4 (a)	15.0	0.14	1.2×10^{-3}	1	0.318	1.147	3.040
5 (a)	10.0	0.46	3.09	10	0.166	3.645	2.250
Fracture (b)	NA	0.9	3.4×10^{2}	1	0.0395	1.29	4.23

a = van Genuchten equations b = Mualem's equations

Figure 2a shows the finite-element discretization of the flow domain consisting of 391 isoparametric bilinear rectangular elements (excluding the fractures) with 432 nodes. Three idealized fracture networks were considered to be present in layer four with identical material properties (see Table I). These networks were discretized by means of linear elements: the first corresponding to a set of 100 orthogonal fractures (i.e., shown in thick lines in Figure 2a), the second to a set of 50 horizontal fractures (Figure 2b), and the third to a set of 50 vertical fractures (Figure 2c). The mean and standard deviation of the length (in meters) of these fractures in their respective sets correspond to (4.25, 3.55), (6.0, 4.35) and (2.5, 0.505).

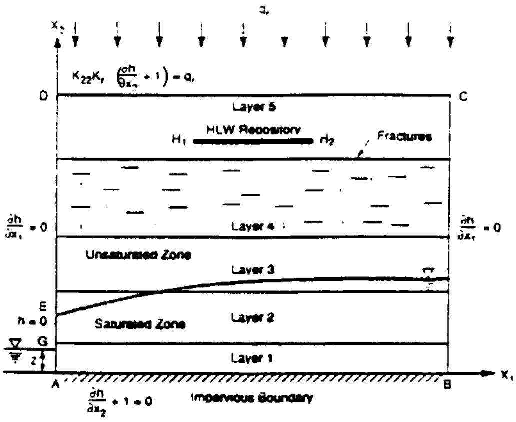

Figure 1. Description of Ditch-Drained Multilayered and Fractured Unconfined Aquifer

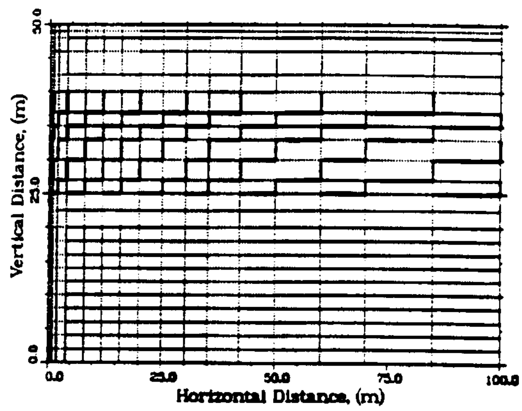

Figure 2a. Finite-Element Mesh, Layer 4 (orthogonal fracture set shown in thick lines)

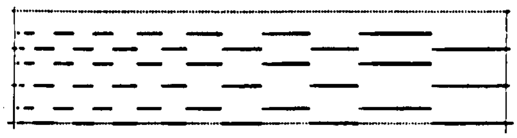

Figure 2b. Horizontal Fracture Set, Layer 4.

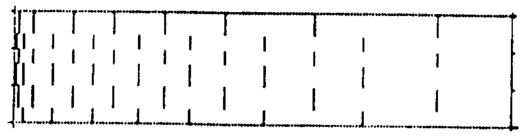

Figure 2c. Vertical Fracture Set, Layer 4.

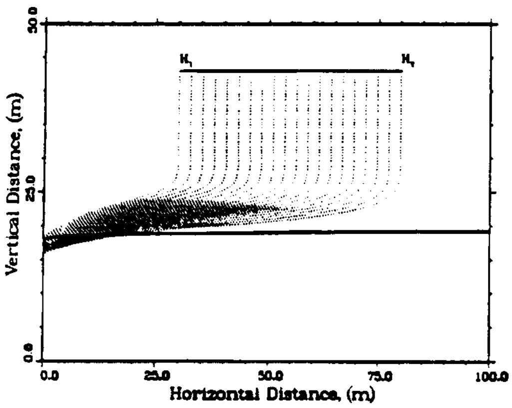

Figure 3a. Pathlines of Water Particles for Baseline Case

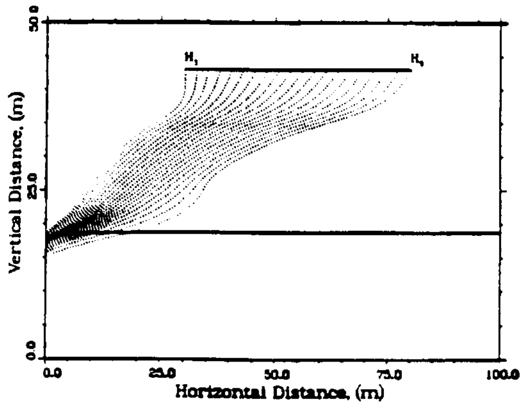

Figure 3b. Pathlines of Water Particles for Orthogonal Fracture Case

The computation of GWTT was performed for two cases: (i) fracture-free case (baseline) and (ii) case with fractures.

Figures 3a and 3b show the computed pathlines of 20 particles released from the repository horizon for both the baseline case and the orthogonal fracture case. The shape of the streamlines highlights the impact of this particular fracture network on the pressure distribution on the flow domain.

Similar investigations were performed on the remaining pair of fracture configurations. Subsequently, groundwater arrival times were computed, describing the relative cumulative flow being discharged through the seepage face as a function of time. The latter were defined as the ratio of the sum of the flow, Q, in successive streamtubes that reaches the seepage face, to the total flow, Qmax, in the streamtubes. Figure 4 shows a summary of the arrival time curves for the baseline case and the three fracture configurations. It may be observed that the orthogonal fracture network (Case 2) exhibits the largest arrival time lag, approximately 4.06×10^3 yrs relative to the baseline case (1), followed by the vertical fracture case (4) with 1.004×10^3 yrs. This lag time drops to an insignificant level (30 yrs) for the horizontal fracture case (3). Noting that the streamlines in layer 4 in the baseline case are nearly vertical, the response registered in the latter case is in conformity with theoretical predictions; that is, fracture zones orthogonal to streamlines offer practically no resistance to fluid flow.

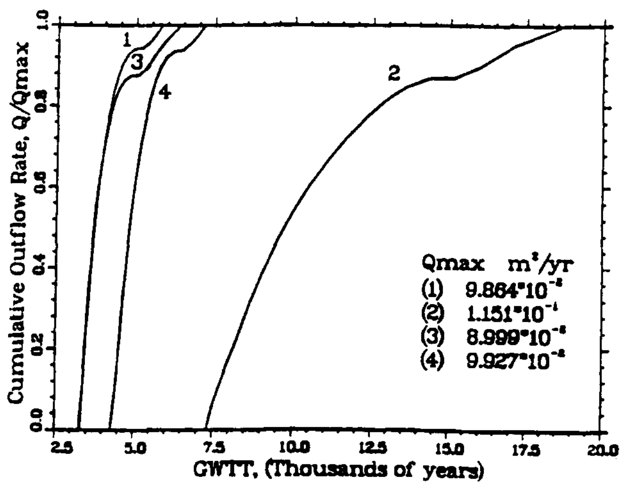

Figure 4. Arrival Time Curve for All Cases. (1) baseline case; (2) orthogonal fracture case; (3) horizontal fracture case; and (4) vertical fracture case

The sensitivity study was performed using the orthogonal fracture case. GWTT is assumed to be essentially a function of uncertainty in hydraulic conductivity of the rock matrix units and fractures, porosity, residual saturation, etc. The sensitivity analysis was performed after selecting the shortest streamline, which crosses layers 5 and 4 and a small portion of layer 3. Based on the computed normalized sensitivity coefficients, the ten most significant parameters were: K_{11_5}, ϕ_5, K_{22_5}, K_{11_4}, ϕ_4, ϕ_3, K_{11_3}, K_{22_3}, S_{r_3}, and K_f where numerical subscripts denote the layer number, and K_f corresponds to the hydraulic conductivity of the fracture. Note that the sensitivity of GWTT to the various material constants arising in the equations of the characteristic curves has not been addressed in this instance.

The system parameters are assumed to be statistically uncorrelated, random variables. The hydraulic conductivity in each layer is assumed to have a log-normal distribution. Porosity and residual saturation are assumed to be normally distributed. For the example problem, the standard deviation of all parameters was extracted from a constant value of the coefficient of variation ($CV = \sigma/\mu$) of 0.2. Results show that the contribution of the uncertainty in the various parameters to the uncertainty in the GWTT, expressed in terms of the standard deviation, corresponds to 6,750 and 169 years for the vertical and horizontal components of the saturated hydraulic conductivities, 199.76 years for porosities, and 9.52 years for residual saturation. These results, interpreted in terms of the coefficient of variation of GWTT, yield for the above-mentioned parameters, K_{11} and K_{22}, ϕ, and S_r, values of 0.92 and 0.03, 0.027, and 1.29×10^{-3}, respectively. Thus, for the example problem, uncertainty in K_{11} plays the most significant role in the computed uncertainty in GWTT.

SUMMARY

In this paper, we presented the development of a deterministic approach for calculating (i) the pathline and travel time of liquid particles in an unconfined aquifer that is partially saturated, fractured and multi-layered, ditch-drained, and subject to a steady infiltration rate, (ii) the sensitivity in GWTT, and (iii) the uncertainty in GWTT. The material properties used in the numerical simulations were based on realistic data with attributes close to the potential HLW repository site.

Preliminary results comparing matrix-flow with fracture-flow simulations suggest that specific fracture configurations restricted to the unsaturated zone could have an appreciable delaying effect on GWTT. We believe that this numerically-based conclusion requires further verification with controlled laboratory experiments.

The sensitivity of GWTT to the various system parameters was estimated by the adjoint sensitivity method, leading to a ranking of the parameters based on the normalized sensitivity coefficients.

Although the adjoint sensitivity method is well suited to the FOSM method for evaluating the uncertainty of an arbitrary performance measure, the information that it provides is only correct for the first order. Consequently, uncertainty predictions for non-linear problems, such as the one dealt with in this paper, should be considered with caution and restricted to parameters with reasonably low coefficients of variation (i.e., ≤ 0.2).

Ranking the importance of the system parameters for the hypothetical HLW repository site and subsequently estimating the uncertainties of the selected performance measure (i.e., GWTT) to these parameters about their mean may be of valuable assistance in performance assessments.

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