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DETERMINISTIC AND PROBABILISTIC PERFORMANCE ASSESSMENT METHODS APPLIED TO RADIONUCLIDE MIGRATION THROUGH FRACTURED GEOLOGIC MEDIUM*

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ABSTRACT

This paper presents a sensitivity and uncertainty study of a hypothetical High Level Waste (HLW) underground repository intersected by a vertical fracture or fault and under saturated conditions. A one-dimensional analytical model based on the Laplace transform method yielding the concentration in the fracture and rock layers and the cumulative mass release of radionuclides at any point within the fracture was developed. In this instance the cumulative mass is adopted as the performance measure. The sensitivity of the performance measure to some of the system parameters affecting the transport process is reported. An efficient probabilistic analysis method is proposed that combines an Advanced Mean Value method and an Adaptive Importance Sampling method. A numerical example related to the transport of Np-237 in a system of layered fractured rock is used to highlight the merit of the above mentioned probabilistic method.

INTRODUCTION

Performance assessment investigations related to the safety aspect of a HLW repository are required to demonstrate compliance with applicable NRC regulations. Sensitivity and uncertainty analyses are currently performed by means of mathematical models designed to address several of the performance criteria required by the licensing process. In order to produce realistic estimates, sources of uncertainties including model uncertainty should be minimized, and disruptive scenarios related to the future states of nature should be relevant to the climatological history and geophysical characteristics of the disposal site. The hypothetical HLW disposal site is assumed to be located in fractured geologic media. Since on the one hand this type of medium is not well understood because of inherent geologic uncertainties and because of the limited ability to quantitatively describe hydrogeological and geochemical processes in such a medium on the other, the adoption of simplified analytical models for a probabilistic assessment of the performance measure becomes a viable alternative. The analytical model adopted here is restricted to investigating radionuclide transport through an idealized semi-infinite system of saturated layered fractured rock but is highly accurate and numerically robust and consequently well suited for long term forecast under such conditions. The selected sensitivity and uncertainty approach which uses the analytically derived local sensitivities is also well known for its accuracy.

In this paper, presentation of analysis method is stressed over application to any specific site. We shall report the equations governing radionuclide transport through an idealized system of fractures connected in series and surrounding rock matrix. The closed form solution pertaining only to the cumulative mass in the fracture will be given in this paper, since the latter was selected as the performance measure of interest. The sensitivity and uncertainty methods adopted here will also be briefly reported. Finally, a scenario of Np-237 migration in a layered rock system assumed to be fully saturated is used to demonstrate the ability of the proposed approach to predict the importance of individual parameters and to calculate the probability of exceeding a regulatory performance limit.

GOVERNING EQUATIONS

The governing one-dimensional equations describing the non-dispersive and isothermal movement of a typical nuclide in the *ith layer of the fracture and saturated rock matrix respectively*[1,2] (see Fig. 1) are given by

(a) Fracture

$$R_i \frac{\partial A_i}{\partial t} + u_i \frac{\partial A_i}{\partial x} + \lambda R_i A_i + \frac{J_i}{b_i} = 0, \quad x_{i-1} < x \le x_i \qquad (1)$$

(b) Rock Matrix

$$R_i' \frac{\partial B_i}{\partial t} - D_{pi} \frac{\partial^2 B_i}{\partial z^2} + \lambda R_i' B_i = 0 \qquad (2)$$

$t > 0,\ x > 0,\ z \ge b_i,\ i = 1, 2, 3, \ldots, n$

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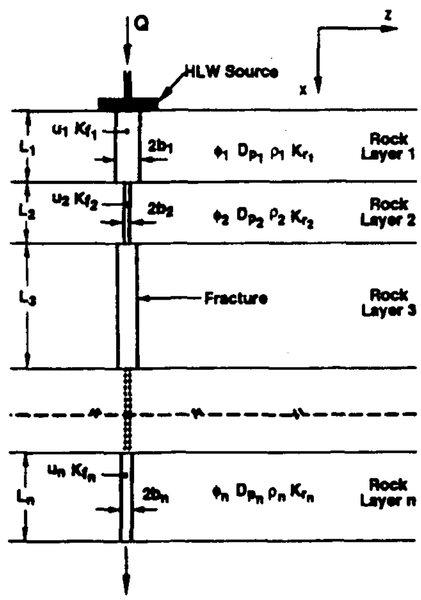

Figure 1. Description of Migration Pathways in a System of Homogeneous Layers of Fractured Rock

where

A_i = concentration in the fracture (ML^{-3})
u_i = average fluid velocity in the fracture (LT^{-1})
b_i = half thickness of fracture (L)
R_i = retardation in the fracture
λ = first-order rate constant for decay (T^{-1})
J_i = diffusive rate of radionuclide at surface of fracture per unit area of fracture surface ($ML^{-2}T^{-1}$)
R_i' = retardation factor in the rock matrix
B_i = concentration in the rock matrix (ML^{-3})
x = spatial coordinate in the fracture (L)
z = spatial coordinate in the rock matrix (L)
t = time (T)
i = index related to the particular layer of fracture and surrounding rock matrix
n = total number of fractured rock layers

The diffusive rate of a nuclide into the ith layer of the rock matrix is assumed to obey Fick's law of diffusion written as

$$J_i = -D_{ei}\frac{\partial B_i}{\partial z}\Big|_{z = b_i} \qquad (3)$$

where D_{ei} is the effective diffusivity in the typical section of the rock matrix[1] defined as

$$D_{ei} = \phi_i D_{pi} \qquad (4)$$

where

ϕ_i = rock porosity
D_{pi} = pore diffusivity (i.e., $D_{pi} = D_d\, g_{fi}$) (L^2T^{-1})
D_d = molecular diffusion of nuclide in water (L^2T^{-1})
g_{fi} = geometric factor (δ_{di}/τ_i^2) where
δ_{di} = pore constrictivity for diffusion (L^0)
τ_i = tortuosity of rock matrix (L^0)

The retardation factor in the ith layer of the fracture (R_i) and the rock matrix (R_i'), respectively[2] are given by:

$$R_i = 1 + \frac{K_{fi}}{b_i} \qquad (5)$$

$$R_i' = 1 + \left[(1-\phi_i)/\phi_i\right]\rho_{ri}K_{ri} \qquad (6)$$

where

ρ_{ri} = bulk rock density (ML^{-3})
K_{fi} = surface distribution coefficient in fracture (L)
K_{ri} = distribution coefficient in rock matrix (L^3M^{-1})

INITIAL AND BOUNDARY CONDITIONS

Equations (1) and (2), are subject to the initial conditions:

$$A_i(x,0) = a_{1i} + a_{2i}e^{-\alpha_i \chi_i},\ x_{i-1} < x \le x_i \qquad (7)$$

where

$$\chi_i = \begin{cases} x, & i = 1 \\ x - x_{i-1} = x - \sum_{j=1}^{i-1} L_j, & i>1 \end{cases} \qquad (8)$$

and:

$$B_i(x,\ z,\ 0) = b_{1i},\ x_{i-1} < x \le x_i,\ x>0,\ z \ge b_i \qquad (9)$$

where a_{1i}, a_{2i}, b_{1i} (all ML^{-3}), and α_i (L^{-1}) are constant for each layer i of the fracture rock system and time invariant, and independent of boundary conditions in the fracture and rock matrix. L_i is the thickness of a typical rock layer i. The boundary conditions in the fracture are given by

$$A_1(0,t) = \bar{A}(t),\ t>0 \qquad (10)$$

$$\frac{\partial A_n(\infty,t)}{\partial x} = 0,\ t>0 \qquad (11)$$

where $\bar{A}(t)$ is the concentration at the source.

For the ith layer of the rock matrix, the corresponding boundary conditions are:

$$B_i(x,b_i,t) = A_i(x,t),\ \ t>0,\ x>0,\ x_{i-1} < x \le x_i \qquad (12)$$

Note that Equations (3) and (12) couple the concentrations in the fracture and the rock matrix.

$$\frac{\partial B_i(x,\infty,t)}{\partial z} = 0,\ t>0,\ x>0,\ x_{i-1} < x <= x_i \qquad (13)$$

CONCENTRATION OF THE SOURCE

For a step release mode, the concentration of a typical nuclide at the source $\bar{A}(t)$ is given by

$$\bar{A}(t) = A^0 e^{-\lambda t},\ t>0 \qquad (14)$$

where A^0 is the concentration of the species at time equals zero.

For a band release mode, the boundary condition at the fracture inlet may be written as

$$\bar{A}(t) = A^0 e^{-\lambda t}\left[U(t) - U(t-T)\right] \qquad (15)$$

where T is the leaching time and U(t) is the Heaviside step function. The general form of the solutions for the band release mode in the ith layer of the fracture and rock matrix based on a boundary condition given by Equation (15) and which uses the superposition method[3] may be written as:

$$\begin{aligned} {}^bA_i(x,t) &= A_i\big(x,t;\ \bar{A}(t), A_i(x,0), B_i(x,z,0)\big)U(t) \\ &\quad - e^{-\lambda T}A_i\big(x,t-T;\ \bar{A}(t-T)\big)U(t-T) \end{aligned} \qquad (16)$$

where ${}^bA_i(x,t)$ corresponds to the band-release solution.

It may be easily shown that at the interface of two consecutive fracture layers the following relation holds:

$$A_i(x,t) = A_{i-1}(x,t),\ i>1 \qquad (17)$$

CUMULATIVE MASS

The closed form solution of the cumulative mass release of the contaminant in the nth fracture layer based on the Laplace transform method is reported below. Details regarding its derivation including those related to the concentrations in the fracture and the rock matrix may be found elsewhere.[4]

The cumulative mass per unit width at any point within the fracture is given by

$$\begin{aligned} M(x,t) &= \int_0^t Q\, A_n(x,\tau)\,d\tau = Q\Bigg[\mathcal{Q}_{01n}(x,t) \\ &\quad - \sum_{i=1}^{n}\sum_{j=1}^{2} {}_j\mathcal{Q}'_{iin}(x,t) + \sum_{i=2}^{n} {}_1\mathcal{Q}'_{i-1in}(x,t) \\ &\quad + e^{-\alpha_i \chi_i}\, {}_2\mathcal{Q}'_{i-1in}(x,t) + \mathcal{Q}_n(x,t)\Bigg] \end{aligned} \qquad (18)$$

where Q is the steady water flow rate in the fracture and $A_n(x,t)$ the concentration in the fracture. In the above equation the components of functions $\mathcal{Q}_{01n}(x,t)$, ${}_1\mathcal{Q}'_{imn}(x,t)$, ${}_2\mathcal{Q}'_{imn}(x,t)$ and $\mathcal{Q}_n(x,t)$ are given by

$$\begin{aligned} \mathcal{Q}_{01n}(x,t) &= A_1^0\Bigg\{-\frac{e^{-\lambda t}}{\lambda}\,\mathrm{erfc}\left[\frac{\theta_{1n}}{2(t-\gamma_{1n})^{1/2}}\right] \\ &\quad + \frac{e^{-\lambda\gamma_{1n}}}{2\lambda}\Bigg[e^{\theta_{1n}\sqrt{\lambda}}\,\mathrm{erfc}\left[\frac{\theta_{1n}}{2(t-\gamma_{1n})^{1/2}} + \sqrt{\lambda(t-\gamma_{1n})}\right] \\ &\quad + e^{-\theta_{1n}\sqrt{\lambda}}\,\mathrm{erfc}\left[\frac{\theta_{1n}}{2(t-\gamma_{1n})^{1/2}} - \sqrt{\lambda(t-\gamma_{1n})}\right]\Bigg]\Bigg\}U(t-\gamma_{1n}) \end{aligned} \qquad (19a)$$

and:

$$\begin{aligned} {}_1\mathcal{Q}'_{imn}(x,t) &= b_{1i}\Bigg\{-\frac{e^{-\lambda t}}{\lambda}\,\mathrm{erfc}\left[\frac{\theta_{mn}}{2(t-\gamma_{mn})^{1/2}}\right] + \\ &\quad \frac{e^{-\lambda\gamma_{mn}}}{2\lambda}\Bigg[e^{\theta_{mn}\sqrt{\lambda}}\,\mathrm{erfc}\left[\frac{\theta_{mn}}{2(t-\gamma_{mn})^{1/2}} + \sqrt{\lambda(t-\gamma_{mn})}\right] + \\ &\quad e^{-\theta_{mn}\sqrt{\lambda}}\,\mathrm{erfc}\left[\frac{\theta_{mn}}{2(t-\gamma_{1n})^{1/2}} - \sqrt{\lambda(t-\gamma_{mn})}\right]\Bigg]\Bigg\}U(t-\gamma_{mn}) \\ &\quad + \frac{(a_{1i}-b_{1i})}{\left(\frac{c_{fi}}{R_i}\right)^2 - \lambda}\Bigg\{\exp\left[\frac{c_{fi}}{R_i}\left(\theta_{mn} - \frac{c_{fi}\gamma_{mn}}{R_i}\right)\right]\exp\left[\left(\left(\frac{c_{fi}}{R_i}\right)^2 - \lambda\right)t\right]\cdot \\ &\quad \mathrm{erfc}\left[\frac{\theta_{mn}}{2(t-\gamma_{mn})^{1/2}} + \frac{c_{fi}}{R_i}(t-\gamma_{mn})^{1/2}\right] - \\ &\quad \frac{\exp(-\lambda\gamma_{mn})}{2}\Bigg[e^{\theta_{mn}\sqrt{\lambda}}\,\mathrm{erfc}\left[\frac{\theta_{mn}}{2(t-\gamma_{mn})^{1/2}} + \sqrt{\lambda(t-\gamma_{mn})}\right]\cdot \\ &\quad \left(\frac{c_{fi}}{R_i\sqrt{\lambda}} + 1\right) - e^{-\theta_{mn}\sqrt{\lambda}}\,\mathrm{erfc}\left[\frac{\theta_{mn}}{2(t-\gamma_{mn})^{1/2}} - \sqrt{\lambda(t-\gamma_{mn})}\right]\cdot \\ &\quad \left(\frac{c_{fi}}{R_i\sqrt{\lambda}} - 1\right)\Bigg]\Bigg\}U(t-\gamma_{mn}) \end{aligned} \qquad (19b)$$

and:

$$2Q'_{imn}(x,t) = \sum_{j=1}^{2} (-1)^j a_{2i}\frac{\beta_{ji}}{q_i}\Bigg\{\exp\left[\beta_{ji}(\theta_{mn}-\beta_{ji}\gamma_{mn})\right]\cdot \frac{e^{(\beta_{ji}^2-\lambda)t}}{\beta_{ji}^2-\lambda}\operatorname{erfc}\left[\beta_{ji}(t-\gamma_{mn})^{1/2}+\frac{\theta_{mn}}{2(t-\gamma_{mn})^{1/2}}\right] - \frac{\exp(-\lambda\gamma_{mn})}{2(\beta_{ji}^2-\lambda)}\Bigg[e^{\theta_{mn}\sqrt{\lambda}}\operatorname{erfc}\left[\frac{\theta_{mn}}{2(t-\gamma_{mn})^{1/2}}+\sqrt{\lambda(t-\gamma_{mn})}\right]\cdot\left(\frac{\beta_{ji}}{\sqrt{\lambda}}+1\right) - e^{-\theta_{mn}\sqrt{\lambda}}\operatorname{erfc}\left[\frac{\theta_{mn}}{2(t-\gamma_{mn})^{1/2}}-\sqrt{\lambda(t-\gamma_{mn})}\right]\cdot\left(\frac{\beta_{ji}}{\sqrt{\lambda}}-1\right)\Bigg]\Bigg\}U(t-\gamma_{mn}) \qquad (19c)$$

and:

$$Q_n(x,t) = \sum_{j=i}^{2}(-1)^j\frac{a_{2n}\beta_{jn}}{q_n}e^{-\alpha_n x_n}\frac{1}{(\beta_{jn}^2-\lambda)}\left[e^{(\beta_{jn}^2-\lambda)t}\operatorname{erfc}(\beta_{jn}\sqrt{t})+\frac{\beta_{jn}}{\sqrt{\lambda}}\operatorname{erf}[(\lambda t)^{1/2}]-1\right] + \frac{b_{1n}}{\lambda}(1-e^{-\lambda t}) + \frac{(a_{1n}-b_{1n})}{\left[\left(\frac{c_{fn}}{R_n}\right)^2-\lambda\right]}\left[\exp\left[\left(\left(\frac{c_{fn}}{R_n}\right)^2-\lambda\right)t\right]\cdot\operatorname{erfc}\left[\frac{c_{fn}}{R_n}t^{1/2}\right]+\frac{c_{fn}}{\sqrt{\lambda}\,R_n}\operatorname{erf}[(\lambda t)^{1/2}]-1\right] \qquad (19d)$$

where

$$c_{fi} = \frac{\phi_i}{b_i}\left(R'_i D_{pi}\right)^{1/2}$$

$$\beta_{ji} = \frac{c_{fi}}{2R_i} + (-1)^j\left[\left(\frac{c_{ji}}{2R_i}\right)^2 + \frac{u_i\alpha_i}{R_i}\right]^{1/2}, \quad j = 1,2$$

$$\overline{\eta}_i = \frac{L_i}{u_i}$$

$$\eta_i = \frac{x - x_{i-1}}{u_i} \qquad (20)$$

$$\theta_{mn} = \sum_{i=m}^{n-1} c_{fi}\overline{\eta}_i + c_{fn}\eta_n$$

$$\gamma_{mn} = \sum_{i=m}^{n-1} R_i\overline{\eta}_i + R_n\eta_n$$

Note that when β_{ji} in the above equation turns negative and the time parameter becomes excessively large, exponential terms with an argument greater (in absolute value) than a computed one are set to zero in order to mitigate overflow problems.[4]

SENSITIVITY ANALYSIS AND SENSITIVITY COEFFICIENT

Sensitivity analysis is concerned with investigating deviations of a physical system from its nominal behavior spurred by deviations of system components and parameters from their nominal values.[5,6]

Considering a response function of n dependent variables $p_1,\ldots,p_n$ and l parameters $\alpha_1,\ldots,\alpha_l$, this function may be represented by:

$$R(\mathbf{p},\alpha) = R(p_1,\ldots,p_n;\alpha_1,\ldots,\alpha_l) \qquad (21)$$

With R set to M(x,t), the sensitivity coefficients $dM/d\alpha_i$ (also referred to as marginal sensitivities) can be loosely interpreted as the change in the value of the performance measure for a unit increase in the value of the parameter (i.e., a first order estimate of the perturbation dM) and written as :

$$\frac{dM}{d\alpha_i} = \frac{\partial M}{\partial \alpha_i} + \frac{\partial M}{\partial \mathbf{p}^T}\mathbf{p}^* \qquad (22)$$

where superscript T denotes the transpose of vector **p** and $\mathbf{p}^* = \partial \mathbf{p}/\partial\alpha$ corresponds to the vector of state sensitivities. The sensitivities for Equation (18) were analytically derived and reported elsewhere.[4]

The above sensitivities can be used to compute the normalized sensitivity of M to a particular parameter, α_i, defined as:

$$S_i = \frac{dM/M}{d\alpha_i/\alpha_i} = \frac{d(\ln M)}{d(\ln\alpha_i)} \qquad (23)$$

which represents the fractional change in the performance measure M due to a fractional change in the value of the parameter.

UNCERTAINTY ANALYSIS AND PROBABILISTIC SENSITIVITY ANALYSIS

In this paper, uncertainty analysis means probabilistic analysis in which the uncertain input variables are modeled as random variables with assigned probability distributions. The goal of the uncertainty analysis is to compute the cumulative probability $F_M(m)$ (or cumulative distribution function, CDF) of a response or performance measure.

Probabilistic sensitivity is defined as the derivative of the cumulative probability, $F_M(m)$, with respect to a parameter, α. The sensitivity, $dF_M(m)/d\alpha$, is evaluated at a specified probability, P, or at a specified response, m. The parameter α is related to the input variables (e.g., a system parameter, or its mean value or standard deviation). Probabilistic sensitivity can be used as a measure in identifying key parameters that contribute to the uncertainty in the CDF response. Based on the Most Probable Point (MPP) approach described below, probabilistic "sensitivity factors"[8] can be developed to measure the relative importance of the random input variables.

There is a fundamental difference between the sensitivity coefficients of Eq. 23 and probabilistic sensitivities. The sensitivity coefficients defined in Eq. 23 are evaluated at a reference point, typically the mean value point. Thus these coefficients are "mean-based" and their use is limited to the region close to the response calculated at the mean point. On the other hand, the probabilistic sensitivities are based on the MPP concept which defines different critical parameter spaces for different m values. Consequently, the probabilistic sensitivities are functions of m and their variations will tend to be large when different transport mechanisms dominate in different parameter spaces. As a result, the dominant random variables might be different for different m values.

EFFICIENT PROBABILISTIC METHODS

Currently, the most commonly used probabilistic methods in repository performance assessment are the Monte Carlo method, the Latin Hypercube sampling method, and the response surface method[7]. For complicated models requiring extensive computer analyses, these methods may be either too time-consuming or not sufficiently accurate. An alternative to these methods is explored in the following.

In the field of structural and mechanical reliability, efficient probabilistic methods have been under development for more than a decade. Methods such as First/Second Order Reliability Method (FORM/SORM)[8] and Advanced Mean Value method (AMV)[9] have been developed for both efficiency and accuracy. These methods are based on the limit-state formulation and the MPP concept.

In the limit state formulation, the performance is investigated at a selected value, for example, $M = m$. Given this "limit", probability of performance being less than (or exceeding) m is computed. A full CDF can be established by selecting a number of limit states, m_i, and performing probability analysis at each of these selected limit states. Numerous combinations of input parameter values lead to limit value m of the performance measure, thus defining a limit state surface.

For each limit state, m, an optimum point on the limit state surface for linearization of the response function is determined. A commonly used optimum point is the MPP. The MPP is determined by first transforming the generally non-normal, dependent random vector **x** of input variables into independent, standardized normal vector **u**. Once in the transformed u-space, the MPP is known to be the minimum distance point, which is the point in the u space that has the highest probability of producing the value m of the response function as illustrated in Fig. 2.

Since the probability is concentrated around the MPP, in its neighborhood, the response function can be approximated by a simple linear or quadratic polynomial function which can then be used to derive the associated probability. Thus, the key step in

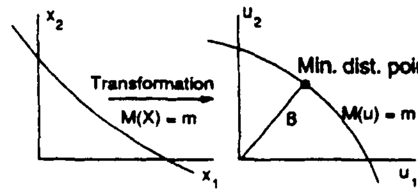

Fig. 2. Transformation and Most Probable Point (MPP)

applying the limit state formulation is in locating the MPP. For complicated numerical models, this step essentially determines the efficiency of the method. In general, the MPP may be found by using various optimization algorithms. When a function evaluation is very expensive, it is important to minimize the total CPU time in locating the MPP.

The AMV method has been developed to approximate the MPP with a minimum number of function evaluations. The AMV method involves evaluating the response function and its gradients at the mean value, computing the approximate MPP locus, and updating the responses on the locus at each probability level.[9] The AMV solution provides a first-order CDF solution as well as other information regarding the behavior of the response function. Based on the AMV solution, an iteration procedure has also been developed to search for the exact MPP. In general, each iteration requires the evaluation of the response and its gradient at an updated MPP.

ADAPTIVE IMPORTANCE SAMPLING METHOD

The approximating function developed around the MPP provides only approximate probability. To confirm the solution, importance sampling methods can be used by sampling more frequently in the region close to the MPP. This reduces the number of samples required to reach a solution with narrower confidence interval as compared with the standard Monte Carlo method.

Various importance sampling schemes are available. A recently developed adaptive importance sampling method[12] is applied in this paper. In this method, the starting sampling region is based on the first or second-order limit state surface developed at the MPP. The sampling region is adjusted by deforming the limit state surface. The deformation is designed to gradually increase the sampling region until it fully covers the "target" region. An example based on changing the curvature of the surface is illustrated in Fig. 3. When the sampling region fully covers the target region, the probability solution will converge, indicating that no more deformation of the surface is required.

DISCUSSIONS AND RESULTS

The test case reported here refers to the one-dimensional

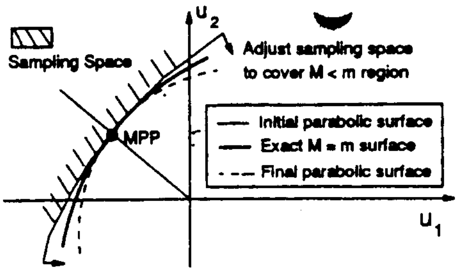

Fig. 3. Concept of Adaptive Importance Sampling

transport of a radionuclide, Np-237, in a layered saturated portion of a fractured rock system composed of five layers (the last extending to infinity, see Fig. 4), with piece-wise constant parameters. The steady flow rate of water Q due to surface ponding per unit width of fracture is 0.1 m^2/yr. The type of solute release mode at the source investigated here corresponds to a band release, where the leaching time T = 5 x 10^3 years. Note that the flow domains in both fracture and rock layers are assigned non-zero initial concentrations (see Equations (7) and (9). The input data pertaining to this test case is presented in Table 1.

Figure 5 depicts the time-dependent evolution of the cumulative mass (per unit width of the fracture) profile at three different observation points in the fracture. These are located at distances of 100, 200 and 500 meters downstream from the source, lying within the second, third and fifth layer respectively. A comparison of our analytical solution results with those yielded by Stefhest's solution[11] indicates excellent agreement. Note that all three profiles tend to become asymptotic to three specific

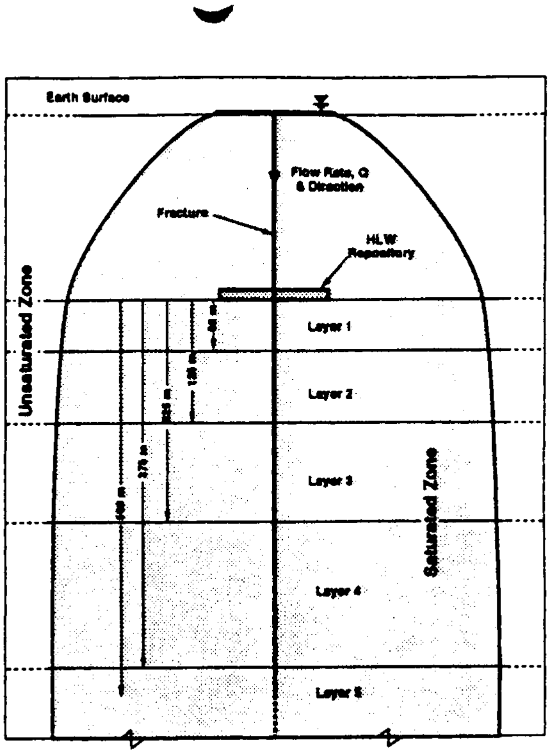

Fig. 4. Vertical cross-section of a layered rock system intersected by a vertical fracture subject to surface ponding.

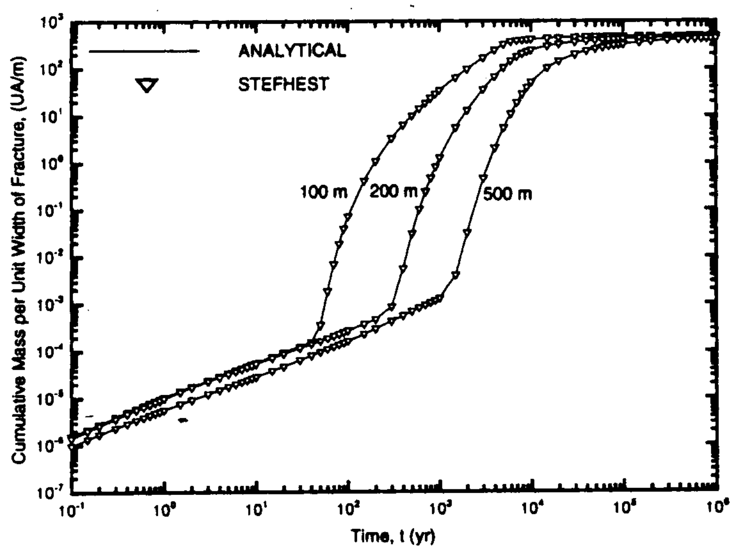

Fig. 5. Cumulative mass of Np-237 per unit in the fracture vs. time at different positions x = 100, 200, and 500 meters (Exponentially decaying source and band release mode)

Table 1. INPUT PARAMETERS

SPECIES: Np-237, $T_{1/2} = 2.3 \times 10^6$ yr, Leaching Time $T = 5 \times 10^3$ yr., $A^o = 1.0^*$, $Q = 0.1$ (m^2/yr).

LAYER	L(m)	b(m)	u(m/yr)	Φ
1	50.0	5.0E-03	10.0	0.01
2	75.0	4.0E-03	12.5	0.008
3	100.0	3.0E-03	16.666	0.006
4	150.0	2.0E-03	25.0	0.004
5	∞	1.5E-03	33.333	0.002

LAYER	ρ(g/cm^3)	D_p (m^2/yr)	K_f(m)	K_r(cm^3/g)
1	2.0	0.01	5.0E-03	0.5
2	2.3	0.02	8.0E-03	0.6978
3	2.6	0.06	2.7E-02	1.158
4	2.65	0.05	1.0E-02	1.059
5	2.7	0.03	3.0E-03	0.741

LAYER	a_1 *	a_2 *	α (m^{-1})	b_1 *
1	1.50E-04	-0.50E-04	0.02	1.00E-05
2	2.00E-04	-0.25E-05	0.02	1.75E-05
3	1.75E-04	-0.20E-05	0.02	1.25E-05
4	2.00E-04	-0.15E-05	0.02	1.05E-05
5	1.50E-04	-0.20E-05	0.02	1.05E-05

* (UA/L^3 = arbitrary units of activity/L^3)

values of the cumulative mass namely, 4.902×10^2, 4.7×10^2 and 4.309×10^2 (Units of Activity/m) at times greater than 10^4 years.

Figures 6a and 6b illustrate the analytically versus numerically computed spatial and temporal variations of sensitivity of the cumulative mass to two typical rock matrix parameters: pore diffusivity and distribution coefficient respectively. These results suggest that for the given range of parameters, pore diffusivity seems to have an overall greater impact on the cumulative mass than the distribution coefficient. In both cases maximum sensitivity seems to be achieved at time close to 2×10^4 years. Note that four observation points coincide with the interface of two successive rock layers and the fifth lies at some 500m downstream from the source. (Figure 4)

The previous example may be used to test the performance of the above-mentioned probabilistic methods. The performance measure is taken as the cumulative mass release at an observation point in the fracture located at a distance 500m downstream from the source (i.e., in the fifth rock layer) and for a simulation time corresponding to 10^4 years. The mean values of the 25 random variables (i.e., b, ϕ, D_p, K_f, and K_r in each layer) are listed in Table 1. All the random variables are assumed to be independent lognormally distributed with coefficient of variations of 0.5. It should be noted, however, that the methodology can apply to correlated and non-normal distributions.

In Figure 7, several CDF solutions are plotted on a standard normal probability plotting paper, where the unit of the vertical axis corresponds to the inverse normal CDF, $\Phi^{-1}(\cdot)$. Initially, a Monte Carlo based reference solution was developed using 5000 simulations. The AMV solution was based on the evaluation of the cumulative mass (response) and its sensitivities at the mean

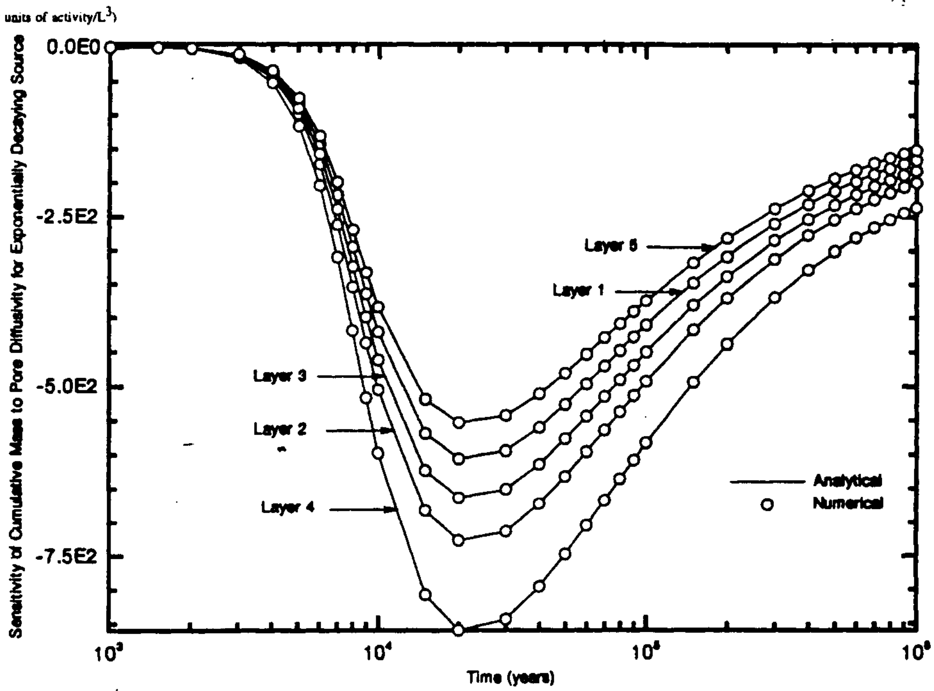

Fig. 6a. Sensitivity of cumulative mass to pore diffusivity vs time for Np-237 (Exponentially decaying source).

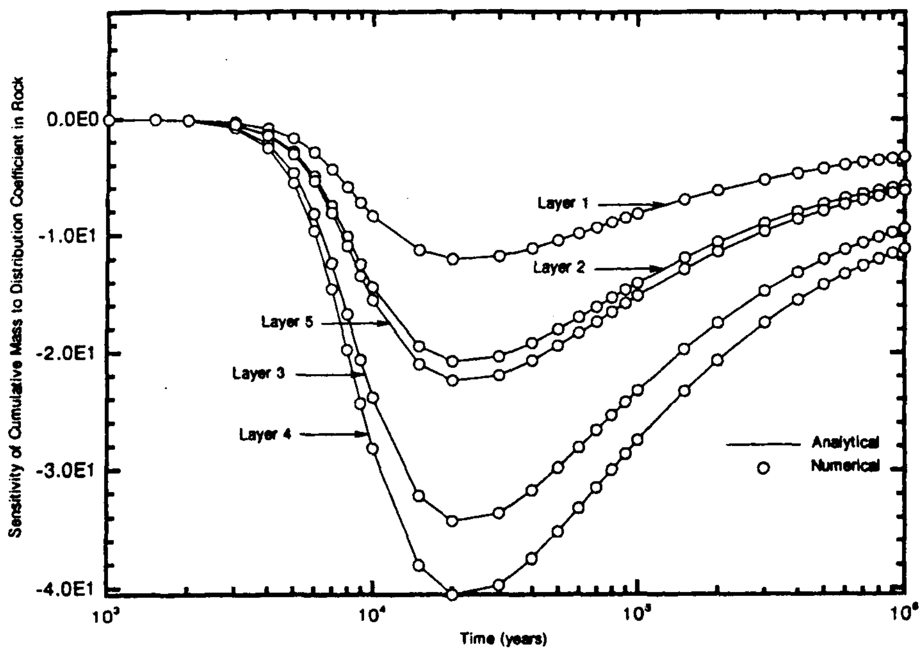

Fig. 6b. Sensitivity of cumulative mass to distribution coefficient in rock vs time for Np-237. (Exponentially decaying source).

value, plus seven response evaluations for seven selected CDF values. Had the sensitivities been calculated through numerical differentiation, a minimum of 33 function evaluations would have been required. The AMV solution produces a CDF whose shape resembles the one obtained through the Monte Carlo method. Subsequently, the converged AMV solution, using the exact MPP, is obtained using three additional iterations. Finally, a quadratic function without product terms was developed. If the sensitivities were calculated by numerical differentiation, a minimum of 129 function evaluations would have been required. The above numbers indicate that the number of function evaluations and the computer time depend on the number of random variables and the way the sensitivities are computed.

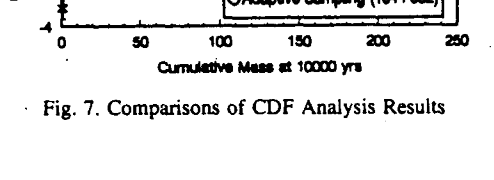

Fig. 7. Comparisons of CDF Analysis Results

Based on the exact MPP, the adaptive sampling scheme is applied to the limit state, M = 223 UA/m. For simplicity, the adaptive surface used has a common curvature at the MPP. Consequently, 532 simulations were needed (after the MPP is found), and the solution agreed very well with the Monte Carlo solution. The required number of simulations could be reduced if separate curvatures are used so that the final sampling region is closer to, but still covers, the target region. Since the efficiency is dominated by the ratio of the target region to the sampling region, the above adaptive sampling method is essentially independent of the probability level or the number of random variables. Thus, the method offers significant advantage for obtaining the CDF tails.

Because the final MPP-based approximate solution ($\Phi(3.08) = 0.99896$) is reasonably good, as confirmed by the adaptive sampling method ($\Phi(3.21) = 0.99934$), it suggests that the MPP-based polynomial function can be used to replace the exact response function. One immediate application is to compute probabilistic sensitivity $dF_M(m)/d\alpha$ based on the polynomial function, rather than the more complicated and time-consuming original function. The probability sensitivity results are not shown here because of space limitations.

Based on the MPPs, the sensitivity factors indicated that at the mean value point, where the corresponding M is 51 UA/m, the six most significant random variables are ϕ_4, D_{p4}, K_{r4}, σ_3,

D_{p3}, K_{r3}, and the importance measures of these six variables are about equal. At M = 223 ŨA/m, the above six variables remain the most dominant ones indicating no significant change in the transport process. In this instance, the sensitivity factors for ϕ_4, D_{p4}, K_{r4} are higher than ϕ_3, D_{p3}, K_{r3}.

CONCLUDING REMARKS

Sensitivity and uncertainty analyses based on a scenario of Np-237 migration through a fractured layered rock have been presented. The solution of the cumulative mass release which is adopted as the performance measure was reported. The results show that probabilistic analysis can be performed effectively by using the advanced mean value method coupled with the adaptive importance sampling method. Since the efficiency of the demonstrated method is independent of the probability levels, the method is particularly useful for problems where the focus is on the tails of the response distribution.

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