PROBABILISTIC SCREENING TOOL FOR GROUND-WATER CONTAMINATION ASSESSMENT

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ABSTRACT: This paper presents a methodology for assessing the effects of source-, chemical-, and aquifer-related parameter uncertainty on the response of a semianalytical transport model using first- and second-order reliability methods. A probabilistic model is developed by coupling the deterministic transport model with a general-purpose probability analysis program. Ground-water contamination risk is addressed by evaluating the probability that a given contaminant exceeds the regulated standards at a well downgradient from a waste source. The general applicability of the methodology is demonstrated on two simple hypothetical case studies of transport of nonreactive and reactive solutes in the subsurface. Sensitivities of the probabilistic outcome to the basic uncertainties in the input random variables are provided through importance factors. The reliability-method results are checked against those obtained using the classical Monte Carlo–simulation method, and the results are in good agreement except for very low probability events in which the reliability methods provide accurate results much more efficiently than the Monte Carlo method. The need for a careful trade-off analysis between accuracy and computer time is highlighted.

INTRODUCTION

Physical parameter uncertainty greatly affects the predictive ability of ground-water flow and contaminant transport models. Failure to rigorously account for parameter uncertainty in contaminant transport analysis would, on the one hand, cast serious doubts on our ability to accurately delineate the contaminant plume at a given site; on the other hand, it would considerably reduce the possibility of success of the remediation scheme intended to clean up the plume within the specified time, simply because of the uncertainty related to the plume delineation. These uncertainties are represented in the intrinsic heterogeneity of the porous media and uncertainty related to the contaminant source, in addition to uncertainties related to the chemical, physical, and biological properties of the transported chemical.

Analytical screening models can provide general information on possible aquifer contamination impacts and are very helpful for assessing the potential of contamination of ground-water supplies. However, many of these models fail to account for the uncertainty inherently present in hydrogeologic setting parameters and chemical characteristics. Several efforts have been directed towards developing probabilistic screening ground-water tools. Examples include the work of Smith and Charbeneau (1990) using first- and second-order uncertainty analysis methods, and that of DelVecchio and Haith (1993) using the Monte Carlo–simulation method.

In the present work, a simple probabilistic screening model for ground-water contamination assessment is developed by extending a deterministic semianalytical contaminant transport model to include the effect of parameter uncertainty. Only soluble contaminant plumes are considered. The use of the semianalytical model precludes the consideration of the spatial variability of aquifer properties, however the emphasis of this work is to provide a simple, fast, and easy-to-use tool for the probabilistic screening for ground-water contamination, and to obtain preliminary information on the effect of parameter uncertainty on transport of the contaminant considered.

UNCERTAINTY ANALYSIS

First- and second-order reliability methods (FORM and SORM, respectively) were originally developed to assess the safety of structural components and structural systems and are now widely used in the study of structural reliability problems (Lu et al. 1994). The methods were recently applied to problems of ground-water flow and contaminant transport (Sitar et al. 1987; Cawlfield and Sitar 1988; Schanz and Salhotra 1992; Wu and Cawlfield 1992; Cawlfield and Wu 1993). To assess the extent of ground-water contamination, the problem is posed in a component reliability context, in which situations with a single failure mode are analyzed. FORM and SORM are selected as the probabilistic methods in this study due to their numerous appealing features. These methods do not require restrictive and limiting assumptions about the problem geometry or properties of the media. Computationally, FORM and SORM are much more efficient than the basic Monte Carlo method for low-probability events. Various levels of statistical information can be easily accommodated, from the second moment information to the full joint probability-density function of the input random variables. FORM and SORM readily provide sensitivity results with respect to both limit-state function and probability-distribution parameters. Finally, FORM and SORM are equally compatible with analytical and numerical transport models.

In the next section a brief review of the reliability methods is presented for the sake of completeness. A full review of the reliability methods can be found in Madsen et al. (1986) and Melchers (1987).

THEORETICAL BACKGROUND

In component reliability, the uncertain parameters involved in describing the aquifer, the contaminant, and the source are represented by a set of n random variables $\mathbf{X} = (X_1, X_2, \ldots, X_n)$. The limit-state function (also called the performance function) is a scalar function of the input random variables $g(\mathbf{X})$. The value $g(x_1, x_2, \ldots, x_n)$ determines the state of the component for the particular realization $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ of the random vector $\mathbf{X}$. The g-function is formulated with the convention that if $g(x_1, x_2, \ldots, x_n) > 0$,

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the component has survived, whereas the component has failed if $g(x_1, x_2, \ldots, x_n) < 0$. So the n-dimensional space R^n of the basic random variables is divided into two domains

$$S = \{\mathbf{x};\ g(\mathbf{x}) > 0\}, \text{ which denotes the safe domain} \quad (1a)$$

$$F = \{\mathbf{x};\ g(\mathbf{x}) < 0\}, \text{ which denotes the failure domain} \quad (1b)$$

The hypersurface $\{\mathbf{x};\ g(\mathbf{x}) = 0\}$ is the limiting condition between failure and survival, and is termed the limit-state surface or failure surface. In the proposed work, the limit-state function is formulated such that the event of interest is the failure event. Thus, for a continuous source, the g-function is given by

$$g(\mathbf{X}) = C_t - C(\mathbf{X}) \quad (2)$$

where C_t = prespecified maximum permissible regulatory target concentration level at the receptor well; and $C(\mathbf{X})$ = actual value of the contaminant concentration at the chosen well. It is obvious that the events described by $\{g(\mathbf{X}) < 0\}$ and $\{C(\mathbf{X}) > C_t\}$ are equivalent. In other words, the failure state in this case means failure to meet regulatory standards regarding the contaminant of interest at the well within required simulation time. Note that for a continuously leaking source, the contaminant breakthrough at the receptor well increases monotonically with time. Therefore once the target concentration at the receptor well is exceeded (and failure occurs), the concentration at the well will always be greater than the target value as time progresses and the failure condition will persist.

In assessing the contamination risk, the event of interest is the failure to meet the regulatory standards at the receptor well, and the probability of such an event, termed the probability of failure, is given by the following n-fold integral:

$$P_F = P[g(\mathbf{X}) \le 0] = P[C_t \le C(\mathbf{X})] = \int_{g(\mathbf{X}) \le 0} f_{\mathbf{X}}(\mathbf{x})\, d\mathbf{x} \quad (3)$$

where $f_{\mathbf{X}}(\mathbf{x})$ = joint probability density function of $\mathbf{X}$ and the integration is carried over the failure domain. A variety of factors complicate the direct estimation of this n-fold integral and prevent the use of the standard methods of integration. The first problem stems from the fact that for large problems, the integration is carried in a high-dimensional space, which makes the numerical integration very time-consuming or even intractable. Hohenbichler et al. (1987) point out that for an n-dimensional integral, if m is the number of calls of the integrand per dimension, the computation time grows as m^n.

Another factor that complicates the estimation of the aforementioned probability integral is that in many cases the absolute value of the integrand is very small and therefore the effect of numerical inaccuracies can be considerably magnified (Breitung 1991). Furthermore, problems arise due to the complex and algorithmic formulation of the integration domain boundaries given by the g-function. This is the case when numerical solutions of the transport equation are obtained using finite elements or finite-difference methods, such that a sequence of solutions of a large numerical transport problem is required to find a single point on the limit-state surface. In addition, problems arise due to the lack of information concerning the multivariate joint probability-density function in many practical situations.

FORM and SORM as Approximation Methods

The primary objective of the reliability methods is to overcome the aforementioned difficulties and to evaluate the multidimensional integral in (3). FORM and SORM are analytical schemes used to approximate the probability integral when the basic variables have strictly increasing continuous joint cumulative distribution functions. FORM and SORM consist of a number of steps (Bjerager, 1990). First, the random vector $\mathbf{X}$ of basic variables is transformed into the vector $\mathbf{U}$ of standardized and uncorrelated normal variates (i.e., zero mean, unit variance, and zero correlation) using a nonlinear one-to-one mapping, $\mathbf{U} = \mathbf{T}(\mathbf{X})$, such that the original joint probability-density function $f_{\mathbf{X}}(\mathbf{x})$ is mapped into the standard normal density function. Such a transformation always exists for random variables having strictly increasing continuous joint cumulative distribution functions. The space of the basic random variables $\mathbf{X}$ is often termed the x-space or physical space, and the standard normal space is called the u-space. In the case of statistically independent random variables, the nonlinear mapping is reduced to the following diagonal transformation: $u_i = \Phi^{-1}[F_x(x_i)]$, $i = 1, \ldots, n$, where $\Phi(\ )$ = standard normal cumulative distribution and $F_{\mathbf{X}}(\mathbf{x})$ = cumulative distribution function of $\mathbf{X}$. In the case of statistical dependence, the joint distributions of the random variables are assumed to be of the Nataf type, as explained by Der Kiureghian and Liu (1986). The Nataf model assumes knowledge of the marginal distributions and correlations between variables. This method has been used in this study when considering the effect of correlation between some of the basic random variables.

The second step involves the transformation of the limit-state surface $g(\mathbf{X}) = 0$ in the x-space to its image in the u-space, the surface $G(\mathbf{U}) = 0$. Fig. 1 illustrates the mapping of the physical space into the standard normal space for a two-dimensional parameter space. The major advantage of the transformation into the standard normal space is the rotational symmetry of the probability density in the u-space, which means that for all hyperplanes of equal distances from the origin, the probability content of the half-space away from the origin is constant (Der Kiureghian and Liu 1986).

The following step is the approximation of the nonlinear limit-state surface in the u-space by an appropriate tangent surface at the point of smallest distance to the origin. This smallest distance, β, is termed the reliability index and is a measure of the reliability of the component under consideration. The point on the limit-state surface that is the closest to the origin in the u-space, $\mathbf{u}^*$, is called the design point, and it is the most likely failure point in the standard normal space. Because the probability density in the u-space decays exponentially with the square of the distance from the origin, the primary contribution to the probability integral in (3) comes from the part of the failure region closest to the origin. Therefore, the design point $\mathbf{u}^*$ is an optimum point at which to approximate the limit-state surface $G(\mathbf{U}) = 0$.

The final step in the FORM/SORM estimation of the n-fold probability integral given in (3) is to compute the failure

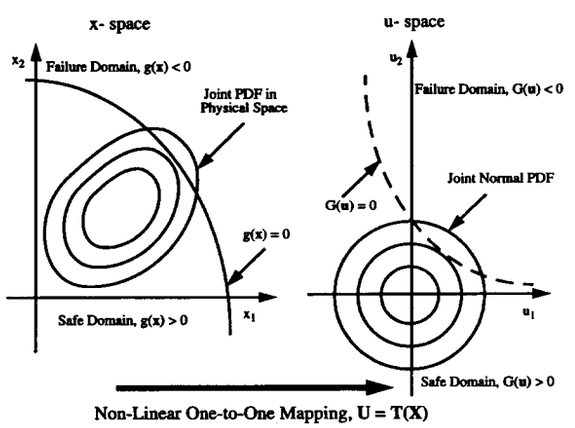

FIG. 1. Mapping of Physical Space into Standard Normal Space

probability corresponding to the approximating failure surface.

It should be emphasized that FORM and SORM are full distribution methods, meaning that the full joint probability-density function or the set of full marginal distributions with correlation matrix can be incorporated. Other methods often cited in the literature include first-order second moment (FOSM) methods, which can only incorporate the second statistical moment information (i.e., mean vector and covariance matrix) of the basic variables $\mathbf{X}$. Nevertheless, FORM and SORM can still be defined in a second moment context (Bjerager 1990).

FORM versus SORM

FORM and SORM differ mainly in their method of failure surface approximation in the u-space (Fig. 2). In FORM, the limit-state surface is approximated by the tangent hyperplane at the design point. The reliability index of the first-order reliability method is given by the inner vector product

$$\beta^{\text{FORM}} = \boldsymbol{\alpha}^* \cdot \mathbf{u}^* \tag{4}$$

where $\boldsymbol{\alpha}^*$ = unit vector normal to the limit-state surface at the design point in the u-space and directed towards the failure region (Fig. 2). The first-order approximation of the probability of failure is then given by

$$P_F \approx P_F^{\text{FORM}} = \Phi(-\beta^{\text{FORM}}) \tag{5}$$

where $\Phi(\,)$ = standard normal cumulative distribution.

The second-order reliability method (SORM), on the other hand, has the ability to accommodate the curvature of the limit-state surface by using a second-order paraboloid approximation at the design point. This becomes necessary in problems characterized by a highly nonlinear limit-state surface and, consequently, a nonflat limit-state surface at the design point.

Two types of paraboloid approximations are used in SORM: curvature-fitted (Fiessler et al. 1979; Breitung 1984) and point-fitted (Der Kiureghian et al., 1987) paraboloid approximation. A number of researchers provide expressions for estimating the probability content in a parabolic set. For example, Breitung (1984) provided an asymptotic formula

$$P_F \approx P_F^{\text{SORM}} \approx \Phi(-\beta^{\text{FORM}}) \prod_{j=1}^{q-1} (1 + \beta^{\text{FORM}} \kappa_j)^{-1/2} \tag{6}$$

$$\beta^{\text{SORM}} = \Phi^{-1}[1 - P_F^{\text{SORM}}] \tag{7}$$

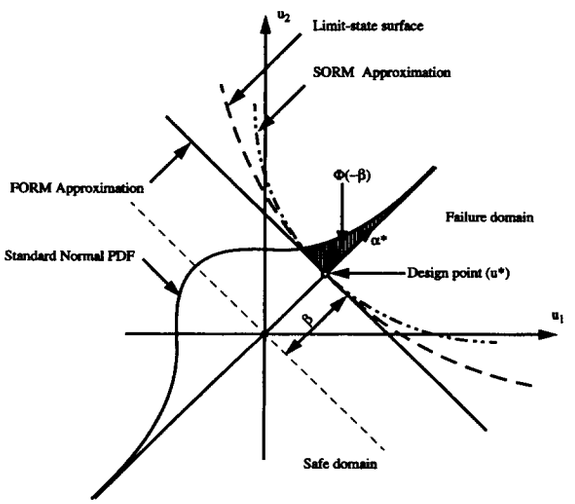

FIG. 2. FORM and SORM Approximation to Failure Surface in Standard Normal Space

In (6), κ_j = $q - 1$ principal curvatures of the limit-state surface in the u-space, with the sign convention that curvatures are negative when the surface curves towards the origin.

The computational effort of SORM should be recognized. In component reliability, the run time required for a FORM analysis grows proportionally with the problem dimensionality, n, whereas the additional computational effort needed for a SORM analysis grows with $n^2/2$. The point-fitted method (Der Kiureghian et al. 1987) has the advantages of reducing the number of g-function evaluations to $2n$, remaining valid for surfaces that are not twice differentiable, and being insensitive to any numerical noise in the limit-state surface that may arise when the limit-state function is only given algorithmically. Nevertheless, SORM is significantly more computationally intensive than FORM.

Design-Point Determination

Finding the design point in the standard normal space constitutes the major effort in reliability analysis. This is particularly true for large problems where the g-function is defined algorithmically, as when using numerical transport procedures. The design point $\mathbf{u}^*$ is the solution of the following nonlinear constrained optimization problem:

$$\text{minimize } |\mathbf{u}| \text{ subject to } G(\mathbf{u}) = 0 \tag{8}$$

This simply means that the objective is to determine a point on the limit-state surface in the standard normal space with the minimum distance from the origin. Various algorithms have been developed to resolve this problem. These include the popular HL-RF method [which was originally developed by Hasofer and Lind (1974) in FOSM reliability analysis, and later extended by Rackwitz and Fiessler (1978) to include distribution information], the gradient projection method, the sequential quadratic programming (SQP) method, and the modified HL-RF method (Liu and Der Kiureghian 1986). The comparison of the optimization methods should be done on the basis of generality, robustness, efficiency and capacity (Liu and Der Kiureghian 1991). The probabilistic model used in this work (Veritas 1992b) employs the SQP method. This reflects the developers trust of the efficiency, robustness, and generality of the SQP algorithm.

Sensitivity Measures

As an integral part of the FORM/SORM analysis, one obtains valuable information including uncertainty importance factors (Hohenbichler and Rackwitz 1986) and parametric sensitivity factors. The latter are sensitivities of both the reliability index and estimate of the failure probability to both probability-distribution parameters and limit-state function parameters (Madsen 1988).

For independent variates, the uncertainty importance factor is defined as the derivative of the first-order reliability index with respect to the corresponding variate in the standard normal space, and is given by

$$\left.\frac{\partial \beta}{\partial u_i}\right|_{\mathbf{u}=\mathbf{u}^*} = \alpha_i \tag{9}$$

where α_i = ith component of the unit normal vector to the limit-state surface at the design point.

Although there exist a number of useful sensitivity information, in this paper only the uncertainty importance factors expressed as $100\alpha_i^2$ have been reported due to the lack of space. For statistically independent variables, it has been shown (Madsen 1988) that omission sensitivity factors (defined as the relative error in the first-order reliability index when a

basic variable X_i is replaced by a deterministic number equal to its median $X_{i,m}$) are given by

$$\frac{\beta(X_i = X_{i,m})}{\beta} = \frac{1}{\sqrt{1 - \alpha_i^2}} \tag{10}$$

It is therefore observed that the uncertainty importance factors, $100\alpha_i^2$, give a measure of the relative importance of modeling the uncertainty of a basic random variable X_i with respect to the final probability outcome.

This concept naturally extends to higher dimensions. The relative error in the first-order reliability index of representing a group of m mutually dependent variables, X_i, $i = 1, \ldots, m$, by their respective median is given by (Veritas 1992a)

$$\frac{\beta(X_i = X_{i,m}, i = 1, \ldots, m)}{\beta} = \frac{1}{\sqrt{1 - \sum_{i=1}^{m} \alpha_i^2}} \tag{11}$$

Therefore, the uncertainty importance factors associated with a group of mutually dependent variables can be expressed by the quantity $100\ \Sigma_{i=1}^{m}\ \alpha_i^2$. In case $m = 1$, the results of (11) reduce to that of (10).

Importance factors allow for the identification of the random variables that have the least impact on the final reliability outcome. Each of these variables can then be replaced, for all practical purposes, by a deterministic value—its median, for example. Therefore, the importance factors are very useful in reducing the number of basic random variables in large-size reliability models.

APPLICATIONS

Probabilistic Screening Model

The probabilistic model used in this work is based on the semianalytical horizontal plane source model (HPS) developed by Galya (1987). HPS uses Green's function solutions and numerical integration to simulate uniform unidirectional advective transport in the x-direction with three-dimensional dispersion in the x-, y-, and z-directions. The model can account for first-order decay and sorption, and can accommodate any number of sources with varying concentrations and any number of receptor locations.

Input to the model includes the seepage velocity; dispersivities in the x-, y-, and z-directions; soil porosity; aquifer thickness; first-order decay coefficient; soil bulk density; organic carbon content; receptor location; along with the source location; source area dimension; source concentration; and infiltration rate. The use of HPS limits the case studies to rather simple geometry and boundary conditions, and all the limitations and weaknesses of the model as outlined by Galya (1987) should be considered. The intention, however, was to provide for a simple tool to explain the proposed probabilistic approach.

Physical-parameter uncertainty is considered by linking the transport model to the general purpose probability analysis program PROBAN (Veritas Research 1992b). This allows for carrying out a wide range of simulation and reliability analyses for both simple and complex problems. PROBAN also contains an extensive built-in distributions library of probability distributions that enables the assignment of a variety of marginal or joint probability-density functions.

Fig. 3 is a schematic presentation of the various elements involved in the proposed approach. The probabilistic transport model can be used by the user as a "black box" without necessitating a great deal of knowledge of the reliability theory from the user's part. Input to the model includes physical-parameter uncertainty as well as deterministic parameters.

Various levels of statistical information can be accommodated by the model. When only incomplete statistical information is available, the first two moments of each random variable are specified, without providing a specific probability distribution. If some, or all, of the random variables are correlated, this information can be readily incorporated into the model through the correlation coefficients. When there is incomplete statistical information, only an ad hoc estimate of the probability of failure can be obtained. On the other hand, if the complete probability information is available, the input random variables are defined by their full joint density function, which can be decomposed into a product of conditional distributions.

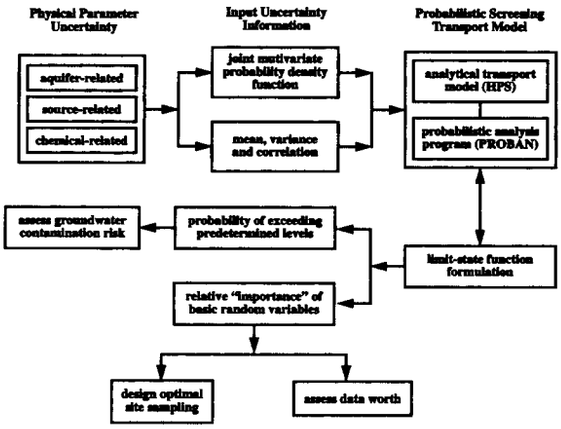

FIG. 3. Flow Chart of Probabilistic Transport Analysis Model

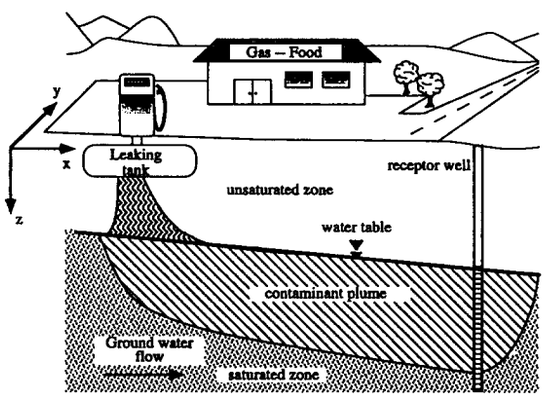

FIG. 4. Schematic of Case-Study Setup

The user is also prompted to formulate the limit-state function for the site-specific conditions, which identifies the performance criteria of the component being considered. It should be noted that the formulation is different in the case of continuous and instantaneous leaking sources, and differs depending on whether ground-water flow or contaminant transport is the primary focus of the study.

The problem of interest in this work is to study the probability that the concentration of a given contaminant leaking continuously from a source exceeds a predetermined target level at a downgradient water supply well during the simulation time of interest. Fig. 4 shows a schematic of the case study setup. The actual mathematical formulation was presented in (2).

Once the limit-state function is formulated and the input variables are provided, the model applies the first- and second-order reliability methods to provide the user with the probability of failure at the receptor well, the reliability index characterizing the transport scenario, and the sensitivity of the failure probability and reliability index to the basic variability in the basic random variables. The decision regarding

the assessment of ground-water contamination risk can be made with the probabilistic outcome available. As described earlier, the sensitivity data can help the user assess the worth of available data and guide in the future data-collection protocols. Monte Carlo simulations of the failure probability, or of the concentration at the receptor well, can be readily provided by the HPS-PROBAN model with minor modifications to the input file.

The interface between PROBAN and HPS is done using FORTRAN user-defined subroutines, and the HPS-PROBAN is run on a SUN SPARCstation 2. In the FORM/SORM analysis, HPS is used at each iteration in the constrained optimization routine used to solve (8) to provide a current estimate of the g-function for the current realization, $\mathbf{x}$, of the random vector $\mathbf{X}$. The search algorithm usually converges to a minimum in less than 20 iterations. To ensure that a global minimum is obtained, the user may choose to run the problem with different starting points, and check whether the algorithm converges to the same solution each time.

Nonreactive-Solute Transport

First, the methodology is demonstrated on a case of transport of a conservative (nonreactive) solute in ground water. This means that the only mechanisms involved in the solute transport are the advection and dispersion. The solute is assumed to undergo no chemical transformations, biological degradation, or adsorption to the soil matrix. The source is assumed continuous. The deterministic parameters to this case study are listed in Table 1. The probability of failure at a receptor well downgradient from the waste source of the source is studied. The well is assumed to be screened from the water table to a depth of 2.0 m below the water table, thus the observation point is taken to be 1.0 m below the water table.

Input random variables to the case study are categorized into aquifer-related and source-related parameters, and are listed in Table 2. Aquifer-related parameters include seepage velocity; dispersivities in the x-, y-, and z-directions; and soil porosity. Source-related parameters include the source dimension parallel to the x- and y-axes. Probability-density functions and relevant parameters for the aquifer-related parameters were obtained from the nationwide survey done for the Environmental Protection Agency (EPA) in 1988 (*Background* 1988), along with the 400-site survey conducted by Newell et al. (1990). The selection of the uniform probability distribution for the source dimensions is arbitrary. The basic random variables are assumed to be mutually statistically independent.

For the case of lognormally distributed variables, the mean and standard deviation are given; for shifted lognormal variables, the mean, standard deviation, and the minimum values are given. Lower and upper limits are provided for the case of uniformly distributed variables.

In this case study, we look at the normalized target concentration at the receptor well, $[C(\mathbf{X})/C_0]$, where $C(\mathbf{X})$ is the actual concentration, and C_0 is the source concentration. Thus the limit-state function is formulated as follows:

$$g(\mathbf{X}) = (C/C_0)_{\text{target}} - C(\mathbf{X})/C_0 \tag{12}$$

where $(C/C_0)_{\text{target}}$ = normalized target concentration at the well.

Instead of performing the analysis for a single normalized target concentration, a set of such target concentrations was considered. In other words, the reliability problem is solved a number of times, varying the term $(C/C_0)_{\text{target}}$ that appears in (12) at each time. Note that the probability distribution of the concentration under consideration can be obtained by varying the target concentration values and using the parametric sensitivity results with respect to limit-state function parameters. This gives a more flexible way of assessing the ground-water contamination risk at the receptor well for any selected target concentration value. The probability of failure at receptor wells at distances of 200 m and 400 m downgradient are shown in Fig. 5. First-order and curvature-fitted second-order reliability methods were used. The decrease in failure probability with target concentration increase is intuitive, because it is less probable for the solute concentration to exceed a high value at the downgradient well than a smaller value for a continuous source.

FORM and SORM failure probabilities were found to be in good agreement for low target concentration values (and hence for higher failure probabilities). However, FORM and SORM results depart from each other for large target concentration values (and lower failure probabilities), which indicates the appreciable nonlinearity of the limit-state surface at the design point. In this case, a second-order method is expected to provide a better approximation of the failure surface at the design point because it accounts for the principal curvature of the limit-state surface in the standard nor-

TABLE 1. Deterministic Input Parameters for Case of Nonreactive Solute Transport

Variable (1)	Unit (2)	Value (3)
Aquifer thickness H	m	30.0
Simulation time t	yr	20.0
x-distance to the well	m	Variable
y-distance to the well	m	10.0
z-distance to the well[a]	m	1.0
Infiltration rate Q	m/yr	1.0
Retardation factor R	—	1.0
First-order decay coefficient λ	yr^{-1}	0.0

[a]z-distance is measured from water table.

TABLE 2. Random Input Variables for Case of Nonreactive Solute Transport

Variable (1)	Unit (2)	Distribution (3)
(a) Aquifer-related parameters		
Seepage velocity U	m/yr	LN (126.7, 227.37)
x-dispersivity α_x	m	SLN (10, 4, 0.01)
y-dispersivity α_y	m	SLN (1, 0.4, 0.001)
z-dispersivity α_z	m	SLN (0.1, 0.04, 0.0001)
Soil porosity θ	—	U (0.3, 0.5)
(b) Source-related parameters		
Source length L_x	m	U (50, 100)
Source width L_y	m	U (50, 100)

Note: LN (mean, standard deviation) = lognormal; SLN (mean, standard deviation, lower limit) = shifted lognormal; U (lower limit, upper limit) = uniform.

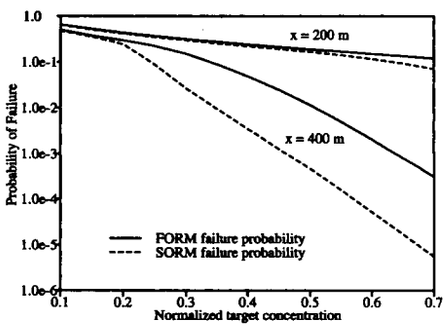

FIG. 5. Effect of Normalized Target Concentration Levels on Probability of Failure for Nonreactive Case

mal space. Although the results contained in Fig. 5 are qualitatively intuitive, the quantitative aspects could not have been obtained without the formal probabilistic computations described in the aforementioned formulation.

Fig. 6 illustrates the effect of changing the normalized target concentration levels at the receptor well on the FORM and SORM reliability index for the 200 m and 400 m cases. Because there is a monotonic one-to-one relationship between the probability of failure and reliability index [see (5)], the same trend of agreement at low normalized target concentration levels and discrepancy at large normalized target concentration levels is observed for the FORM and SORM results. The reliability index is a measure of the component reliability—it increases for decreasing probability of failure.

The discrepancy between the FORM and SORM results are further investigated by estimating the percentage difference between the results for varying normalized target concentration and distances from the source. The absolute value of the percentage difference was estimated as follows:

$$\text{absolute percentage difference} = \text{absolute}\left(\frac{P_F^{\text{FORM}} - P_F^{\text{SORM}}}{P_F^{\text{FORM}}}\right) \times 100 \tag{13}$$

This is shown in Fig. 7. FORM and SORM failure probabilities were found to be in good agreement for low target concentration values, or for high target concentration values at closer distances to the source. In other words, the agreement between the FORM and SORM results is good for cases with high probability of failures (above 10^{-1} for this particular case study and for the prescribed probability distributions). FORM and SORM results depart significantly from each other, however, for large target concentration values, or for small target concentrations at larger distances from the source, which indicates the appreciable nonlinearity of the limit-state surface at the design point, in which case the use of SORM is warranted.

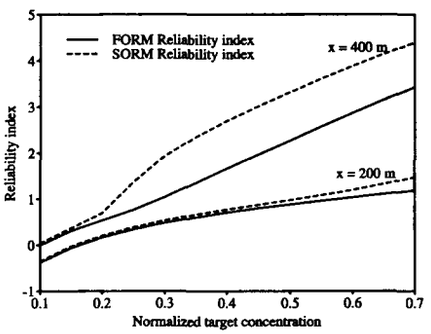

FIG. 6. Effect of Normalized Target Concentration Levels on Reliability Index for Nonreactive Case

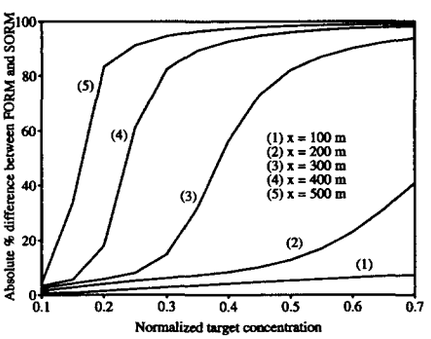

FIG. 7. Percentage Difference between FORM and SORM Results for Nonreactive Case

The previous discussion draws the attention to an important issue regarding the choice of SORM versus FORM as the reliability analysis option. In many practical situations, FORM and SORM results would be in good agreement, provided that the limit-state surface at the design point in the standard normal space is nearly flat. On the other hand, when the limit-state function contains highly nonlinear terms, or when the input random variables have an accentuated nonnormal character, SORM tends to produce more accurate results than FORM. However, it should be recognized that SORM requires more computational effort than FORM. As discussed before, in component reliability, the run time required for a FORM analysis grows proportionally with the problem dimensionality, n, whereas the additional computational effort needed for a SORM analysis grows with $n^2/2$. Consequently, the selection of the reliability method should be done based on problem dimensionality, available computer resources, and the required level of accuracy. In other words, one should always conduct a careful trade-off analysis between computational and accuracy requirements. In this case study, the run times (user + system times) for FORM and SORM were in the order of 1 min and 2.5 min, respectively.

The combined effect of the distance from the receptor well to the leaking source and the normalized target concentration levels on the failure probability is shown in Fig. 8. In this case, both the target concentration and distance from the source are varied, and the resulting curvature-fitted SORM failure probabilities form the shown "failure probability surface." It is clear from the figure that for a specified normalized target concentration, the failure probability decreases with increasing downgradient distance from the source, and that for a specified distance from the source, the failure probability decreases with increasing target concentration. This analysis would be useful if we look at a number of locations downgradient from the leaking source, so that we can identify the failure probability related to a given leaking source for any given well and desired target concentration level.

The importance factors presented in the theoretical background section indicate the sensitivity of the probabilistic outcome to the basic uncertainty in the input random variables. The change of the importance factors with changing normalized target concentration levels is shown in Fig. 9. It is evident that over the range of target concentrations selected, and for the probability distributions prescribed for this case study, the probability of failure at the receptor well is most sensitive to the basic variabilities in the seepage velocity, z-dispersivity, and source length L_x. The importance factors for the remaining variables were less than 1.0% and were not

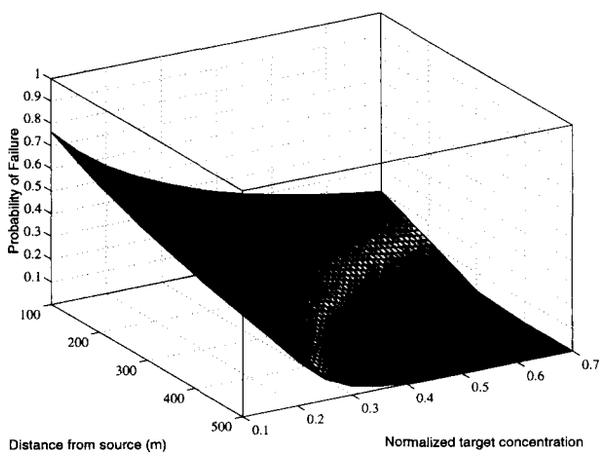

FIG. 8. Curvature-Fitted SORM Failure Probability Surface for Nonreactive Case

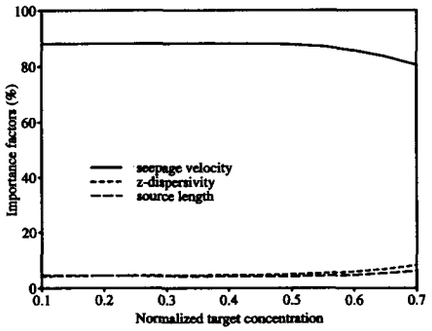

FIG. 9. Effect of Normalized Target Concentration on Importance Factors in Nonreactive Case

TABLE 3. Deterministic Input Parameters for Case of Reactive Solute Transport

Variable (1)	Unit (2)	Value (3)
Simulation time t	yr	20.0
x-distance to well location	m	100.0
y-distance to well location	m	1.0
z-distance to well location[a]	m	1.0
Infiltration rate Q	m/yr	1.0
Source concentration (C_0)	mg/L	200.0
Contaminant type	—	o-xylene

[a]z-distance is measured from water table.

plotted. Therefore, although the impact of seepage velocity on the probabilistic outcome is evident, the significance of the source-related uncertainty should also be recognized, and failure to account for these uncertainties could result in erroneous contamination risk assessment. Note that when correlation between some of the input random variables was included, the resulting probability of failure was within about 3% of the uncorrelated case.

Reactive-Solute Transport

As an example of transport of a reactive solute in the subsurface, the proposed methodology is applied to the case of transport of o-xylene. A continuous leaking source is also used in this case. The concentration at a well 100.0 m downgradient, and 1.0 m off the centerline (x-axis) is studied. The deterministic parameters used in the case study are listed in Table 3 and the input random variables to the model are listed in Table 4.

The input random variables are classified into three categories: aquifer-related, source-related, and chemical-related parameters. Basic random variables are assumed mutually statistically independent.

First-order kinetics have been widely used to describe processes like natural biodegradation, chemical reactions, and radioactive decay. For the purpose of this work, it is assumed that o-xylene undergoes natural anaerobic biodegradation by indigenous microorganisms following first-order kinetics. Due to changing depths of ground-water elevation and fluctuation in levels of nutrients and electron acceptors, there is uncertainty in the value of the first-order decay coefficient for the contaminant. This is taken into account by assuming the decay coefficient to be random. The choice of the range of equally likely values of the first-order decay coefficient used in this work takes into account actual rates for natural biodegradation reported by Wilson et al. (1993) for o-xylene. As for the organic carbon partition coefficient K_{oc}, the range of values were obtained from the listed values given by Fetter (1993).

In this case study, we look at actual o-xylene concentration

TABLE 4. Random Input Variables to Case of Reactive Solute Transport

Variable (1)	Unit (2)	Distribution (3)
(*a*) Aquifer-related parameters		
Seepage velocity U	m/yr	LN (126.7, 227.37)
Dispersivity (x-direction) α_x	m	SLN (10, 4, 0.01)
Dispersivity (y-direction) α_y	m	SLN (1, 0.4, 0.001)
Dispersivity (z-direction) α_z	m	SLN (0.1, 0.04, 0.0001)
Soil porosity θ		U (0.3, 0.5)
Soil bulk density ρ_b	g/cm^3	U (1.2, 1.8)
Fraction of organic carbon f_{oc}	% weight	SLN (0.0031, 0.0003, 0.001)
(*b*) Source-related parameters		
Source length L_x	m	U (50, 100)
Source width L_y	m	U (50, 100)
(*c*) Chemical-related parameters		
Organic carbon partition coefficient K_{oc}	cm^3/g	U (200.0, 900.0)
First-order decay coefficient λ	yr^{-1}	U (1.456, 5.72)

Note: LN (mean, standard deviation) = lognormal; SLN (mean, standard deviation, lower limit) = shifted lognormal; U (lower limit, upper limit) = uniform.

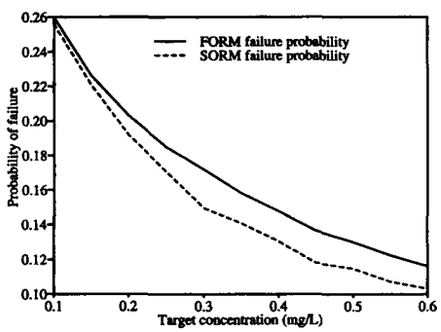

FIG. 10. Effect of o-xylene Target Concentration Levels on Probability of Failure

at the receptor well, resulting from the continuous leaking source. Note that the o-xylene undergoes adsorption to the soil matrix and biodegradation in addition to advection and dispersion, thus the actual concentration of o-xylene at the receptor well will be much smaller than that of a similar leak of a nonreactive solute. The limit-state function for this case is formulated as follows:

$$g(\mathbf{X}) = C_t - C(\mathbf{X}) \tag{14}$$

The effect of changing the target concentration levels at the receptor-well location on the probability of failure is illustrated in Fig. 10. Both FORM and SORM (curvature-fitted) were used for the component reliability analysis. As was observed and explained in the nonreactive case, there is a similar trend in decreasing the failure probability with increasing target concentration. For this application, FORM and SORM results agree reasonably well for the whole range. A similar trend was also noted in good agreement between FORM and SORM reliability index for the whole range of target concentration levels. For the sake of brevity, this result is not presented. The effect of correlation between some of the input random variables in this case was similar to that of the nonreactive case, and the resulting difference in the prob-

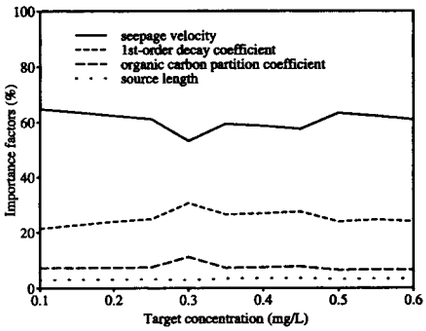

FIG. 11. Effect of o-xylene Target Concentration on Importance Factors

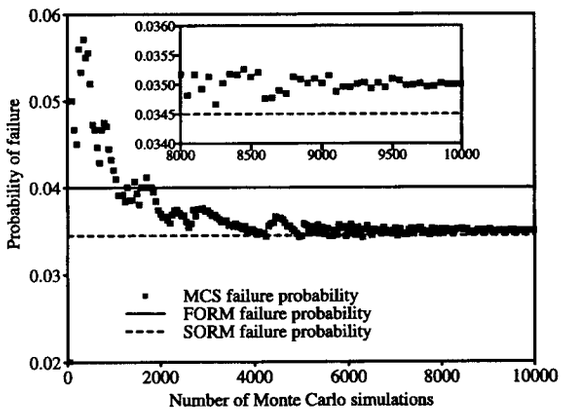

FIG. 12. Comparison of FORM, SORM, and Monte Carlo–Simulation Estimate of Probability of Failure

ability of failure was within about 5% of the uncorrelated case.

The importance factors for a range of o-xylene target concentration levels is shown in Fig. 11. It is clear that over the range of target concentration selected, and for the probability distributions prescribed for this case study, the probability failure at the receptor well is most sensitive to the basic uncertainty in the seepage velocity, the first-order decay coefficient, the organic carbon partition coefficient, and, to a lesser extent, the source length L_x. Therefore, although the impact of seepage velocity on the probabilistic outcome is pronounced, the significance of the chemical-related and source-related uncertainty should be recognized, and failure to account for these uncertainties would cast shadows of doubt over the risk-assessment results. The importance factors for other variables were negligible (below 1.0%), therefore they were not plotted. The apparent oscillation in the results are spurious numerical artifact due to the fact that the level of accuracy of the reliability algorithm varies slightly with the level of target concentration levels resulting from the nonlinear nature of the limit-state surface at the design point in the standard normal space. The trend of the true behavior of the solution, however, remains clear.

In Fig. 12, the failure probabilities obtained by FORM, curvature-fitted SORM, and the classic Monte Carlo simulation are plotted. The MCS and SORM results seem to be in a very good agreement (as shown in the inset). FORM results, however, departs considerably from the "true" solution predicted by the ensemble mean of the large number of Monte Carlo simulations. It should be emphasized that 10,000 Monte Carlo simulations were required to get a reliable estimate of the probability of failure (i.e., a coefficient of variation of the estimate within the permissible limits, 0.02 in this case). FORM and SORM results were obtained in less than 20 iterations, and the required run time (user + system time) on a SUN SPARCstation 2 was in the order of 2 min and 3 min, respectively. The 10,000 Monte Carlo results, on the other hand, were obtained in about 60 min of run time on the same machine.

This clearly illustrates the power and computational efficiency of SORM through which the results can be obtained at a small fraction of the computational cost required for the Monte Carlo–simulation results. The figure also indicates the inaccuracy of the FORM results in this case. Nevertheless, the FORM results were obtained in a very short run time, thus it could be used to provide a first estimate of the failure probability. The asymptotic convergence of the classic Monte Carlo simulation is evident by the way the simulation estimate converges to the failure probability that is predicted by SORM.

CONCLUSIONS

The significant role that the parameter uncertainty plays in modeling ground-water contaminant transport has been recognized by environmental engineers as well as regulatory agencies. Recently there have been considerable attempts to address such an issue using the various stochastic hydrogeology approaches. In this work we have presented a simple and efficient screening tool for the probabilistic assessment of ground-water contamination at a given receptor well receiving contamination from an upgradient source. The model is based on a semianalytical model of simple structure, thus it does not take into account the spatial variability of the aquifer parameters. Nevertheless, the intention was twofold: to perform a proof-of-concept type of study for illustrating the potential power of the reliability methods; and to develop a probabilistic tool that can provide general indication of contamination risk, along with sensitivity of the results with respect to the various basic sources of uncertainty, in a framework that can explicitly account for aquifer-related, source-related, and, in the case of reactive solutes, chemical-related parameter uncertainty.

We have shown that first- and second-order reliability methods (FORM and SORM, respectively) can be a potential alternative to the classical Monte Carlo–simulation method when dealing with ground-water contamination events that have very small probability of occurrence, therefore requiring thousands of Monte Carlo simulations to provide reliable results. In this work, FORM and SORM were used to assess the probability that a given contaminant exceeds a certain target concentration level at a given point in space and time in the solution domain, and to provide the sensitivity of such a probabilistic event with respect to the basic variability in the input variables. Contamination scenarios with both reactive and nonreactive solutes were presented for demonstration purposes.

FORM and SORM results were compared and were tested against those obtained using the classical Monte Carlo–simulation method. In selecting the analysis method, it should be emphasized that SORM is more accurate than FORM, but computationally more expensive. In this paper, because the problem analyzed was fairly simple, computer time required for SORM was still very low (on the order of a few minutes on a SUN SPARCstation 2) and the use of SORM was warranted. However, for larger problems, and when using more complex numerical models (based on finite-difference or finite-element methods) this becomes a matter of considerable significance, and a careful trade-off analysis between computational effort and accuracy should be conducted to determine which approximation method to use. We also showed that FORM results are sometimes very different from SORM results, and in such cases, SORM analysis is warranted, even with the extra computational effort required.

The impact of the basic uncertainty in seepage velocity was identified. However, chemical-related and source-related parameter uncertainty have also appeared as significant factors to consider in the probabilistic analysis of ground-water transport problems, and their importance should not be overshadowed by the aquifer-related parameter uncertainty.

Although the probabilistic model used in this work is based on a semianalytical transport code, the methodology is equally applicable to more sophisticated and realistic numerical models as well. The writers are currently working on the integration of FORM and SORM with a three-dimensional numerical finite-element transport code in order to account for the effect of spatial correlation structure of the relevant aquifer- and chemical-related parameters.

ACKNOWLEDGMENT

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APPENDIX II. NOTATION

The following symbols are used in this paper:

C = actual concentration of contaminant at receptor well (M/L^3);
C_t = deterministic target concentration at receptor well (M/L^3);
C_0 = source concentration (M/L^3);
F = failure domain of component of interest;
$F_{\mathbf{X}}(\mathbf{x})$ = joint cumulative distribution function of $\mathbf{x}$;
f_{oc} = fraction of organic carbon (percentage by weight);
$f_{\mathbf{X}}(\mathbf{x})$ = joint probability density function of $\mathbf{x}$;
$G(\mathbf{U})$ = limit-state function in standard normal space;
$g(\mathbf{X})$ = limit-state function in physical space;
H = aquifer thickness (L);
L_x = length of leaking source in x-direction (L);
L_y = width of leaking source in y-direction (L);
P_F = probability of failure;
P_F^{FORM} = FORM approximation to probability of failure;
P_F^{SORM} = SORM approximation to probability of failure;
Q = infiltration rate (L/T);
R = retardation factor;
S = survival domain of component of interest;
U = seepage velocity (L/T);
$\mathbf{u}^*$ = design point in standard normal space;
u-space = standard normal space;
$\mathbf{X}$ = n-dimensional random vector;
$\mathbf{x}$ = particular realization of random vector $\mathbf{X}$;
x-space = physical space of random variables;
$\boldsymbol{\alpha}^*$ = unit vector normal to limit-state surface at design point in standard normal space;
α_x = dispersivity in x-direction (L);
α_y = dispersivity in y-direction (L);
α_z = dispersivity in z-direction (L);
β^{FORM} = first-order reliability index;
β^{SORM} = second-order reliability index;
θ = aquifer porosity;
κ_j = principal curvatures of limit-state surface in standard normal space;
λ = first-order decay coefficient;
ρ_b = soil bulk density (M/L^3); and
Φ = standard normal cumulative distribution function.