Development of Geologic Repository Models for Site Selection and Design Optimization

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ABSTRACT

This paper presents a new radionuclide transport model to evaluate performance of a geologic repository for high-level radioactive waste. The model is based on a compartment model, and a Markov-chain model. A domain is divided into an array of compartments, and a transition probability matrix describes transport among the compartments. The model is demonstrated for a hypothetical repository in porous rock formations. A three-dimensional, non-uniform groundwater flow field is created numerically using the finite element method. The transition probability matrix is constructed based on the velocity field and hydraulic dispersion coefficients. The results show that this transport model can capture the change of hydraulic properties in the domain by the repository structure and material degradation. They also suggest that the impact of engineered barrier systems should be evaluated in comparison with the site conditions such as the ambient hydraulic head gradient.

Key Words: Geologic Disposal, Compartment model, Markov-chain process

1. INTRODUCTION

As a final disposal for high-level radioactive waste, many countries have proposed the deep geologic disposal under a water table. In Japan, the repository will be constructed in the water-saturated region at 300-500m deep from the surface. It consists of an array of tunnels containing the waste canisters, ranging over several square kilometers.

Previous performance assessments [1] are based on a simplified radionuclide transport model with conservative parameters and assumptions. It assumed a uniform flow of groundwater through repository, neglecting the repository structure. Although such a model is sufficient to evaluate the safety margin of the repository, it is not suitable to optimize the repository design, since each component should be analyzed in terms of its impact on the radionuclide transport.

For example, degraded concrete wall and excavation-damaged zone (EDZ) around tunnels could become a fast path of transport. In order to hinder the flow through the repository, several engineered barrier system will be introduced such that the tunnels will be filled by clay material, and concrete/clay plugs will be installed at the end of tunnels. The transport model must capture such differences of hydraulic properties, in order to compare the different designs. In addition, in order to analyze many different designs, the model has to be flexible and computationally inexpensive.
Previous works proposed compartment-model approach to describe the transport in the repository region [2]-[3]. In the compartment models, the domain is divided into an array of compartments. A Markov-chain process describes the transport by using transition probabilities of particles among the compartments. The advantage of this approach is its flexibility to include different geometries and various phenomena by probabilistic interpretation. It can also utilize results from the particle-tracking methods in a small-scale domain, to simulate the transport in larger domain with less computational power.

The previous models, however, only consider the uniform groundwater velocity field and one-dimensional domain. This paper presents the extension of compartment model in a non-uniform and three-dimensional domain. The transition probability is derived from more fundamental interpretation of transport process for a non-uniform domain.

We apply the model to a hypothetical repository in porous rock formations. Several repository designs and degradation of concrete wall are considered. A three-dimensional, non-uniform groundwater flow field is calculated numerically using the finite-element method for each set of the repository parameters. The transport is simulated to obtain a release rate to the downstream.

2. MODEL

2.1. Compartment Model

The domain is divided into an array of $n$ compartments ($i = 1, 2 \ldots n$). Let $N_{s,i}$ and $N_{a,i}$ denote the number of solute particles and sorbed particles in compartment $i$, respectively. The mass balance equations are written as a first-order differential equation with time as,

$$
\frac{dN_{s,i}}{dt} = -r_{a,i}N_{s,i} + r_{d,i}N_{a,i} + \sum_{j=1}^{n} q_{ij}N_{s,j} - \sum_{j=1}^{n} q_{ij}N_{s,i} - \lambda N_{s,i},
$$

$$
\frac{dN_{a,i}}{dt} = r_{a,i}N_{s,i} - r_{d,i}N_{a,i} - \lambda N_{a,i},
$$

where $r_{a,i}$ and $r_{d,i}$ are the adsorption and desorption coefficient, respectively. $q_{ij}$ is the transfer rate of solute particle from compartment $i$ to compartment $j$. $\lambda$ is the radioactive decay constant. Although decay chains are not considered here, Equation (1) can be easily extended. The relationship between solute particles and sorbed particles is usually assumed to be linear as $N_{s,i} = \alpha N_{a,i}$.

Although Marseguerra et.al. derived the transfer rate $q_{ij}$ by the analogy to an advection-dispersion equation [3], they considered only a uniform domain. We take a different approach to derive the transport parameters, in a similar manner to Costa et.al.[4].

First, we consider the discrete-time frame by the forward Euler method as,
\[ N_{s,i}(t + \Delta t) = N_{s,i}(t) + \left( \frac{r_{a,i}}{\alpha_p - r_{a,j}} \right) \Delta t N_{s,j} + \sum_{j=1}^{n} q_{j,i} \Delta t N_{s,j} - \sum_{i=1}^{n} q_{j,i} \Delta t N_{s,i} - \lambda \Delta t N_{s,i}. \]  \hspace{1cm} (2)

We define a transition probability, \( P_{ij} \), for a particle to move from compartment \( i \) to \( j \) in a time interval \( \Delta t \). Since the number of particles is large, the weak low of large numbers is applied. We consider “averaged” movement of particles so that the transition probability is interpreted to the transfer rate as \( P_{ij} = q_{ij} \Delta t \).

In the numerical calculation, the number of particles in each compartment at \( t = k \Delta t \) is stored in a vector \( a^{(k)} = (N_{s,1}(t), N_{s,2}(t), \ldots, N_{s,n}(t)) \). The transport in one interval is described by the matrix-vector operation as,

\[ a^{(k+1)} = a^{(k)}[P] + a^{(k)}[r] - \lambda \Delta t a^{(k)}. \]  \hspace{1cm} (3)

where \( [P] \) is an \( n \) by \( n \) transition probability matrix defined as \( [P] = P_{ij} \) and \( [r] \) is a sorption-term matrix defined as \( [r] = (r_{d,i}/\alpha_p - r_{a,i}) \Delta t \) for \( i = j \) and \( [r] = 0 \) otherwise.

### 2.2. Derivation of Transition Probability

First, we consider the transition probabilities from compartment \( i \) in a one-dimensional array. It is assumed that particles stay in the original compartment or move only to the adjacent compartments in a small time interval \( \Delta t \). The destination compartments are prescribed as \{\( i-1, i, i+1 \)\}. Let \( X_i = \{-1, 0, +1\} \) be the magnitude of displacement of a particle in \( \Delta t \). We can define three transition probabilities as \( P_{i,i-1}, P_{i,i} \) and \( P_{i,i+1} \). The expectation and the variance of \( X_i \) is obtained as,

\[ E[X_i] = P_{i,i+1} - P_{i,i-1}, \]
\[ \text{Var}[X_i] = \left( P_{i,i+1} + P_{i,i-1} \right) - \left( P_{i,i+1} - P_{i,i-1} \right)^2 \]  \hspace{1cm} (4)

They can be directly determined by the particle-tracking method. Here we consider the transport in a non-uniform porous medium, where the hydraulic dispersion causes the distribution of particles. The hydraulic dispersion coefficient is the sum of a diffusion coefficient and a mechanical dispersion coefficient.

Consider three compartments \{\( i-1, i, i+1 \)\}, having different length of compartments \{\( d_{i-1}, d_i, d_{i+1} \)\}, porosities \{\( \varepsilon_{i-1}, \varepsilon_i, \varepsilon_{i+1} \)\}, and dispersion coefficients \{\( D_{i-1}, D_i, D_{i+1} \)\}. The concentration gradient is assumed to drive the dispersion, following common working hypothesis. The transition probabilities by dispersion from \( i \) to \( i+1 \) and from \( i \) to \( i-1 \) are obtained by multiplying the average dispersive flux by the time interval as,

\[ P_{\text{disp},i,i+1} = \frac{\Delta t}{\varepsilon_i d_i} \frac{\varepsilon_i D_i + \varepsilon_{i+1} D_{i+1}}{d_i + d_{i+1}}, \quad P_{\text{disp},i,i-1} = \frac{\Delta t}{\varepsilon_i d_i} \frac{\varepsilon_i D_i + \varepsilon_{i-1} D_{i-1}}{d_i + d_{i-1}} \]  \hspace{1cm} (5)
The expectation value and variance are determined as $E_{\text{disp}}[X_i]$ and $\text{Var}_{\text{disp}}[X_i]$ from definitions. The total expectation and variance is obtained by adding the advection term $v_i \Delta t / d_i$ as,

$$
E[X_i] = \frac{v_i \Delta t}{d_i} + E_{\text{disp}}[X_i]
$$

$$
\text{Var}[X_i] = \text{Var}_{\text{disp}}[X_i]
$$

(7)

The transition probabilities are obtained by substituting Equation (8) in Equation (4). The time-step size and compartment size is restricted to avoid the probabilities to be negative.

For multi-dimensional cases, the transition probabilities are obtained in the same manner by considering each direction independently.

3. DEMONSTRATION

Figure I shows a three-dimensional hypothetical repository. It consists of tunnels (inner cross-sectional area $2 \times 2 \text{m}^2$), which are surrounded by concrete wall (0.4 m thick) and EDZ (0.6m thick), and host rock. 6 waste forms ($0.8 \times 0.8 \times 0.8 \text{ m}^3$) are located in the tunnels. Clay Plugs (0.6m thick) are installed at the end of the tunnels.

The domain is divided into $n = 86,112$ compartments. The number of compartments in each direction is $(n_x, n_y, n_z) = (78, 48, 23)$. The boundary condition is applied as an equi-potential plane at the right and the left side plane ($x = -15.8$ and $x = 15.8$) in Figure I (a). The ambient constant hydraulic gradient is set to be $c = 1 \times 10^{-3}$ or $1 \times 10^{-4}$ from left to right.

Table I shows input parameters, which are hydraulic conductivities $K$, porosities $\varepsilon$, and pore diffusion coefficients $D$. Each material is assumed to be a uniform porous medium. Since the repository scale is small, only effective diffusion coefficient is considered.
Table I. Hydraulic and transport parameters for each material in the repository region.

<table>
<thead>
<tr>
<th>Material</th>
<th>Rock</th>
<th>EDZ</th>
<th>Concrete</th>
<th>Backfill</th>
<th>Plug</th>
<th>Waste Form</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-\log K$ (m/s)</td>
<td>8*</td>
<td>6*</td>
<td>5*/13*</td>
<td>6***/12*</td>
<td>12*</td>
<td>K = 0***</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.347*</td>
<td>0.366*</td>
<td>0.333*</td>
<td>0.333*</td>
<td>0.307*</td>
<td>0.100***</td>
</tr>
<tr>
<td>$D$ (m$^2$/yr)</td>
<td>4.37E-3**</td>
<td>2.37E-3**</td>
<td>4.37E-3**</td>
<td>4.62E-2**</td>
<td>4.37E-3***</td>
<td>4.37E-3***</td>
</tr>
</tbody>
</table>

* From Reference [5], ** From Reference [6], *** Assumed values

Different hydraulic conductivities are assumed for intact or degraded concrete ($1 \times 10^{-13}$m/s or $1 \times 10^{-5}$m/s), and clay backfill or rock backfill ($1 \times 10^{-13}$m/s or $1 \times 10^{-6}$m/s). The impact of plugs is also compared. The following cases are considered:

1. No Plug / Clay backfill / Intact concrete
2. No Plug / Clay backfill / Degraded concrete
3. No Plug / Rock backfill / Degraded concrete
4. Plug / Clay backfill / Intact concrete
5. Plug / Clay backfill / Degraded concrete
6. Plug / Rock backfill / Degraded concrete

The non-uniform groundwater velocity field is formulated by the Darcy’s law, assuming time-independent and incompressible flow. It is calculated numerically by the finite element method. Transport is simulated based on the model described in the previous section. It is assumed that particles are released at the waste form locations at time 0, diffuse out from the waste form and transport thought the repository region. Absorbing boundary conditions are prescribed at the six planes. Decay and sorption is neglected, in order to focus on the effect of hydraulic properties. Although the release from the domain occurs at all the six planes, only the release from the downstream plane ($x=15.8$) is evaluated, since it has the highest peak.

Figure II and III shows the release rate from $x=15.8$ plane to down-stream for the case with $c =$
$1 \times 10^3$ and $1 \times 10^{-4}$, respectively. It can be considered that Figure II is an advection-dominant case and Figure III is a diffusion-dominant case.

Figure II shows the effect of the plugs to reduce the peak release rate by factor of 1.5. Although the degradation of concrete increases the release rate, the impact is relatively small. The difference of backfill material does not have impact, since a fast transport path in the degraded concrete region dictates the transport.

In Figure III, peaks of the release rate are lower than those in Figure II. Since the diffusion is dominant, the release from the other planes is increased. In this case, the plugs and degradation of concrete, and the difference of backfill material do not show significant difference.

This could suggest that the engineered barrier system should be designed based on the site conditions. If the hydraulic head gradient is small, the hindrance of groundwater flow will not contribute to enhance the safety. In fact, this demonstration is quite simplified so that it does not take into account the change of chemical condition by concrete degradation, nor sorption by clay material. More realistic chemical and geochemical processes should be included in the model.

### 3. CONCLUSIONS

This paper has presented a new transport model concept based on the compartment model and the Markov-chain model. The transition probabilities are derived for the transport in the non-uniform porous medium, by conserving the expectation and variance of the displacement. The model has been demonstrated for a hypothetical repository with three-dimensional, non-uniform groundwater flow field. It has shown that this model can capture the difference of the repository design and material degradation. The results suggest that the impact of such difference also depends on the site conditions. The model should be further improved to include chemical and geochemical processes to be used for the actual optimization of the repository design.

### REFERENCES