Annals of Nuclear Energy 37 (2010) 861–866

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

Monte Carlo estimation of radionuclide release at a repository scale

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ARTICLE INFO

Article history:
Received 9 September 2009
Received in revised form 18 February 2010
Accepted 19 February 2010
Available online 3 April 2010

Keywords:
Radioactive waste repository
Radionuclide migration
Compartment model
Monte Carlo simulation

ABSTRACT

Prediction of radionuclide release is a central issue in the performance assessment of nuclear waste repositories. This requires modeling of the radionuclide migration processes through the repository barriers, accounting for the related uncertainties. The present paper illustrates a Monte Carlo simulation-based compartment model in which detailed, local-scale modeling feeds a global-scale analysis of the repository, at reasonable computational expenses. An application to a realistic case study is presented to verify the feasibility of the approach.

1. Introduction

The objective of the engineered and natural barriers of a radioactive waste repository is to prevent the release of radionuclides and retard their migration to the groundwater, and eventually to the biosphere (IAEA, 1999a).

The assessment of the performance of these barriers, both in the repository design and operative phases, is a complex task which entails (Helton and Sallaberry, 2009; Yim and Simonson, 2000): (i) the identification of the scenarios that influence the repository behavior throughout its lifetime; (ii) the estimation of their probabilities of occurrence; (iii) the estimation of their consequences associated to the release of the radionuclides, typically in terms of the expected dose received by the defined critical group of people; and (iv) the evaluation of the uncertainties associated to the aforementioned estimates.

In this framework, the quantitative analysis of the processes of radionuclide migration across the barriers of the repository to the main intake paths, plays a fundamental role. Eventually, the analysis is to be made at the repository scale, accounting also for macroscopic effects such as those due to the spatial arrangements of the waste containers in the repository structures (Kawasaki et al., 2005; Kawasaki and Ahn, 2006) and the heterogeneity of the media (Tsujimoto and Ahn, 2005; Williams, 1992; Williams, 1993). For example, the assumption of radionuclides point release, often made for ease of computation, may lead to inaccuracies in the estimation of the repository safety performance, since there might be non-linear interactions among the radionuclides released by different canisters in the same groundwater stream and the radionuclide travel time across the barriers of the repository may vary by orders of magnitude. In practice, this can lead to significant computational expenditures if the analysis is performed by extension to the repository scale of the detailed flow and mass transport codes used at the single waste package scale.

Also, various national Nuclear Regulatory Agencies are issuing new licensing standards for radioactive waste repositories, which require the estimation of the expected dose to some defined critical groups and the associated uncertainty of both aleatory (stochasticity of the future system behavior) and epistemic (lack of knowledge of the model parameter values) types (Helton and Sallaberry, 2009). This also can lead to quite substantial computational efforts with the flow and transport codes classically used.

An approach which seems suitable for effectively handling the above issues is that of proceeding to a compartmentalized modeling of the radionuclide migration at the different scales of the media of the repository. Detailed modeling would be applied to the smaller domain to characterize the migration process in a single compartment; the results of this modeling would serve as input of the model of the repository area compartments, based on a coarser discretization and, thus, computationally less intensive.

Simplifying Markovian hypotheses are often introduced to model the stochasticity of the transfer process across the compartments (Kawasaki et al., 2005; Kawasaki and Ahn, 2006; Lee and Lee, 1995; Xu et al., 2007). In this paper, instead, we resort to Monte Carlo simulation for modeling particle migration in a compartmentalized repository; the simulation scheme allows modeling realistic features of system behavior without encountering

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doi:10.1016/j.anucene.2010.02.011

the difficulties (or simplifications thereof) brought by the need of finding analytical or numerical solutions, and naturally accounting for the aleatory uncertainty related to the stochasticity of the migration process.

The proposed approach is illustrated through its application to a near surface repository design concept studied by ENEA, the Italian New technologies, Energy and Environment Agency (Marseguerra et al., 2001). The results are compared to those obtained by application of the detailed model to the full repository scale.

The paper is organized as follows. In Section 2, the formulation of the process of radionuclide migration within a compartmentalized medium and 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 (Kawasaki et al., 2005; Marseguerra et al., 2001). Finally, some conclusions on the advantages and limitations of the proposed approach are provided in Section 4.

2. Compartment model of radionuclide migration

For simplicity, but with no loss of generality, let us assume that the radionuclide migration occurs within a two-dimensional medium discretized into $N = N_x \times N_y$ compartments (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 the characterization of the migration process, radioactive decay is here neglected; its inclusion within the Monte Carlo simulation modeling schemes poses no particular additional challenge.

Let us also suppose that the radionuclide migration across the compartments can be modeled by a continuous-time Markov process. The state variable $X(t)$ represents the position state of a single radionuclide migrating within the compartment matrix, i.e., $X(t) = n$ implies that the radionuclide is in compartment n at time t, $n = 1, 2, \dots, N + 1$ (IAEA, 1999b). The stochastic process of radionuclide migration described by the state variable $X(t)$ is completely described by the row vector

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

where $P_n(t)$ is the probability that the radionuclide is in state n at time t, i.e., $X(t) = n$.

Accounting for 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., $0 \leqslant u < t$); in other words, given the present state (compartment) $X(t)$ occupied by the radionuclide, its future behavior is independent of the past (Zio, 2009):

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

The conditional probabilities

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

are called the transition probabilities of the Markov process.

If the transition probabilities do not depend on the 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:

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

Considering a time interval $v = \Delta t$ sufficiently small that only one transition can occur and applying the Taylor expansion of Eq. (4), the one-step transition probability from compartment i to compartment j can be written as:

$$p_{ij}(\Delta t) = P[X(t+\Delta t) = j|X(t) = i] = \lambda_{ij} \cdot \Delta t + \theta(\Delta t) \tag{5}$$

where λ_{ij} is the rate of the transition from state (compartment) i to state (compartment) j, and $\lim_{\Delta t \to 0} \frac{\theta(\Delta t)}{\Delta t} = 0$.

In the continuous time domain (i.e., for an infinitesimal time interval $\Delta t \to 0$), the stochastic time T_{ij} that the radionuclide resides in state (compartment) i before making a transition to state (compartment) j is, then, exponentially distributed with parameter λ_{ij} and the migration process is probabilistically described by the following system of ordinary differential equations:

$$\frac{dP}{dt} = \mathbf{P}(t) \cdot \Lambda \tag{6}$$

where

$$\Lambda = \begin{bmatrix} -\sum_{j=2}^{N+1} \lambda_{1j} & \lambda_{12} & \cdots & \lambda_{1N+1} \\ \lambda_{21} & -\sum_{j=1,\ j\neq 2}^{N+1} \lambda_{2j} & \cdots & \lambda_{2N+1} \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \tag{7}$$

is the transition rate matrix.

In principle, Eq. (6) allows finding analytical solutions for the dynamics of the state probabilities $\mathbf{P}(t)$, provided the values of the compartment transition rates λ_{ij} (7) 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, the transition times between the compartments can no longer be described by exponential distributions and analytic solutions are often not available, thus rendering numerical approximation schemes mandatory.

In this regard, Monte Carlo simulation can offer an effective procedure for estimating the probabilities $P_n(t)$ that a radionuclide is in compartment n at time t, $n = 1, 2, \dots, N + 1$ and, consequently, the probability density function of the release in the environment $pdf_{env}(t)$. The stochastic migration process of a large number M of radionuclides in the $N_x \times N_y$ domain is simulated by repeatedly sampling the transitions of each individual radionuclide particle across all compartments, from the proper transition probability density functions. The random walk of the individual radionuclide is simulated either until it exits the domain to the $N + 1$ compartment "environment", or until its lifetime crosses the time horizon T of the analysis. The time horizon T is subdivided in N_t time instants at a distance Δt to each other; a counter $C(n,k)$ is associated to each compartment $n = 1, 2, \dots, N + 1$ and each discrete time instant $k = 1, 2, \dots, N_t$. During the simulation, a one is accumulated in

$n_x = 1$	n=1	2	...	N_y
2	$N_y + 1$	$N_y + 2$	...	$2N_y$
3	⋮	⋮	⋮	⋮
⋮	⋮	⋮	⋮	⋮
⋮	⋮	⋮	⋮	⋮
N_x				$N = N_x \times N_y$
	$n_y = 1$	2	...	N_y

Fig. 1. An $N_x \times N_y$ matrix of N compartments.