Uncertainty Quantification of Contaminant Transport Through Geological Repository using 2D Monte Carlo Simulation

D. Datta, M. Pandey, Brij Kumar and P. S. Sharma
Health Physics Division

Abstract
The safety of a radioactive waste or spent nuclear fuel repository is related to its capacity to confine radioactivity and isolate it from the biosphere. The most likely process leading to the release of radionuclides from a radioactive waste repository in a geological formation is the transport by groundwater. Entry of radionuclide into the biosphere after traveling through geosphere may possess a risk per year to the people living in the vicinity of the site. Therefore, this study has been developed to assess the risk in presence of the uncertainty of the parameters that constitute the governing model for describing the migration of the radionuclide through geological repository. The risk addressed here is due to drinking of water possibly contaminated with the migrated nuclide. Double Monte Carlo simulation is applied for modeling and the basic reason is due to the uncertainties of the bounds of the parameter of the specified distribution function. The paper demonstrates the simulation by an example problem in which migration of I-129 radionuclide released from waste disposal facility and migrated through a geological repository to a biosphere is focused.

Introduction
Subsurface contamination by leakage and spill of radioactive liquid effluent from any nuclear industry has resulted in many environmental concerns for a period of many years. Environmental risks of such contamination need to be analyzed to provide support for decisions related to remediation of the contamination problems. The safety of a radioactive waste or spent nuclear fuel repository is related to its capacity to confine radioactivity and isolate it from the biosphere. The most likely process that can lead to the release of radionuclides from a repository to the geosphere is transport by groundwater. Consequently, waste disposal-related safety analyses must assess the importance of the migration of radionuclides (i.e., their mobility) in the conservative assumption of leaching by groundwater (i.e., after the destruction of the engineered barriers). However, many models and relevant field studies have recognized that the contaminant fate in subsurface is substantially influenced by uncertainties inherent in natural porous media, path length of the geosphere travelled by the radionuclide, fractional release rate, retardation factor and containment period. Presence of uncertainty not only increases the computational load but also provides a best estimate approach of safe design of a geological repository. Moreover, uncertainty of the parameters of the specified probability distribution (e.g., mean and standard deviation of a normal probability distribution) that characterizes the model parameters also yields a bound of the uncertainty and this bound can be very helpful while making any decision related to design of the waste package and its disposal into the geological repository. Mathematical models used for carrying out this time dependent risk assessment (risk analysis of a waste repository) include parameters having values varying within some ranges. Literature study shows that traditional 1D Monte Carlo simulation has been applied to estimate
the risk in presence of uncertainty. Examples of this kind of approach of risk assessment are elsewhere found [1]. In this context, the assessment and presentation of the effects of uncertainty are widely recognized as important parts of analyses for such complex systems [1]. Generally, most of the earlier studies used the stochastic approaches to accommodate the uncertainties associated with contaminant transport models [2-3]. This paper presents the double Monte Carlo based modeling of contaminant migration through geological repository. The outcome of this study is the assessment of time dependent risk to the public through the drinking of groundwater contaminated by the migrated water-borne radionuclide. In this modeling very often, the parameters of the probability distribution itself are expressed in the form of range or interval which is due to lack of proper analysis of the experimental data. This demands the double Monte Carlo simulation and the result of this simulation is expressed in terms of bounds generally attributed as lower cumulative probability and upper cumulative probability [4-5].

The physical processes which are responsible for migration of the contaminant include dispersion, advection, adsorption and decay. Time profile of the risk along with its two bounds is presented in this paper. The structure of the paper is as follows. Section 2.0 describes the double Monte Carlo simulation and sampling scheme required to generate the random numbers from the specific probability distribution. Section 3.0 presents the problem statement considered for the purpose of modeling. Numerical results of the outcome of this modeling are presented in section 4.0 and finally conclusion is presented in section 5.0.

2D Monte Carlo Method

The Monte Carlo method is a numerical solution to a problem that models objects interacting with other objects or their environment based upon simple object-object or object environment relationships. It represents an attempt to model nature through direct simulation of the essential dynamics of the system in question. In this sense the Monte Carlo method is essentially simple in its approach - a solution to a macroscopic system through simulation of its microscopic interactions. A solution is determined by random sampling of the relationships, or the microscopic interactions, until the result converges. Thus, the mechanics of executing a solution involves repetitive action or calculation. To the extent that many microscopic interactions can be modeled mathematically, the repetitive solution can be executed on a computer. However, the Monte Carlo method predates the computer and is not essential to carry out a solution although in most cases computers make the determination of a solution much faster. There are many examples of the use of the Monte Carlo method [5] that can be stated in short as simple random sampling of the uncertain parameters with respect to the specific probability distribution. Latin hypercube sampling [5] is applied here as the main sampling scheme.

Illustration with Example

Suppose our sample model is as follows:

\[ Z = (X + Y)/(X \cdot Y) \], where \( x \) any \( y \) are uncertain parameters due to their randomness. Uncertainty of these parameters is assumed as follows:

\[ X = N(\mu_x, \sigma_x), Y = U(a_y, b_y) \]

Let the values of all these constants be:

\[ \mu_x = 10, \sigma_x = 20, \mu_y = 0.2, \sigma_y = 0.5; \]
\[ a_y = 100, b_y = 300, b_y = 400; \]

Sampling strategy in double Monte Carlo is as follows:

Sample values of \( X \) and \( Y \) are generated using the following scheme as:

\[ X_1 = N(\mu_1, \sigma_1), X_2 = N(\mu_2, \sigma_2), X_3 = N(\mu_3, \sigma_3) \text{ and } X_4 = N(\mu_4, \sigma_4) \]
\[ Y_1 = U(a_1, b_1), Y_2 = U(a_2, b_2), Y_3 = U(a_3, b_3) \text{ and } Y_4 = U(a_4, b_4) \]
Construct a temporary matrix, say XX as $XX = [X_1, X_2, X_3, X_4]$. Compute the minimum and maximum of each rows of XX matrix.

Cumulative probability distribution with minimum values of each row of XX will be termed as lower cumulative probability of $X$ and the same with maximum values of each row of XX will be termed as upper cumulative probability of $X$. Repetition of the similar task with $Y_1, Y_2, Y_3,$ and $Y_4$ will generate the lower and upper cumulative probability of $Y$.

Now substituting the simulated min-max values of $X$ and $Y$ we have the following values of the model output as

$$Z_1 = \frac{\text{min}(X) + \text{min}(Y)}{\text{min}(X) \cdot \text{min}(Y)};$$

$$Z_2 = \frac{\text{min}(X) + \text{max}(Y)}{\text{min}(X) \cdot \text{max}(Y)};$$

$$Z_3 = \frac{\text{max}(X) + \text{min}(Y)}{\text{max}(X) \cdot \text{min}(Y)};$$

$$Z_4 = \frac{\text{max}(X) + \text{max}(Y)}{\text{max}(X) \cdot \text{max}(Y)};$$

Construct a temporary matrix ZZ with $Z_1, Z_2, Z_3,$ and $Z_4$. Compute the minimum and maximum values of each row of ZZ and labeled them as $Z_{\text{min}}$ and $Z_{\text{max}}$. Cumulative probability distribution of $Z_{\text{min}}$ and $Z_{\text{max}}$ can be now constructed and labeled as lower and upper cumulative probability of the model $Z$. $2.5^{th}, 50^{th}$ and $95^{th}$ percentile from lower and upper cumulative probability will provide the uncertainty band of the model output $Z$. The outcome of the complete simulation is as depicted in Figs. 1-3.

**Problem Formulation**

Double Monte Carlo simulation [5-6] based modeling has been applied to estimate the time dependent radiological risk to the human with respect to the migration of water-borne radionuclide through a geological repository. Accordingly the scenario considered in the model tracks the one dimensional migration of typical water borne radionuclide through two geo-spherical layers characterized by different hydro geological properties. Statement of the problem is as follows:

The processes being considered in the model are radioactive decay, dispersion, advection and chemical reaction between the migrating radionuclide and porous medium. Radioactive waste (conditioned) contained within a steel canister is disposed in the
form of a package in the geological repository, which can be represented as point source for the purpose of modeling. The migration of the radionuclide through the geosphere is the core of the present modeling. The governing equation covering all the processes mentioned is represented as

$$\frac{\partial C(x,t)}{\partial t} - v \frac{\partial^2 C(x,t)}{\partial x^2} - \frac{\partial C(x,t)}{\partial x} - R C(x,t)$$

(1)

where, $C(x,t) =$ concentration of radionuclide at position $x$, in the geosphere at time $t$, $R =$ retardation factor, $v =$ water travel velocity in the geosphere layer (m/y), $d =$ dispersion length in the geosphere layer (m), and $\lambda =$ decay constant of the radionuclide in per year. The modeling of the biosphere is expressed via risk to the human from the ingestion of the drinking water containing the migrating radionuclide [7-9]. This biosphere modeling is given by accordingly,

$$\text{Risk (}/\text{yr}) = C(l, t) * B$$

(2)

where, $B =$ biosphere risk factor evaluated from the drinking capacity of each individual in a year. The model for computing the biosphere risk factor can be given as

$$B = \frac{W}{W} - \varepsilon$$

(3)

where, $w =$ water ingestion rate (m$^3$/y), $W =$ stream flow rate (m$^3$/y) and $\varepsilon =$ risk factor (}/y).

The aim of this problem is to quantify the probability bounds of risk (}/yr) with random uncertain input parameters.

Solution:

Equation (1) has been solved analytically by using Green’s function method with proper initial and boundary condition and the final solution [7-9] of $C (L, t)$ is written as

$$C(L,t) = 0.5^{\nu} \zeta^2 B \kappa^2 \exp(-\theta + \mu \zeta - \eta) \nu$$

(4)

where, $\theta =$ initial inventory of the radionuclide in the repository, $\mu = L / (2 \Delta t^2)$, $\zeta = R \Delta \nu + 1$, $\eta = v \nu (4 \Delta t)$, and $T =$ containment period (y).

The factor $\xi$ is as follows:

$$\xi = (\kappa(x_1) + \kappa(x_2)), \kappa(x) = \nu \exp(x) \ast \exp(x),$$

$$\zeta_1 = (\nu \ast \nu)_{\frac{1}{2}}$$

The uncertain input parameters of this model are:

- $\xi =$ fractional release rate (}/y),
- $T =$ Containment period (y),
- $R =$ retardation factor,
- $L =$ geosphere path length (m),
- $d =$ dispersivity (m$^2$/y),
- $v =$ groundwater velocity (m/y)

Computational Issues

Uncertain input parameters are characterized by the specific probability distribution suggested by the domain experts. Experts also provide the bounds of the parameters of their probability distributions. Probability distributions representing the uncertainty of the input parameters are of two types: (a) log-uniform and (b) uniform. Accordingly sample values of the specific input parameters following the double Monte Carlo simulation are generated. Each random uncertain input parameter is expressed in terms of a probability bound addressed by lower and upper cumulative probability. Substitutions of these bounds in the model with the fixed value of the deterministic input parameters yield the probability bounds (lower and upper) of the risk. Uncertainty of the model output in this case is expressed in terms of these probability bounds. The function may be complex and is known as Faddeeva function [9]. Hence computation of this function has been carried out by following an algorithm given in [10].

Computation of the error function with complex argument is the computational issue of the factor $\xi$ of equation (4). Lower and upper bounds of the estimated risk at different time have been computed. 50th percentile values from lower and upper cumulative probability of the time dependent risk are used as the mean risk at any specific time.

Numerical Results

Uncertain input parameters of the model as presented in Eq.(1-4) are: (a) leach rate, $k$ (}/y), (b) retardation factor, $R$, (c) water travel velocity,
v (m/y), (d) containment period, T (y), (e) path length, L(m) travelled by the radionuclide within geosphere before coming to biosphere, and (f) the stream flow rate, W(m³/y). Probability distribution of all these uncertain parameters is suggested by experts. As per expert’s opinion, leach rate is log-uniformly distributed, but the limits of the log uniform distribution cannot be precisely specified and that is the reason, the limits of the leach rate distribution are provided by the experts in the form of an interval. Similarly, retardation factor is uniformly distributed and the limits (lower and upper) are again given as an interval. So, random sample values of leach rate and the retardation factor has been generated using double Monte Carlo simulation (section 2.1). Probability distribution of the water travel velocity, stream water velocity, containment period are considered as log uniform as per expert’s opinion. Geosphere path length is taken as uniform distribution.

The deterministic parameters are given in Table 1. Probabilistic uncertain parameters having lower and upper bounds in terms of an interval (as illustrated in section 2.1) are called as type II uncertain parameters. Parametric uncertainty of type II parameters of the model is as shown in Table 2. Parametric uncertainty of all type 1 probabilistic input parameters are presented in Table 3. A sample size of 1000 on the basis of Latin hypercube sampling has been used for simulation business.

Table 1: Deterministic input Parameters

<table>
<thead>
<tr>
<th>Parameter Description</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₀ (Bq)</td>
<td>3.7E10</td>
</tr>
<tr>
<td>d (m)</td>
<td>20</td>
</tr>
<tr>
<td>(\lambda) (y⁻¹)</td>
<td>4.414E-8</td>
</tr>
<tr>
<td>w (m³/y)</td>
<td>0.73</td>
</tr>
<tr>
<td>(\varepsilon) (Bq)</td>
<td>2.18E-10</td>
</tr>
</tbody>
</table>

Table 2: Type-II Probabilistic Parameters

<table>
<thead>
<tr>
<th>Input</th>
<th>Distribution</th>
<th>Lower Bound</th>
<th>Higher bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\lambda)</td>
<td>Log-uniform</td>
<td>(10^3)</td>
<td>(10^6)</td>
</tr>
<tr>
<td>(R)</td>
<td>Uniform</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5</td>
<td>10</td>
</tr>
</tbody>
</table>

The lower and upper cumulative probabilities of double Monte Carlo simulated samples of leach rate and retardation factor are as shown in Figs 4 and 5.

The histograms of type I probabilistic parameters T, v and L are as shown in Figs. 6-8.
Probability distribution of the time dependent risk through ingestion of water-borne radionuclide migrated through geological and biosphere is generated for a time interval of $10^4 \text{ y} - 10^6 \text{ y}$ by using the uncertainty distribution as shown in Figs. 4-8. Lower and upper cumulative probability distribution of the estimated time independent risk are used to compute the corresponding mean value of the risk at each observation time. The profile of the lower and upper bounds of the time dependent risk is presented in Fig. 9.

Bounds of risk per annum at each time can be easily predicted by drawing a line parallel to the ordinate at a specific time. Therefore, bounds of risk at that specific time will be the intersection points of the line drawn and the lower and upper bound risk profile. It can be concluded from Fig. 9 that for the present problem, the interval of risk at time, $t = 40000 \text{ y}$ is found as $[4.0E-14, 3.5E-12]$ per year. Time profile of intervals of risk in a similar way can be easily generated to make some effective decisions on the issue of safe disposal of radioactive waste.

**Conclusions**

Risk assessment using Monte Carlo simulation is known as probabilistic risk assessment that requires careful interpretation when the spread of the variables represents uncertainty due to scarcity of...
data rather than a genuine and measurable random distribution. Specific problems arise when the risk is dominated by a specific probability distribution of one of the parameter with a particular combination of other parameter values, as frequently occurs in assessments of nuclear waste repositories. In these circumstances, traditional methods may be computationally inefficient and, in any case, their results tend to accentuate the arbitrariness of much of the input data. Not only that, imprecise information of the parameters of a probability distribution will modify the spread of the output and hence in this context, double Monte Carlo simulation has been applied. In this paper, double Monte Carlo simulation based modeling of transport of radionuclide through a geological repository has been presented. Double Monte Carlo based modeling addresses the type II probabilistic parameters. Type II parameters play a major role in the simulation. Probability distributions of uncertain parameters are taken by expert’s opinion. Presence of bounds of the risk can provide in making the decisions about the performance of the geological repository. That is to say that if the geological repository is perfect, it will restrict to migrate the radionuclide into the biosphere.

References


