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Monte Carlo-based assessment of the safety performance of a radioactive waste repository

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ABSTRACT

The present paper illustrates a Monte Carlo simulation-based compartment model for evaluating the expected dose to the critical group from direct intake of contaminated water. An application to a realistic case study is presented to demonstrate the feasibility of the approach.

1. Introduction

The performance assessment of a radioactive waste repository aims at evaluating the harm caused by the potential release of radioactive wastes from repositories and intake by humans [1,2]. Models of subsurface radionuclide transport are typically used to analyze return of radionuclides through groundwater pathways back to the biosphere [3,4].

From the Regulatory Agency viewpoint, new licensing standards are being issued for radioactive waste repositories, requiring estimation of expected dose to some defined critical groups and associated uncertainty of both aleatory (stochasticity of future system behavior) and epistemic (lack of knowledge of model parameter values) nature [5,6].

Given the different spatial and temporal scales of the processes involved, a suitable approach is that of modeling radionuclide migration through compartments of the repository and geologic media, at different scales of detail; this allows keeping the analysis manageable by adapting the level of detail in the model description of migration processes occurring at different physical scales; the output information provided by the modeling at a given scale is used to determine parameters of the stochastic transition process of migration across compartments at the next higher scale. Within this modeling paradigm, Markovian hypotheses can be introduced to analytically model stochasticity of the transfer process across compartments [7–10].

In this paper, Monte Carlo simulation is used for modeling particle migration in medium compartments; the simulation scheme is adopted because it allows realistic modeling of system behavior without encountering difficulties (or simplifications thereof) brought by the need of finding analytical or numerical solutions, and naturally accounting for the aleatory uncertainty related to stochasticity of the migration process [11]; the simulation environment also lends itself to propagation of epistemic uncertainties in model parameters, with no additional burden on modeling.

The approach is illustrated with reference to radionuclide releases out of a near surface repository design concept studied by ENEA, the Italian New Technologies, Energy and Environment Agency [12,13]. After being released from the repository, the radionuclides start migrating through the unsaturated zone and the saturated groundwater zone beneath. The groundwater mass flow and radionuclide transport processes are followed in a two-dimensional array of compartments, whereas, for simplicity, the unsaturated zone is modeled by simply introducing a delay in times of migration of the radionuclides. The expected radionuclide concentrations in groundwater compartments and dose intensities released to a critical person are outputs of the analysis by Monte Carlo simulation.

The paper is organized as follows. In Section 2, the stochastic process of radionuclide migration within a compartmentalized medium is formalized in the framework of Markov analysis and

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the basic principles of Monte Carlo simulation are recalled. In Section 3, the Monte Carlo simulation model of radionuclide migration is applied to the ENEA case study [12–14]. Finally, some conclusions of the proposed approach are drawn.

2. Compartment model for the simulation of radionuclide migration

A two-dimensional medium discretized into $N=N_xN_y$ compartments is considered (Fig. 1), where N_x and N_y are the number of compartments along the x- and y-axes, respectively. An additional compartment $N+1$ is added to represent the environment in which the domain is embedded. For simplicity of illustration, and with no loss in characterization of the migration process, radioactive decay is here neglected; its inclusion within the Monte Carlo simulation modeling schemes poses no particular additional challenge.

Under specific assumptions, the stochastic process of radionuclide migration across compartments can be modeled by a continuous-time Markov process. Let us denote by $X(t)$ the state variable representing the position state of a radionuclide particle migrating within the compartment matrix, i.e., $X(t)=n$ implies that the radionuclide is in compartment n at time t, $n=1,2,\ldots,N+1$ [15]. The outcome of the stochastic process of radionuclide migration described by the state variable $X(t)$ is completely described by the row vector

$$\mathbf{P}(t)=[P_1(t)\;\;P_2(t)\;\;\ldots\;\;P_{N+1}(t)] \tag{1}$$

where $P_n(t)$ is the probability that the radionuclide is in state n at time t, i.e., $X(t)=n$. Introducing the Markov property, if the radionuclide is in state (compartment) i at time t (i.e., $X(t)=i$), the probability of reaching state j at time $t+v$ does not depend on the states (compartments) $X(u)$ visited by the radionuclide at times u prior to t (i.e., $0<u<t$); in other words, given the present state (compartment) $X(t)$ occupied by the radionuclide, its future behavior is independent of the past [15]:

$$P[X(t+v)=j|X(t)=i,X(u)=x(u),0<u<t]=P[X(t+v)=j|X(t)=i] \tag{2}$$

The conditional probabilities

$$P[X(t+v)=j|X(t)=i],\quad i,j=1,2,\ldots,N+1 \tag{3}$$

are called the transition probabilities of the Markov process.

If the transition probabilities do not depend on time instants t and $t+v$ but only on the width of the separating time interval v, then the Markov process is said to be homogeneous:

$$P[X(t+v)=j|X(t)=i]=p_{ij}(v),\quad t,v>0\quad\text{and}\quad i,j=1,2,\ldots,N+1 \tag{4}$$

Under these hypotheses, it can be shown [16] that the stochastic time T_{ij} that the radionuclide resides in state (compartment) i before making a transition to state (compartment) j is exponentially distributed with parameter λ_{ij}. Consequently, the probability of the process undergoing a transition from state (compartment) i to state (compartment) j in the time interval v is [16]

$$p_{ij}(v)=1-e^{-\lambda_{ij}v} \tag{5}$$

Considering a time interval $v=\Delta t$ sufficiently small that only one transition can occur and applying the Taylor expansion of Eq. (5), the one-step transition probability from compartment i to compartment j can be written as

$$p_{ij}(\Delta t)=P[X(t+\Delta t)=j|X(t)=i]=\lambda_{ij}\,\Delta t+O(\Delta t) \tag{6}$$

where λ_{ij} is density of transition from state i to state j, and $\lim_{\Delta t\to 0}O(\Delta t)/\Delta t=0$. Thus, the conditional probability of a transition from state i to state j in the time interval Δt is $\lambda_{ij}\,\Delta t$, whereas the number of radionuclides migrating from compartment i to compartment j in the time interval $(t,t+\Delta t)$ is $MP_i(t)\lambda_{ij}\,\Delta t$, where M is the total number of particles in the system and $P_i(t)\lambda_{ij}\,\Delta t$ the unconditional probability of a transition from i to j in $(t,t+\Delta t)$.

$n_x=1$	$n=1$	2	…	N_y
2	N_y+1	N_y+2	…	$2N_y$
3	⋮	⋮	⋮	⋮
⋮	⋮	⋮	⋮	⋮
⋮	⋮	⋮	⋮	⋮
N_x				$N=N_x\cdot N_y$
	$n_y=1$	2	…	N_y

Fig. 1. N_xN_y matrix of N compartments.

The migration process is then probabilistically described by the following system of ordinary differential equations:

$$\frac{d\mathbf{P}}{dt}=\mathbf{P}(t)\mathbf{\Lambda} \tag{7}$$

where

$$\mathbf{\Lambda}=\begin{bmatrix} -\sum\limits_{j=2}^{N+1}\lambda_{1j} & \lambda_{12} & \cdots & \lambda_{1N+1} \\ \lambda_{21} & -\sum\limits_{\substack{j=1\\ j\neq 2}}^{N+1}\lambda_{2j} & \cdots & \lambda_{2N+1} \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \tag{8}$$

is the transition rate matrix. In principle, Eq. (7) allows finding analytical solutions for the dynamics of state probabilities $\mathbf{P}(t)$, provided the values of compartment transition rates λ_{ij} (8) are available.

However, in many realistic cases, some of the above assumptions must be relaxed, e.g. to account for non-homogeneities in time and space. In such cases, transition times between compartments can no longer be described by exponential distributions and analytical solutions are often not available, thus rendering numerical approximation schemes mandatory.

In these cases, Monte Carlo simulation offers a viable alternative for estimating probabilities $P_n(t)$ that a radionuclide is in compartment n at time t, $n=1,2,\ldots,N+1$ and, consequently, the probability density function of the release in the environment $pdf_{\text{env}}(t)$. The stochastic migration process of a large number M of radionuclides in the N_xN_y domain is simulated by repeatedly sampling transitions of each individual radionuclide particle across the compartments, from the proper transition probability density functions. The random walk of individual radionuclides is simulated either until they exit the domain to the $N+1$ compartment "environment", that is an absorbing state from which particles are not allowed to come back to the migration domain, or until their lifetime crosses the time horizon T of the analysis. The time horizon T is discretized into N_t equally spaced time instants; a counter $Count(n,k)$ is associated to each compartment $n=1,2,\ldots,N+1$ and each discrete time $k=1,2,\ldots,N_t$. During the simulation, a one is accumulated in the counter $Count(n,k)$ if a