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Development of compartment models with Markov-chain processes for radionuclide transport in repository region

Haruko Murakami *, Joonhong Ahn

Department of Nuclear Engineering, University of California, Berkeley, CA 94720-1730, United States

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ABSTRACT

This paper presents a new radionuclide transport model for performance assessment and design of a geologic repository for high-level radioactive waste. The model uses compartmentalization of a model space and a Markov-chain process to describe the transport. The model space is divided into an array of compartments, among which a transition probability matrix describes radionuclide transport. While similar to the finite-difference method, it has several advantages such as flexibility to include various types of transport processes and reactions due to probabilistic interpretation, and higher-order accuracy resulting from direct formulation in a discrete-time frame.

We demonstrated application of this model with a hypothetical repository in porous rock formation. First we calculated a three-dimensional steady-state heterogeneous groundwater flow field numerically by the finite-element method. The transition probability matrix was constructed based on the flow field and hydraulic dispersion coefficient. The present approach has been found to be effective in modeling radionuclide transport at a repository scale while taking into account the effects of change in hydraulic properties on the repository performance. Numerical exploration results indicate that engineered barrier configuration and material degradation have substantial effects on radionuclide release from the repository.

1. Introduction

Japan has been planning to construct a geologic repository in a water-saturated region at depth of more than 300 m from the surface. It consists of an array of waste tunnels containing waste canisters connected by access tunnels, which will be several hundred meters long (Sugita et al., 2005).

The previous performance assessment (JNC, 2000) was based on a radionuclide transport model with conservative parameters and assumptions for the single-canister configuration in a hypothetical repository without specifying the site location. Although such a model is sufficient to investigate feasibility of the generic geologic disposal concept, it is not suitable for optimizing the repository design or for comparing several proposed sites, since the simplification obscures parameter sensitivity of each component. Recently, Nuclear Waste Management Organization of Japan (NUMO) conducted groundwater flow analysis including a repository structure (Sugita et al., 2005), but effects of the repository design and structure on radionuclide transport have not been investigated yet.

The important detail structure of the repository currently considered (Sugita et al., 2005) includes several engineered barrier components that hinder groundwater flow through the repository, such as clay backfill in the tunnels and clay plugs at the end of the waste tunnels. Degraded concrete walls and excavation-damaged zones (EDZ) around the tunnels could become a fast path of radionuclide transport. In order to compare different designs and proposed site, the transport model must capture the difference in hydraulic properties and the effect of material degradation. In addition, the model has to be flexible and computationally inexpensive to accommodate many different designs.

Previous work proposed a compartment-model approach to describe the radionuclide transport in the repository region (Ahn et al., 2002; Kawasaki et al., 2005; Lee and Lee, 1995; Marseguerra et al., 2003). The compartment approach is widely used in various types of contaminant transport models, especially for multimedia systems in biosphere such as the domain including biota and surface water in addition to groundwater (McKone, 1993). The basic principle is to divide a domain into an array of compartments, and describe the transport process inside and among the compartments. For the radionuclide transport applications, Ahn et al. (2002) utilized this approach to describe the transport through one-dimensional array of canisters. They treated transport processes associated with each canister (e.g. release from a canister and diffusion in surrounding clay buffer) as the process inside each compartment, and described the transport process among the compartment

* Corresponding author. Tel.: +1 510 642 5107; fax: +1 510 643 9685.
E-mail address: harukom@nuc.berkeley.edu (H. Murakami).

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by first-order differential equations. Kawasaki et al. (2005) and Marseguerra et al. (2003) introduced Markov-chain (MC) processes to describe the transport among the compartments.

While the compartment model with MC is fundamentally similar to an explicit scheme of finite-difference methods to solve partial differential equations, the advantage of this approach is its flexibility to include different geometries and various phenomena by probabilistic interpretation. Kawasaki et al. (2005) suggested that the model could be used to upscale the results from particle-tracking methods in a small-scale domain, which is helpful to reduce the computational time for simulating the transport in a larger domain.

The previous models, however, consider only a uniform groundwater velocity field or one- or two-dimensional domains. In order to use this approach for realistic and practical purposes, it is necessary to demonstrate its applicability to a non-uniform and three-dimensional domain with a groundwater flow model coupled.

In this paper, we first formulate the transport process in a manner different from Kawasaki et al. (2005) and Marsequerra et al. (2003) such that we consider the transport in a discrete-time and discrete-space frame directly. In addition, we use the probabilistic interpretation to include radionuclide decay and sorption phenomena. The transition probability is derived from physical interpretation of transport processes for a non-uniform domain.

We apply our model to a hypothetical repository in porous rock formations, which has two rows of waste tunnels connecting by two access tunnel, surrounded by concrete walls and the EDZ. We evaluate several different repository designs and conditions, such as with or without clay plugs sealing the waste tunnels, and degradation of concrete wall. Based on the three-dimensional, non-uniform groundwater flow field numerically obtained from the finite-element method, we construct the transition probability matrix and simulate the transport in the domain. We consider the peak release rate of the radionuclide at the downstream plane of the model space as the performance metric to observe and compare the design cases.

2. Model

2.1. Compartment model with a Markov-chain process

We first divide a model domain into an array of n compartments ($i = 1, 2, \ldots, n$). Let N_i denote the number of radionuclides in Compartment i. We consider a transport process of the radionuclides directly in a discrete-time frame as evolution of N_i in one time step between time t and $t + \Delta t$. The change in N_i between time t and $t + \Delta t$ is,

$$\Delta N_i(t) = N_i(t+\Delta t) - N_i(t). \tag{1}$$

A Markov-chain process describes the transport of each particle among the compartments at every time step. As a Markov property, we assume that a particle moves between the current and next time step, depending only on the environment at the current and next positions such as groundwater velocity, diffusivity and dispersivity, not on the past course that the particle has taken to reach the current position. This central assumption of a Markov-chain process generally holds, since the radionuclides move mindlessly without memory.

In the compartment model, the number of each compartment represents a position of the particle. Let P_{ij} be a probability for a radionuclide to move from Compartment i to j in a time interval Δt, which is defined as a transition probability in a Markov-chain process. The transition probability P_{ij} depends only on the environment in Compartment i and j.

This transition probability, representing the transport of each radionuclide, needs to be related to evolution of the number of radionuclides in each compartment. A large number of radionuclides allow us to apply the weak law of large numbers. We consider the average number of radionuclides moving among compartments, such that the number of radionuclides moving from Compartment i to j in Δt is written as $N_i P_{ij}$.

ΔN_i is equal to the number of radionuclides moving into Compartment i minus the number moving out from Compartment i, which is written as,

$$\Delta N_i(t) = \sum_{\substack{j=1\\ j\neq i}}^{n} N_j(t)P_{ji} - \sum_{\substack{j=1\\ j\neq i}}^{n} N_i(t)P_{ij}. \tag{2}$$

Kawasaki et al. (2005) applied the weak law of large numbers to all the existing radionuclides in the domain so that it was necessary to normalize the number of radionuclides in the domain as well as ones potentially entering the domain over time. Such normalization is not necessary in the present model, since we apply the law to the number of radionuclides moving at every time step. The present approach is more flexible to include any form of source release rates usually pre-calculated by the other source-term models.

When we have a pre-calculated source release rate into Compartment i, denoted by $g_i(t)$, the number of radionuclides entering Compartment i between t and $t + \Delta t$ is,

$$G_i(t) = \int_t^{t+\Delta t} g_i(t)dt. \tag{3}$$

We can add Eq. (3) to the mass balance equation (Eq. (2)).

It is straightforward to include radioactive decay, using probabilistic interpretation, since the decay process is known to have the Markov property. Since the probability for a particle not to decay in Δt is $\exp(-\lambda\Delta t)$ with decay constant λ, we can modify Eq. (2) as,

$$\Delta N_i(t) = \left(\sum_{\substack{j=1\\ j\neq i}}^{n} N_j(t)P_{ji} - \sum_{\substack{j=1\\ j\neq i}}^{n} N_i(t)P_{ij} \right) e^{-\lambda\Delta t} - N_i(t)\left(1 - e^{-\lambda\Delta t}\right). \tag{4}$$

The first term represents the number of radionuclides moving in and out Compartment i with decay and the second term represents the radionuclides decaying in Compartment i. The number of the radionuclides at the next step is written as,

$$N_i(t+\Delta t) = \left(\sum_{\substack{j=1\\ j\neq i}}^{n} N_j(t)P_{ji} - \sum_{\substack{j=1\\ j\neq i}}^{n} N_i(t)P_{ij} \right) e^{-\lambda\Delta t} + N_i(t)e^{-\lambda\Delta t}. \tag{5}$$

We can compare this formulation to the one developed by Marseguerra et al. (2003), which discretize a continuous-time mass balance equation. The continuous-time mass balance equation is given as,

$$\frac{dN_i(t)}{dt} = \sum_{\substack{j=1\\ j\neq i}}^{n} N_j(t)q_{ji} - \sum_{\substack{j=1\\ j\neq i}}^{n} N_i(t)q_{ij} - \lambda N_i(t). \tag{6}$$

where q_{ij} is the particle transition rate from Compartment i to j. The forward time-discretization of Eq. (6) is written as,

$$\Delta N_i(t) = \sum_{\substack{j=1\\ j\neq i}}^{n} N_j(t)q_{ji}\Delta t - \sum_{\substack{j=1\\ j\neq i}}^{n} N_i(t)q_{ij}\Delta t - \lambda\Delta t N_i(t). \tag{7}$$

In Eq. (7), the radionuclides moving into and out from Compartment i are not subject to decay. Our direct discrete-time formulation