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STOCHASTIC ANALYSIS OF CONTAMINANT TRANSPORT:
ONE-DIMENSIONAL NON-REACTIVE AND REACTIVE CASES

by

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ABSTRACT

A reliability approach for probabilistic modeling of one-dimensional non-reactive and reactive transport in porous media provides two important quantitative results: (1) an estimate of the probability that dimensionless concentration equals or exceeds some specified level and, (2) the sensitivity of the probabilistic outcome to likely changes in each uncertain variable. The reliability approach is particularly attractive because it can incorporate various marginal probability density functions (PDF) for any of the uncertain variables. In this work uncertain variables include: groundwater flow velocity, diffusion coefficient, dispersivity, distribution coefficient, porosity and bulk density. The primary objective is to examine how the probabilistic outcome is influenced by choice of marginal PDF, correlation and magnitude of uncertainty for the variables. Because little information exists concerning the statistical characteristics of these uncertain variables, the investigation assumes a wide range of PDF types and statistical values in order to identify and isolate the most critical issues for further study. Results indicate that, even for very slow mean velocity, the probability estimate for non-reactive transport is most sensitive to uncertain flow velocity. For practical analysis, it appears acceptable to treat dispersivity as a deterministic constant. For non-reactive transport, correlation between flow velocity and diffusion coefficient has a slight impact, but correlation among other combinations of uncertain variables is not important. The marginal PDF assigned to diffusion coefficient is not important; however, the marginal PDF assigned to flow velocity can significantly influence the probability estimate. In the case of reactive transport, the probability estimate is again quite sensitive to changes in uncertain flow velocity, but uncertainty associated with porosity, distribution coefficient and bulk density are also important.

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I. INTRODUCTION

The goals and objectives of the current research effort include the development of one- and two-dimensional stochastic analytical models, and development of a two-dimensional stochastic numerical model of advective-dispersive transport in porous media. In the following progress report, the results of the one-dimensional stochastic modeling effort are emphasized. Results from the two-dimensional analytical modeling are currently being evaluated. In addition, the two-dimensional numerical modeling effort is in progress.

The uncertainty associated with analysis of subsurface flow and contaminant transport has led to a great interest in probabilistic (or stochastic) models of these processes. Over the past 15 years or so, many studies have dealt with the uncertainty of porous media material properties, spatial correlation characteristics of these properties, and modeling approaches which incorporate the statistical measures into the analysis. Current emphasis by the public and scientific community on environmental risk indicates that methods of probabilistic analysis for subsurface flow and transport will be even more important in the coming years.

The work presented here uses a method of probabilistic analysis based on a reliability approach to investigate the one-dimensional advection-dispersion equation for contaminant transport in porous media. This work expands upon the developments of Sitar et al. (1987) and Cawfield and Sitar (1988) who used the reliability approach to investigate subsurface flow. The reliability approach is used to estimate the probability of exceeding a specified contaminant concentration, and also

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provides sensitivity measures for each uncertain variable. Further, the method allows designation of any marginal probability density function (PDF) for each uncertain variable. For this work, uncertain parameters (or random variables) include average fluid velocity, dispersivity, diffusion coefficient, distribution coefficient, porosity and bulk density.

The primary objective of this work is to investigate how each of the uncertain parameters influence the probabilistic outcome for some hypothetical examples. Of particular interest is the influence of marginal PDF type and the effect of correlation between variables. Information concerning the actual marginal PDF type and correlation values expected for these uncertain variables is lacking; therefore, this investigation assumes a wide range of PDF type and correlation values in order to identify and isolate the most critical issues for further study. Since the reliability approach provides an approximate measure of probability, results concerning the accuracy of the approximation are also presented. Both diffusive (low flow velocity) and advective (high flow velocity) cases are examined, and non-reactive examples are compared to reactive transport examples.

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II. PREVIOUS WORK

Sitar et al. (1987) give an introduction to the use of reliability methods for the development of stochastic flow and transport models. They use the First Order Reliability Method (FORM) to estimate the probability associated with specified flow events for three different problems: one-dimensional saturated flow in porous media, drawdown in a cut slope, and one-dimensional transport in porous media. The deterministic solution to each of these problems consists of relatively simple analytical forms; therefore, the application of the FORM is fairly straightforward. Sitar et al. (1987) show that the FORM estimates of probability match Monte Carlo simulation results very closely for both one-dimensional flow and drawdown in a cut slope. They did not compare FORM and Monte Carlo results for the one-dimensional transport problem.

Some recent work with the FORM focuses on utilizing numerical solution schemes in combination with the reliability algorithms. Cawfield and Sitar (1988) use the FORM in conjunction with a finite element solution for probabilistic analysis of two-dimensional groundwater flow in porous media. They show a derivation of the reliability sensitivity terms from direct differentiation of the numerical equations.

The reliability approach for estimating probabilities associated with groundwater flow and contaminant transport has certain advantages over other common methods for stochastic analysis, such as Monte Carlo simulation and the so-called small perturbation methods. Monte Carlo simulation provides a probability estimate and is quite flexible with respect to type of solution technique (i.e., analytical or numerical). However, Monte Carlo simulation requires a great deal of computer time and is

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especially inefficient for calculating sensitivity measures. Sources often cited for the Monte Carlo approach include Freeze (1975), Smith and Freeze (1979), Smith and Schwartz (1980) and Clifton and Neuman (1982).

The small perturbation approach encompasses a wide range of specific solution techniques; the reader is referred to such works as Gelhar (1976), Dagan (1982) and Gelhar and Axness (1983). The small perturbation method yields closed form expressions for expected value and covariance associated with a given flow event; however, the technique does not directly provide probability information and is restricted to relatively simple problem geometry and boundary conditions. A recent work by Chrysikopoulos et al. (1990) utilizes the small perturbation approach to evaluate stochastic transport with an uncertain retardation factor. A particular type of small perturbation method known as the First Order Second Moment approach (FOSM) uses a Taylor series approximation at the mean points to estimate second moments of a particular subsurface flow outcome (e.g., Dettinger and Wilson, 1981; Devary and Doctor, 1982; and Townley and Wilson, 1985). A recent work by Jones (1989) compares Monte Carlo moment estimates to FOSM estimates for steady groundwater flow. Many authors have noted the potential for error in using the FOSM method when the uncertainty of the variables is relatively high (e.g., Townley, 1984; and Jones, 1989). More complete comparison and reviews of these stochastic techniques are given elsewhere (e.g., Neuman, 1982; Gelhar, 1986; Dagan, 1986; and Cushman, 1987).

In summary, the reliability approach appears to have several advantages for probabilistic analysis: it provides a probability estimate and sensitivity information, it does so relatively efficiently, and it can be flexibly utilized with existing analytical or

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numerical deterministic solution algorithms. In addition, only second-moment values for each uncertain variable are required, but marginal distributions or bounds may also be incorporated into the solution. The reliability approach is approximate, however, and the accuracy of the approximation is discussed in later sections.

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III. RELIABILITY METHOD

Sitar et al. (1987) and Cawfield and Sitar (1988) provide brief introductions to the FORM as applied in subsurface flow. The reliability method has been used for some time in structural mechanics and discussions of the method and its history are available in a number of sources (e.g., Madsen et al., 1986). For completeness, a brief review of the general approach follows, with special emphasis on the incorporation of marginal distribution information. The nomenclature and derivations presented here generally follow those of Der Kiureghian and his coworkers (e.g., Der Kiureghian and Liu, 1986).

The reliability approach consists of essentially two major concepts: (1) the problem is expressed in terms of a performance criterion (also called a performance function) which is mathematically formulated as a function of the uncertain parameters, and (2) the problem is transformed into the canonical space of standard variates, where an estimate is made of the probability associated with the performance criterion.

The performance criterion may be formulated in general as:

$$Z = g(\mathbf{X}) = g(X_1, X_2, \dots, X_n) \quad (1)$$

where Z is a scalar value of the function, X_i is uncertain parameter i , and n is the number of uncertain parameters. As a convention, the performance criterion is formulated such that the probability of interest corresponds to the probability that $Z = g(\mathbf{X}) \leq 0$. That is, the method evaluates the probability that the performance function takes on values less than or equal to zero. In transport problems, the performance function might typically be formulated to compare a selected target value

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of concentration to the output from a solution algorithm. For example, the probability that $(\frac{C}{C_0}) \geq 0.5$ is estimated using the following performance criterion:

$$Z = g(X) = 0.5 - \frac{C}{C_0} \quad (2)$$

where C and C_0 are the concentration and source concentration, respectively. The uncertain variables might include flow velocity, dispersivity and diffusion coefficient, and they enter $g(X)$ implicitly through $C = f(X)$.

The physical space of the uncertain variables (X) is next transformed to the space of uncorrelated standard variates (Y), each with mean equal to 0 and variance equal to 1.0. The transformation $Y = T(X)$ is a one-to-one mapping which depends on the amount of statistical information available concerning the X uncertain parameters. In this work, second statistical moments and a marginal PDF are assigned to each uncertain variable, although the basic reliability algorithm only requires second moments as a minimum. The uncertain variables (X) are transformed into the space of uncorrelated standard normal variables (Y) as follows:

$$Y = \Gamma_0^{-1} Z \quad (3)$$

where Z is a vector of correlated standard normal variates obtained by $Z_i = \Phi^{-1}[F_{X_i}(x_i)]$. Γ_0 is a lower-triangular matrix resulting from the decomposition of the correlation matrix of the Z variables. $\Phi^{-1}(\cdot)$ is the inverse of the widely tabulated standard normal cumulative distribution function and $F_{X_i}(x_i)$ is the cumulative distribution function (CDF) of uncertain parameter X_i . Equation (3) utilizes the so-called Nataf model (Liu and Der Kiureghian, 1986), which is convenient for problems in which marginal CDF forms are known. The correlation coefficients for the

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Z variables ($\rho_{z,i,j}$) are related to the correlation coefficients for the X variables ($\rho_{i,j}$) through an integral relation given by Liu and Der Kiureghian (1986) as follows:

$$\rho_{i,j} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left[\frac{x_i - \mu_i}{\sigma_i} \right] \left[\frac{x_j - \mu_j}{\sigma_j} \right] \phi_2(z_i, z_j, \rho_{z,i,j}) dz_i dz_j \quad (4)$$

In (4), μ_i and σ_i are the mean and standard deviation of each X_i and $\phi_2(z_i, z_j, \rho_{z,i,j})$ is the bivariate normal density with zero means, unit standard deviations and correlation coefficient $\rho_{z,i,j}$. Liu and Der Kiureghian (1986) provide empirical formulae relating $\rho_{z,i,j}$ to $\rho_{i,j}$.

The probability of interest is given exactly by

$$P[g(X) \leq 0] = \int_{g(X) \leq 0} f_X(x) dx \quad (5)$$

in which $f_X(x)$ is the joint PDF of X. For n uncertain variables, (5) is an n-fold integral over the generally complex region where $g(X) \leq 0$. Further complicating evaluation of (5), the joint PDF of X will seldom be known; therefore, an exact evaluation is virtually impossible.

Because of the difficulty in exactly evaluating (5), reliability methods have arisen which approximate $P[g(X) \leq 0]$. The performance function is transformed to standard space and the limit-state surface is defined as $G(Y) \equiv g(X) = 0$. Next, (5) is approximated by fitting a first- or second-order surface to the limit state surface in standard space at a *design point* (y^*). The design point is also considered the *most likely point* leading to $P[G(Y) \leq 0]$. This definition arises because the probability content in

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the standard normal space will be greatest at the origin (i.e., the mean point $Y = 0$), and the probability will decrease rapidly moving away from the origin in any direction.

Determination of y^* requires solution of a constrained optimization problem where β , which is the distance between the design point and the origin in standard space, is minimized subject to the design point being on the limit-state surface $G(Y) = 0$. Liu and Der Kiureghian (1988) generally recommend the so-called HL-RF optimization algorithm given by:

$$y_{l+1} = y_k + \omega_k d_k \quad (6)$$

$$d_k = \frac{1}{|\nabla G(y_k)|^2} [\nabla G(y_k) y_k - G(y_k)] \nabla G(y_k)^T - y_k \quad (7)$$

$$m(y_{k+1}) = \frac{1}{2} \left| y_{k+1} - \frac{\nabla G(y_{k+1}) y_{k+1}}{|\nabla G(y_{k+1})|^2} \nabla G(y_{k+1}) \right|^2 + \frac{1}{2} c G(y_{k+1})^2 \quad (8)$$

Starting at an initial point (commonly the mean point is used), (6) provides a sequence of trial points in which d_k is a search direction vector, ω_k is a step length and $m(\cdot)$ is a *merit function* with positive constant c . The search direction d_k is determined at the current point k , and the step length is selected in order to provide sufficient decrease in the merit function. The new trial point is then calculated and the entire process repeats until convergence. The $\nabla G(y_k)$ terms are evaluated using the appropriate transformation, the chain rule of differentiation, and values of $\frac{\partial g}{\partial X_i}$ obtained by direct differentiation or finite difference approximation. Although experience indicates this algorithm is quite effective, there is no guarantee that it will converge to the global minimum for β . If necessary, a number of initializing points for the algorithm may be selected to test for the global minimum.

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Once the design point y^* is determined, a first-order approximation of (5) is given by

$$P[g(X) \leq 0] \cong \Phi(-\beta) \quad (9)$$

where $\beta = |y^*|$ and $\Phi(\cdot)$ is the standard normal CDF. The approximation in (9) is first-order exact when a marginal PDF for each X uncertain parameter is available and (3) is used for the transformation.

If the limit-state surface is not extremely non-linear near the design point, (9) will approximate (5) well because most of the probability content in the region where $g(X) \leq 0$ is concentrated near y^* . If the limit-state surface is extremely non-linear near the design point, second-order approximations may be needed (e.g., Madsen et al., 1986; and Der Kiureghian et al., 1987). The second-order reliability method (SORM) consists of approximating the limit-state surface in standard space with a paraboloid tangent at the design point. Breitung (1984) gives a second-order formulation and Der Kiureghian et al. (1987) discuss methods for fitting the second-order surface. Der Kiureghian et al. (1987) indicate that roughly $8n$ additional computations of $g(X)$ are necessary for SORM, where n is the number of uncertain variables in the problem.

Sensitivity measures play an important role in the reliability approach, and these measures result directly from intermediate calculations. The most elementary measure is the sensitivity of β to changes in the individual uncertain parameters. In standard space,

$$\alpha = \frac{y^*}{|y^*|} = \nabla_y \beta \quad (10)$$

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In words, α is a vector of gradients of β with respect to components of the vector y^* .

A sensitivity measure in the space of the original uncertain parameters (X) is perhaps more meaningful. Der Kiureghian and Liu (1985) provide a measure scaled by the standard deviation of the X variable as follows:

$$\gamma = \frac{(\nabla_x \cdot \beta)D}{|(\nabla_x \cdot \beta)D|} \quad (11)$$

The γ vector provides a measure of the sensitivity of β to *equally likely changes* in the uncertain parameters (X). Other sensitivity measures are available. Madsen et al. (1986) give formulations for calculating sensitivity with respect to deterministic parameters in the performance criterion, and with respect to distribution parameters for the uncertain variables.

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IV. DISCUSSION OF RESULTS

The primary objective of the one-dimensional modeling effort is to examine a number of possible influences on the probability estimate for one-dimensional advective-dispersive transport. The goal is to determine the relative importance of the marginal PDF form selected for each of the uncertain variables, as well as the influence of the magnitude of the variance and correlation for those variables. The FORM algorithm is used in conjunction with the solution for one-dimensional flow given by Javendal et al. (1984). The governing equation for steady state uniform flow is given as follows:

$$D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} - \lambda R C = R \frac{\partial C}{\partial t} \quad (12)$$

Boundary condition: $C(0,t) = C_0$

Initial condition: $C(x,0) = 0$

D : Dispersion coefficient

C : Concentration of the contaminant

v : Average flow velocity

λ : Radioactive decay reaction

R : Retardation factor = $1 + \frac{\rho_b K_d}{\eta}$

ρ_b : Bulk mass density

K_d : Distribution coefficient

η : Porosity

x : Distance from source

t : Time.

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Radioactive decay is not considered for this work ($\lambda = 0$). The solution given by Javendal et al. (1984) follows:

$$\frac{C}{C_0} = A(x, t) ; 0 < t \leq t_0 \quad (13)$$

$$\frac{C}{C_0} = A(x, t) - A(x, t - t_0) ; t_0 < t \quad (14)$$

$$A(x, t) = \frac{1}{2} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \left[\frac{v^2 t}{\pi DR}\right]^{1/2} \exp\left[-\frac{(Rx - vt)^2}{4DRt}\right] - \frac{1}{2} \left[1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right] \exp\left[\frac{vx}{D}\right] \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right] \quad (15)$$

$$D = D^* + \alpha v \quad (16)$$

where v is the average flow velocity, D^* is the diffusion coefficient, and α is the dispersivity. In (13) and (14), t is the total elapsed time and t_0 is the total time the contaminant source is active.

Any of the parameters appearing in the solution may be treated as uncertain variables. Very little experimental work has been devoted to determining the statistical characteristics of these uncertain variables. Most statistical work in flow and transport has concentrated on the hydraulic conductivity spatial variation (e.g., Freeze, 1975; Smith, 1981; Hoeksma and Kitanidis, 1985; and Sudicky, 1986). This emphasis is logical, because the hydraulic conductivity variability is a direct influence on the variability of flow velocity. However, the uncertainty of the other variables may be significant in some situations. It is possible that the uncertainty of some variables may

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have little impact on the probability estimate, and the analysis may be simplified by treating such variables as deterministic constants.

Four hypothetical cases are examined to determine the relative importance of various uncertain parameters and their statistical characteristics under different conditions of flow. Both low flow velocity (the so-called diffusion controlled case) and high flow velocity (the so-called advection controlled case) are considered. Within these two categories three uncertain parameters are first examined: flow velocity, diffusion coefficient and dispersivity. Finally, the uncertainty of the individual variables which constitute retardation (R) are included; these three variables are the distribution coefficient, bulk density and porosity. Due to lack of information concerning the statistical characteristics of the uncertain variables, the approach here is to assume a wide range of PDF types and correlation values in order to identify and isolate the most critical issues for further study. Results from probabilistic modeling of these hypothetical examples are summarized in the following four sections.

1. Non-Reactive Diffusive Transport With Uncertain Flow Velocity, Diffusion Coefficient and Dispersivity.

Low velocity (diffusive) processes are important in evaluating the integrity of low permeability barriers such as waste disposal liner systems and low permeability layers in natural deposits. In this example, a constant concentration source (C_0) releases contaminants over some finite time period (t_0) into a one-dimensional uniform flow system with mean average flow of μ_v . The contaminant is non-reactive ($R=1$) with mean diffusion coefficient of μ_D . The porous medium exhibits mean dispersivity of μ_α .

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Consider a 1 meter thick low permeability barrier with a contaminant source on one side and uniform (but uncertain) average flow through the barrier. After $t = 30$ years of constant source concentration, evaluate the probability that $\frac{C}{C_0} \geq 0.5$ on the other side of the barrier ($x = 1.0$ m). The performance criterion given in (2) is used for this estimation. Such an evaluation may be part of the engineering risk analysis for the closure and post-closure plan at a waste management facility.

The results of Perkins and Johnston (1963) are used to select typical mean values for the uncertain parameters which will correspond to a diffusion controlled flow regime under average conditions. The mean values selected are as follows:

$$\mu_v = 8.64 \times 10^{-5} m/d$$

$$\mu_{D^*} = 6.11 \times 10^{-5} m^2/d$$

$$\mu_\alpha = 3.5 \times 10^{-4} m$$

As a starting point, the uncertain parameters are assumed to be statistically independent with standard deviations equal to 10% of their mean value. Three different marginal PDF types are assigned to the uncertain parameters in various combinations; the three PDF types are normal (Gaussian), lognormal, and uniform. These are common PDF types and they represent a broad range from symmetric and peaked (normal) to skewed (lognormal) to flat (uniform).

All possible combinations of the three PDF types were examined; however, the PDF chosen for dispersivity had no effect on the outcome. Therefore, the results in Table 1 assume dispersivity is lognormally distributed. Table 1 primarily demonstrates the

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influence of the PDF choice for flow velocity and diffusion coefficient. The results indicate that the probability estimate is not extremely sensitive to type of PDF chosen for diffusion coefficient. The type of PDF chosen for flow velocity is more important to the probability estimate, although choice between normal or lognormal only changes the estimate by about 20%. Choice of a uniform PDF for flow velocity has a dramatic effect on the probability estimate. The uniform PDF is commonly used when very little information is available; it indicates that all values of an uncertain variable are equally likely between a lower and upper bound. Because values much higher and much lower than the mean velocity are equally likely, the probability that $\frac{C}{C_0} \geq 0.5$ is much lower for a uniformly distributed flow velocity. In practical and physical terms, there is really no strong reason to favor any of these three PDF types. A normal PDF might be justified based on the central limit theorem and the effect of a large number of individual factors. The lognormal is commonly used to characterize hydraulic conductivity, and perhaps it is reasonable to expect that the flow velocity would exhibit some of the skewness in distribution which hydraulic conductivity often shows.

Table 1 also provides values for the sensitivity measure γ . The magnitude of this sensitivity measure indicates the relative importance of each of the uncertain variables to the probabilistic outcome. The probabilistic solution is most sensitive to likely changes in the average flow velocity -- even though this example is a "diffusion controlled" problem in a deterministic sense (e.g., Perkins and Johnston, 1963). The probabilistic outcome is less sensitive to likely changes in the diffusion coefficient, and the outcome is not at all sensitive to the uncertain dispersivity. Therefore, dispersivity may be treated for practical purposes as a deterministic constant. The implication of the sensitivity measures to practical modeling of this problem follows: concentrate on

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reducing the uncertainty of the average flow velocity and, to a lesser degree, the diffusion coefficient. The uncertainty of the dispersivity is not important to the probabilistic outcome.

The results in Table 1 and conclusions just discussed are strictly valid only for the particular problem under consideration. Changing the target value in the performance function or the statistical moments of the uncertain variables will influence the probability estimate and the sensitivity measures. However, for one-dimensional non-reactive transport, the general conclusions as outlined above hold over a wide range of statistical input and problem formulation. As shown in Table 2, even assuming a wide range of correlation between the uncertain variables had little effect on the general conclusions. It may be argued that all three uncertain variables should be correlated in some way, due to their dependence on porous media material characteristics. However, little statistical information exists concerning field determined correlation between these variables. For this work, a wide range of values is examined to determine which correlation measures are critical to the probability estimate. In order to isolate the influence of correlation, results in Table 2 assume all uncertain variables have lognormal marginal PDF. Table 2 shows that the probability estimate is only influenced by correlation between flow velocity and diffusion coefficient, and changing that correlation from 0 to 0.75 causes the probability estimate to vary only from about 0.026 to 0.041. These results indicate that, for this one-dimensional non-reactive example, correlation between the three uncertain variables is not extremely important to the probabilistic outcome; therefore, the effort required to carry out actual field analysis of correlation for these variables may be unwarranted. At the very least, data analysis need only concentrate on correlation between flow velocity and diffusion coefficient.

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Table 3 illustrates the influence of increasing the uncertainty of the variables so that the standard deviation equals the means. Of course the probability estimate changes (it increase dramatically), but the general conclusions still hold -- the outcome is most sensitive to the uncertain flow velocity. Note that the probability estimate for this high uncertainty case is not as sensitive to the assumption of uniform PDF for flow velocity as in the previous case. Because of the higher uncertainty, all of the PDF forms have become much flatter and more dispersed about the mean values, so the uniform and normal PDF are more alike. However, the lognormal PDF becomes more skewed as the variance increases; therefore, the probability estimate is about 30 to 40% lower for lognormal flow velocity.

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Table 1. Influence Of PDF Type On Probability Estimate or Non-Reactive Diffusive Transport With $\sigma_{x_i} = .10 \mu_{x_i}$

Uncertain Variable			Probability Estimate	Sensitivity Measure		
V	D*	α	$P[C/C_0 > 0.5]$	γ_v	γ_{D^*}	γ_α
N	N	L	0.03320	0.9883	0.1525	0.0001
N	L	L	0.03370	0.9891	0.1475	0.0001
N	U	L	0.03450	0.9805	0.1965	0.0001
L	N	L	0.04073	0.9916	0.1297	0.0001
L	L	L	0.04125	0.9920	0.1261	0.0001
L	U	L	0.04183	0.9853	0.1711	0.0001
U	N	L	0.00820	0.8064	0.5914	0.0003
U	L	L	0.00750	0.8174	0.5761	0.0004
U	U	L	0.00980	0.8623	0.5063	0.0004

Probability Density Function (PDF) :

N = Normal, L = Lognormal, U = Uniform

Uncorrelated Uncertain Variables.

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Table 2. Influence Of Correlation Between Uncertain Variables For Non-Reactive Diffusive Transport, Random Variables Are Lognormally Distributed With $\sigma_{x_i} = .10 \mu_{x_i}$

Correlation Coefficient			Probability Estimate	Sensitivity Measure		
$\rho_{v\alpha}$	$\rho_{\alpha D}$	ρ_{vD}	$P[C/C_0 > 0.5]$	γ_v	$\gamma_{D'}$	γ_{α}
0.00	0.00	0.00	0.04125	0.9920	0.1261	0.0001
0.25	0.00	0.00	0.04124	0.9920	0.1261	0.0001
0.50	0.00	0.00	0.04124	0.9920	0.1261	0.0001
0.75	0.00	0.00	0.04124	0.9920	0.1261	0.0001
0.00	0.25	0.00	0.04125	0.9920	0.1261	0.0001
0.00	0.50	0.00	0.04125	0.9920	0.1261	0.0001
0.00	0.75	0.00	0.04125	0.9920	0.1261	0.0001
0.00	0.00	0.25	0.03636	0.9914	0.1305	0.0001
0.00	0.00	0.50	0.03124	0.9908	0.1357	0.0001
0.00	0.00	0.75	0.02609	0.9899	0.1418	0.0001
0.25	0.25	0.00	0.04124	0.9920	0.1261	0.0001
0.50	0.50	0.00	0.04124	0.9920	0.1261	0.0001
0.75	0.75	0.00	0.04170	0.9921	0.1253	0.0001
0.00	0.25	0.25	0.03636	0.9914	0.1305	0.0001
0.00	0.50	0.50	0.03124	0.9908	0.1357	0.0001
0.00	0.75	0.75	0.02630	0.9900	0.1413	0.0001
0.25	0.00	0.25	0.03635	0.9914	0.1305	0.0001
0.50	0.00	0.50	0.03123	0.9908	0.1357	0.0001
0.75	0.00	0.75	0.02664	0.9901	0.1405	0.0001
0.25	0.25	0.25	0.03635	0.9914	0.1305	0.0001
0.50	0.50	0.50	0.03123	0.9908	0.1357	0.0001
0.75	0.75	0.75	0.02608	0.9899	0.1418	0.0001

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Table 3. Influence Of PDF Type On Probability Estimate For Non-Reactive Diffusive Transport With $\sigma_{x_i} = \mu_{x_i}$

Uncertain Variable			Probability Estimate	Sensitivity Measure		
V	D'	α	$P[C/C_0 > 0.5]$	γ_v	$\gamma_{D'}$	γ_α
N	N	L	0.4272	0.9883	0.1525	0.0001
N	L	L	0.4444	0.9960	0.0897	0.0001
N	U	L	0.4279	0.9780	0.2087	0.0001
L	N	L	0.2700	0.9876	0.1567	0.0001
L	L	L	0.2839	0.9958	0.0916	0.0001
L	U	L	0.2722	0.9766	0.2153	0.0001
U	N	L	0.4467	0.9937	0.1119	0.0000
U	L	L	0.4596	0.9978	0.0657	0.0000
U	U	L	0.4470	0.9881	0.1538	0.0000

Probability Density Function (PDF) :

N = Normal, L = Lognormal, U = Uniform

Uncorrelated Uncertain Variables.

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2. Non-Reactive Advective Transport With Uncertain Flow Velocity, Diffusion Coefficient and Dispersivity.

Advective transport tends to be dominant in relatively coarse grained porous media such as alluvial aquifers containing sands and gravels. These types of porous media are typical of the most productive and important groundwater reservoirs used for residential and industrial supplies. A probabilistic evaluation of advective transport might be required for risk analysis related to siting of a waste management facility above a sand or gravel aquifer. The risk analysis may require the assumption that contaminants will reach the sand or gravel aquifer beneath the facility. Given a certain source concentration and the assumption of one-dimensional transport in uniform flow of uncertain magnitude, a model can be developed to estimate the probability of exceeding a selected concentration at some time and location (perhaps a nearby municipal well).

The example used here assumes the following arbitrarily selected mean values for a hypothetical high velocity flow regime:

$$\mu_v = 8.64 \times 10^{-1} m/d$$

$$\mu_{D^*} = 6.11 \times 10^{-5} m^2/d$$

$$\mu_\alpha = 1.75m$$

with $t = 4$ yr. and $x = 1300$ m. The performance function is again formulated as in (2), and the uncertain variables are assumed to be uncorrelated with standard deviations equal to 10% of the mean values.

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Table 4 shows results for various combinations of PDF forms. As might be expected the probabilistic outcome for the high velocity regime is completely dominated by likely changes in the uncertain flow velocity. The probabilistic outcome is not at all sensitive to likely changes in either diffusion coefficient or dispersivity. Therefore, for practical analysis, both diffusion coefficient and dispersivity may be treated as constant deterministic parameters. Table 4 indicates that the particular form of the PDF chosen to represent the uncertain variables does not appear to be a critical consideration, at least for this particular example.

Table 5 indicates that, even when the uncertainty of the variables is increased such that each standard deviation equals the mean value, the probabilistic outcome is not very sensitive to PDF form. However, choice of lognormal PDF for flow velocity in this high standard deviation case does decrease the probability estimate relative to choice of uniform or normal PDF. This is consistent with the results and discussion related to Table 3. Although no results are shown here, correlation between variables for this advective case had very little effect on the probabilistic outcome. Correlation is not significant because the probabilistic solution is completely dominated by the uncertainty of the flow velocity.

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Table 4. Influence Of PDF Type On Probability Estimate For Non-Reactive Advective Transport With $\sigma_{x_i} = .10 \mu_{x_i}$

Uncertain Variable			Probability Estimate	Sensitivity Measure		
V	D'	α	$P[C/C_0 > 0.5]$	γ_v	$\gamma_{D'}$	γ_α
N	N	L	0.3826	1.0000	0.0000	0.0000
N	L	L	0.3826	1.0000	0.0000	0.0000
N	U	L	0.3826	1.0000	0.0000	0.0000
L	N	L	0.3651	1.0000	0.0000	0.0000
L	L	L	0.3651	1.0000	0.0000	0.0000
L	U	L	0.3651	1.0000	0.0000	0.0000
U	N	L	0.4138	1.0000	0.0000	0.0000
U	L	L	0.4138	1.0000	0.0000	0.0000
U	U	L	0.4138	1.0000	0.0000	0.0000

Probability Density Function (PDF) :

N = Normal, L = Lognormal, U = Uniform

Uncorrelated Uncertain Variables.

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Table 5. Influence Of PDF Type On Probability Estimate For Non-Reactive Advective Transport With $\sigma_{x_i} = \mu_{x_i}$

Uncertain Variable			Probability Estimate	Sensitivity Measure		
V	D*	α	$P[C/C_0 > 0.5]$	γ_v	γ_{D^*}	γ_α
N	N	L	0.4881	1.0000	0.0000	0.0000
N	L	L	0.4881	1.0000	0.0000	0.0000
N	U	L	0.4881	1.0000	0.0000	0.0000
L	N	L	0.3258	1.0000	0.0000	0.0000
L	L	L	0.3258	1.0000	0.0000	0.0000
L	U	L	0.3258	1.0000	0.0000	0.0000
U	N	L	0.4914	1.0000	0.0000	0.0000
U	L	L	0.4914	1.0000	0.0000	0.0000
U	U	L	0.4914	1.0000	0.0000	0.0000

Probability Density Function (PDF) :

N = Normal, L = Lognormal, U = Uniform

Uncorrelated Uncertain Variables.

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3. Diffusive Transport Including Uncertain Retardation Factor.

It is now of interest to expand the breadth of the one-dimensional transport problem to include three additional uncertain variables: distribution coefficient (K_d), porosity (η) and bulk density (ρ_b). These variables make up the term known as the retardation factor (R), which is used to model adsorption/desorption. The mean values selected for the three additional uncertain variables are as follows:

$$\mu_{K_d} = 2.29 \text{ cm}^3/\text{g}$$

$$\mu_{\eta} = 0.50$$

$$\mu_{\rho_b} = 1.37 \text{ g/cm}^3.$$

These mean values were arbitrarily selected as typical for results from column experiments reported by Cameron and Klute (1977) and Travis (1978) for some selected contaminants.

Because adsorption is included, down gradient concentrations are much lower than in the non-reactive case, and the performance criterion of (2) gives trivial results (i.e., the probability estimate is 0.0). Therefore a new performance criterion is used as follows:

$$Z = g(\mathbf{X}) = 0.05 - \frac{C}{C_0}. \quad (17)$$

The target value of 0.05 is selected to provide an example with very low probability, as a contrast to the previous examples which yielded relatively high estimates of

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probability. The mean values for v , D^* and α are the same as given in the low flow velocity case discussed earlier. The uncertain parameters are first assumed to be uncorrelated with standard deviation equal to 10% of their mean value.

Table 6 shows the sensitivity measures for the six uncertain variables, and illustrates the effect of PDF form on the results. Bulk density and distribution coefficient are the most significant uncertain variables for this example. Porosity and flow velocity exhibit somewhat lower sensitivity measures, as does the diffusion coefficient. As in previous cases, dispersivity can effectively be treated as a deterministic constant because it has little influence on the probabilistic outcome.

The effect of PDF type chosen to represent the uncertain variables does not follow a clear pattern as in the previous cases, because five of the six uncertain variables are relatively important to the outcome. In addition, it may be expected that PDF type will be more critical when evaluating relatively low probability events, versus relatively higher probability events. An estimate of low probability is much more sensitive to slight differences in the PDF forms, especially the extremes (tails) of the distributions.

Table 7 provides results for four levels of correlation between all six of the uncertain variables; that is, each variable correlated with all others with correlation of 0.0, 0.25, 0.50 and 0.75. All variables are assumed to be lognormally distributed. As is evident from the results of Table 7, correlation between the variables is much more important to the probabilistic outcome for this case than for the non-reactive cases considered previously. This is a result of the relative importance of five of the six uncertain variables; therefore, correlation between these variables is also important.

Table 6. Influence Of PDF Type On Probability Estimate For Reactive Diffusive Transport With $\sigma_{x_i} = .10$ μ_{x_i}

Uncertain Variable			Probability Estimate		Sensitivity Measure							
V	D*	α	ρ	η	K_d	$P[C/C_0 > 0.05]$	γ_v	γ_{D^*}	γ_a	γ_e	γ_η	γ_{K_d}
N	N	L	N	N	N	7.444E-5	0.3174	0.2219	0.0001	0.5883	0.3971	0.5883
N	L	L	N	N	N	7.325E-5	0.3162	0.2392	0.0001	0.5857	0.3959	0.5857
N	U	L	N	N	N	8.840E-5	0.3183	0.2168	0.0001	0.5885	0.3988	0.5885
L	N	L	N	N	N	7.663E-5	0.3504	0.2197	0.0001	0.5804	0.3940	0.5804
L	L	L	N	N	N	7.536E-5	0.3491	0.2366	0.0001	0.5779	0.3927	0.5779
L	U	L	N	N	N	9.085E-5	0.3511	0.2156	0.0001	0.5804	0.3956	0.5804
U	N	L	N	N	N	9.123E-5	0.2687	0.2253	0.0001	0.5977	0.4032	0.5977
U	L	L	N	N	N	8.981E-5	0.2680	0.2428	0.0001	0.5949	0.4018	0.5949
U	U	L	N	N	N	1.093E-4	0.2706	0.2201	0.0001	0.5976	0.4049	0.5976
N	N	N	N	N	N	7.445E-5	0.3174	0.2219	0.0001	0.5883	0.3971	0.5883
N	L	N	N	N	N	5.010E-5	0.3341	0.2342	0.0001	0.6504	0.4183	0.4854
N	U	N	N	N	N	5.580E-5	0.3517	0.2468	0.0001	0.7097	0.4404	0.3432
N	L	N	N	L	N	8.300E-5	0.3126	0.2184	0.0001	0.5719	0.4478	0.5719
N	L	N	N	L	U	5.849E-5	0.3277	0.2294	0.0001	0.6250	0.4740	0.4740
N	L	N	N	L	U	6.806E-5	0.3440	0.2412	0.0001	0.6750	0.5006	0.3423
N	U	N	N	U	N	8.752E-5	0.3266	0.2285	0.0001	0.6122	0.3024	0.6122
N	U	N	N	U	L	2.552E-4	0.3466	0.2576	0.0001	0.6702	0.3031	0.5219
N	U	N	N	U	U	6.083E-5	0.3656	0.2568	0.0001	0.7608	0.3148	0.3500

Probability Density Function (PDF) :

N = Normal, L = Lognormal, U = Uniform

Uncorrelated Uncertain Variables.

Probability Density Function (PDF) :

N = Normal, L = Lognormal, U = Uniform

Uncorrelated Uncertain Variables.

Table 7. Influence Of Correlation Between Uncertain Variables For Reactive Diffusive Transport, Random Variables Are Lognormally Distributed With $\sigma_{x_i} = .10$ μ_{x_i}

Correlation Coefficient	Probability Estimate	Sensitivity Measure						
		$P[C/C_0 > 0.05]$	γ_v	γ_{D^*}	γ_a	γ_p	γ_n	γ_{K_d}
0.00	3.740E-5	0.3919	0.2656	0.0001	0.5085	0.5085	0.5085	0.5085
0.25	2.563E-6	0.3904	0.2646	0.0001	0.5091	0.5091	0.5091	0.5091
0.50	1.424E-8	0.3876	0.2627	0.0001	0.5101	0.5101	0.5101	0.5101
0.75	5.773E-15	0.3812	0.2582	0.0002	0.5125	0.5125	0.5125	0.5125

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4. Advective Transport Including Uncertain Retardation Factor.

As a final hypothetical example, consider high flow velocity (advective) transport, including uncertain bulk density, distribution coefficient and porosity. The same mean values for average flow velocity, diffusion coefficient and dispersivity are used as in the high velocity case discussed previously. The mean values for distribution coefficient, porosity and bulk density are the same as those used in the previous section which considered diffusive transport and uncertain retardation.

Table 8 shows typical results when the performance criterion of (17) is used and uncorrelated uncertain variables with standard deviations equal to 10% of their mean values are assumed. The probabilistic outcome is most sensitive to likely changes in the uncertain flow velocity. Porosity, distribution coefficient and bulk density are also relatively important. The sensitivity measures indicate that the dispersivity and diffusion coefficient can be treated as deterministic constants for this probabilistic analysis. It is interesting to note that, for this case of relatively high flow velocity, the dispersivity is actually more important to the probabilistic outcome than is the diffusion coefficient. Also, the choice of PDF type for the uncertain variables does not seem to be a critical issue for this case. This is primarily due to the relatively high value of the probability for this event; therefore, differences between the distributions are not as critical.

Table 8. Influence Of PDF Type On Probability Estimate For Reactive Advective Transport With $\sigma_{x_i} = .10$ μ_{x_i}

Sensitivity Measure												
Uncertain Variable		Probability Estimate		Sensitivity Measure								
V	D*	α	ρ	η	K_d	$P[C/C_0 > 0.05]$	γ_v	γ_{D^*}	γ_a	γ_p	γ_η	γ_{K_d}
N	N	L	N	N	N	0.4909	0.5555	0.0000	0.0378	0.4799	0.4789	0.4799
N	L	L	N	N	N	0.4909	0.5555	0.0000	0.0378	0.4799	0.4789	0.4799
N	U	L	N	N	N	0.4909	0.5555	0.0000	0.0378	0.4799	0.4789	0.4799
N	N	L	N	N	N	0.4799	0.5550	0.0000	0.0378	0.4805	0.4782	0.4805
L	N	L	N	N	N	0.4799	0.5550	0.0000	0.0378	0.4805	0.4782	0.4805
L	L	L	N	N	N	0.4799	0.5550	0.0000	0.0378	0.4805	0.4782	0.4805
L	U	L	N	N	N	0.4920	0.6780	0.0000	0.0334	0.4242	0.4234	0.4242
U	N	L	N	N	N	0.4920	0.6780	0.0000	0.0334	0.4242	0.4234	0.4242
U	L	L	N	N	N	0.4920	0.6780	0.0000	0.0334	0.4242	0.4234	0.4242
N	N	N	N	N	N	0.4917	0.5555	0.0000	0.0380	0.4799	0.4789	0.4799
N	L	N	N	N	N	0.4988	0.5565	0.0000	0.0380	0.4795	0.4796	0.4784
N	U	N	N	N	N	0.4924	0.5051	0.0000	0.0345	0.4362	0.4354	0.6032
N	N	L	N	N	N	0.4822	0.5548	0.0000	0.0380	0.4806	0.4784	0.4806
N	L	L	N	N	N	0.4917	0.5561	0.0000	0.0380	0.4804	0.4788	0.4788
N	L	L	N	N	N	0.4838	0.5044	0.0000	0.0345	0.4365	0.4347	0.6041
N	U	L	N	N	N	0.4924	0.5055	0.0000	0.0345	0.4365	0.6018	0.4365
N	N	U	N	N	N	0.4989	0.5060	0.0000	0.0345	0.4360	0.6028	0.4350
N	U	U	N	N	N	0.4930	0.4666	0.0000	0.0319	0.4028	0.5556	0.5571

Probability Density Function (PDF) :

N = Normal, L = Lognormal, U = Uniform

Uncorrelated Uncertain Variables.

Probability Density Function (PDF) :

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Uncorrelated Uncertain Variables.

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5. Accuracy of the Reliability Approximation.

In general, the FORM results for the one-dimensional examples just presented agree very closely with SORM and Monte Carlo results evaluated using the CALREL program of Liu et al. (1989). Table 9 shows typical results comparing the three methods for non-reactive, diffusive transport. The results are all within a few percent of each other, except when flow velocity is assigned a uniform PDF. Since flow velocity dominates the non-reactive transport probabilistic solution, a uniformly distributed flow velocity is carried through the transformation and creates a standard space within which probability content is spread out rather broadly from the origin. Therefore, even minor differences between the first-order approximation and the limit state surface results in a fairly inaccurate approximation of the probability measure. The difference is especially critical for relatively low probability events. Note that the SORM estimate is much closer to the Monte Carlo result than the FORM, because the second-order approximation reflects more of the true limit state surface at some distance away from y^* .

Table 10 shows results for non-reactive advective transport, where the FORM, SORM and Monte Carlo results are nearly identical for all PDF combinations. Due to the relatively high magnitude of the probability estimate in this case, minor differences between the first-order surface and the true limit state surface are not as significant.

Even for rather small probabilistic problems such as these (only three uncertain parameters), the computational efficiency of the reliability methods versus Monte Carlo simulation is noticeable. A microcomputer may take a few minutes to finish a

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Monte Carlo simulation, while FORM or SORM may take only a few seconds. Exact difference in time depends on the number of realizations used for the Monte Carlo simulation. Although the computation time difference between FORM and SORM is negligible for these examples, recall that SORM requires about $8n$ more computations than FORM.

These conclusions regarding the accuracy of the FORM approximation are strictly valid only for the one-dimensional analysis, and do not imply that FORM will always provide probability estimates with accuracy comparable to SORM and Monte Carlo simulation. There is evidence that SORM or Monte Carlo simulation is required for accuracy when numerical solutions of the transport problem are used, and the variability of the uncertain parameters becomes extremely large (N. Sitar, personal communication, 1990). The question of accuracy of FORM, SORM and Monte Carlo simulation for numerical solutions of transport in porous media is the subject of ongoing research.

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Table 9. Comparison Of Probability Estimate Between First-Order, Second-Order, And Monte Carlo Analyses, For Non-Reactive Diffusive Transport.

Uncertain Variable			Probability Estimate $p[C/C_0 > 0.5]$		
V	D*	α	First-Order	Second-Order	Monte Carlo
N	N	L	0.03296	0.03300	0.03320
N	L	L	0.03346	0.03297	0.03310
N	U	L	0.03427	0.03321	0.03270
L	N	L	0.04040	0.04053	0.04010
L	L	L	0.04091	0.04039	0.03990
L	U	L	0.04152	0.04066	0.03970
U	N	L	0.008108	0.005160	0.004900
U	L	L	0.007404	0.004075	0.003700
U	U	L	0.01110	0.005926	0.004500
<p>Probability Density Function (PDF) :</p> <p>N= Normal, L= Lognormal, U= Uniform</p> <p>Uncorrelated Uncertain Variables, with $\sigma_{x_i} = .10 \mu_{x_i}$</p>					

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Table 10. Comparison Of Probability Estimate Between First-Order, Second-Order, And Monte Carlo Analyses, For Non-Reactive Advective Transport.

Uncertain Variable			Probability Estimate $p[C/C_0 > 0.5]$		
V	D'	α	First-Order	Second-Order	Monte Carlo
N	N	L	0.3826	0.3826	0.3823
N	L	L	0.3826	0.3826	0.3823
N	U	L	0.3826	0.3826	0.3823
L	N	L	0.3651	0.3651	0.3650
L	L	L	0.3651	0.3651	0.3650
L	U	L	0.3651	0.3651	0.3650
U	N	L	0.4138	0.4138	0.4112
U	L	L	0.4138	0.4138	0.4112
U	U	I	0.4138	0.4138	0.4112

Probability Density Function (PDF) :

N = Normal, L = Lognormal, U = Uniform

Uncorrelated Uncertain Variables, with $\sigma_{x_i} = .10 \mu_{x_i}$

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V. PROGRESS ON TWO-DIMENSIONAL AND NUMERICAL STOCHASTIC MODELS

The reliability approach has been used to develop a two-dimensional stochastic analytical model of transport in porous media. A deterministic analytical solution for two-dimensional transport in porous media with unidirectional steady state flow is given by Javendal et al. (1984). This solution is combined with the reliability algorithm to form a stochastic model with the following uncertain variables: flow velocity, longitudinal dispersivity, lateral dispersivity and diffusion coefficient. The objective is to examine the relative importance of these uncertain variables to the probabilistic outcome; methodology follows a similar approach to the one-dimensional results mentioned in the preceding section.

We are still examining some of the hypothetical examples for combinations of PDF, correlation and variance for each of the uncertain variables. At this time general conclusions are incomplete. Our intent is to focus on the relative importance of the two dispersivity parameters (longitudinal and lateral). Preliminary results indicate that the probabilistic outcome is not too sensitive to variation in the lateral dispersivity. This is consistent with the one-dimensional results which indicate the probabilistic outcome is not too sensitive to likely variations in uncertain dispersivity.

Progress on the development of a two-dimensional finite element numerical stochastic model continues on schedule. At this time, a working version of the model is nearly complete. The stochastic numerical model is being developed by combining an existing two-dimensional finite element model of transport called SUTRA with a reliability algorithm. The resulting stochastic finite element model will include the

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following uncertain variables: element hydraulic conductivity, porosity, dispersivity and diffusion coefficient. The experimental methodology for examining the numerical stochastic model parallels the methodology utilized for the one- and two-dimensional analytical stochastic studies previously described. Of primary concern is the relative importance of the marginal PDF, variance, and correlation for the uncertain variables. We anticipate that results will indicate one or more of the uncertain variables may be effectively treated as deterministic parameters for the probabilistic analysis. Such results will allow great efficiency in carrying out field sampling programs, as well as efficiency in the probabilistic analysis.

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VI. CONCLUSIONS

The reliability approach is an attractive tool for probabilistic analysis of one-dimensional transport in porous media. Results from a first-order reliability transport model include an estimate that the concentration at a specified time and location in the flow region exceeds a target concentration selected by the analyst. In addition, sensitivity measures are evaluated which indicate the relative importance of each uncertain variable in the problem. Uncertain variables in the one-dimensional non-reactive model include flow velocity, diffusion coefficient and dispersivity. For the reactive model, uncertain variables include the previous three plus porosity, distribution coefficient and bulk density. Each uncertain variable is assigned a mean value, variance and a marginal PDF form. Correlation between the variables may also be included.

The primary objective of this work is to investigate the relative importance of the marginal PDF type, correlation and magnitude of uncertainty for the uncertain variables. Major conclusions are as follows:

(1) For one-dimensional non-reactive transport with relatively low flow velocities, the probabilistic outcome is most sensitive to likely changes in the uncertain flow velocity. The PDF selected for flow velocity is also important. The probabilistic outcome is less sensitive to likely changes in the diffusion coefficient, and the PDF selected to characterize the diffusion coefficient does not significantly influence the results. The probabilistic outcome is not sensitive to likely changes in dispersivity; for practical analysis dispersivity may be treated as a deterministic constant. Correlation between flow velocity and diffusion coefficient will alter the probabilistic outcome slightly; other correlation combinations do not significantly alter the solution.

(2) For non-reactive transport with relatively high flow velocity, the probabilistic outcome is only sensitive to likely changes in the uncertain flow velocity. For practical analysis, diffusion coefficient and dispersivity may be treated as deterministic constants. The PDF type chosen for flow velocity can be relatively important, although the influence may be slight for high probability events.

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(3) For reactive transport with low velocity, the probabilistic outcome is most sensitive to likely changes in distribution coefficient and bulk density. Likely changes in porosity, flow velocity and diffusion coefficient are also important. The PDF type chosen for these uncertain variables may be significant, especially for low probability events. Because most of the uncertain variables are relatively important, correlation between these variables can have a significant influence on the probabilistic outcome.

(4) For reactive transport with high flow velocity, the probabilistic outcome is most sensitive to likely changes in flow velocity, porosity, bulk density and distribution coefficient. Both diffusion coefficient and dispersivity may be treated as deterministic constants for practical analysis. PDF type and correlation between the uncertain variables will have a significant influence on the probabilistic outcome.

(5) For the one-dimensional non-reactive transport examples, the FORM approximation provides relatively accurate estimates of the probability measure, as compared with SORM and Monte Carlo results. A uniformly distributed flow velocity creates some inaccuracy in the FORM estimate for the low velocity example, because the probability content is more dispersed throughout standard space and minor differences between the first-order approximation and the true limit state surface may be relatively important. The FORM estimate is much closer to SORM and Monte Carlo simulation when a relatively high probability event is examined, because the difference between the first-order approximation and the limit state surface introduces only small errors relative to the magnitude of the estimate.

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VII. ACKNOWLEDGEMENTS

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