

A Nuclide Transport Model in the Fractured Rock Medium Using a Continuous Time Markov Process

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연속시간 마코프 프로세스를 이용한 균열암반매질에서의 핵종이동 모델

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Abstract

A stochastic way using continuous time Markov process is presented to model the one-dimensional nuclide transport in fractured rock matrix as an extended study for previous work [1]. A nuclide migration model by the continuous time Markov process for single planar fractured rock matrix, which is considered as a transient system where a process by which the nuclide is diffused into the rock matrix from the fracture may be no more time homogeneous, is compared with a conventional deterministic analytical solution. The primary desired quantities from a stochastic model are the expected values and variance of the state variables as a function of time. The time-dependent probability distributions of nuclides are presented for each discretized compartment of the medium given intensities of transition. Since this model is discrete in medium space, parameters which affect nuclide transport could be easily incorporated for such heterogeneous media as the fractured rock matrix and the layered porous media. Even though the model developed in this study was shown to be sensitive to the number of discretized compartment showing numerical dispersion as the number of compartments are decreased, with small compensating of dispersion coefficient, the model agrees well to analytical solution.

요 약

이전에 제시된 시간 균일적인 경우의 모델 [1]에 대한 확장으로 균열암반내 핵종이동에 관한 연속시간 마코프 프로세스를 이용한 통계적 방법에 의한 모델이 제시되었다. 단일 평판 균열을 갖는

암반매질에서 핵종이 균열로부터 암반조직내로 확산 이동하는 경우 더 이상 균일시간적인 마코프 모델을 적용할 수 없으므로 암반으로의 확산향을 시간에 따라 변화하는 과정으로 보아 모델을 제시한 후 기존의 결정론적 해석해와 비교하였다. 통계적모델의 최종 결과는 시간의 함수로서의 상태변수에 대한 기대값과 그 분산치일 것이다. 핵종의 시간 종속적인 확률분포가 전이강도가 주어질 때 매질내의 특성이 균질하다고 볼 수 있도록 나누어진 암반매질의 각 구획에 대해 주어지게 된다. 이 모델은 매질공간에 대해 불연속적이므로 핵종이동에 영향을 주는 변수들이 쉽게 균열암반이나 다중매질 등과 같은 비균질한 매질에 적용되어 질수 있다. 매질을 나눈 구획수가 수치적 분산에 민감한 것으로 나타났지만 분산계수의 보정에 의해 해석해와 잘 일치되는 것을 알 수 있었다.

1. Introduction

A stochastic approach by which the concentration distribution of nuclides in heterogeneous media could be modeled is using continuous time Markov process concept. In a companion paper, Lee et al. [1] have successfully used a continuous time Markov process to model the nuclide distributions in one dimensional geological systems. By extending this concept, the fractured rock matrix can be considered as a series of discretized compartments and the concentration of nuclides, or equivalent number of nuclides can be considered as a time-dependent random variable. Upon the base of the model in previous paper, we present an extended approach, by which transient system where a process of rock matrix diffusion from the fracture is considered can be modeled.

A nuclide in a given time interval could make a transition to any compartment by groundwater flow or could also disappear from any present compartment due to, e. g., radioactive decay or diffusive loss. All these processes are obviously conditional only on the present location of the nuclide regardless of its previous history utilizing the Markov conceptualization of the geologic system.

Meanwhile, the repository in such crystalline rock as granite, recently, has been favored because of highly low permeability of the rock matrix. However, in general, as the fracture offers principal groundwater flow path due to its higher

permeability than the rock matrix, nuclide transport will be dominated along the fracture. Although this is true, the rock matrix adjacent to the fracture plays an important role in overall nuclide transport. A convenient way to study such transport is to consider the rock matrix has a single planar fracture.

Since Neretnieks [2] showed the diffusion into the rock matrix can enhance retardation of the nuclide transport along the fracture, many analytical and numerical models are proposed [3, 4]. These studies, however, have been performed in deterministic way. In this regard, the objective of this research is to use continuous time Markov process to describe one-dimensional transport of nuclides through the fracture in the rock matrix in the vicinity of the radioactive waste repository. The primary desired quantities from a stochastic model are the mean values and variance of the state variables as a function of time.

2. Nuclide Distributions in the Fracture

A continuous-time Markov process $\{X(t), t \geq 0\}$ is a stochastic process having the property that the conditional distribution of the future state j at a time $t+s$, given the present state i at time s and all past states, depends only on the present state i and is independent of the past.

In matrix notation, the relation between the rate of change of the transition probability and the intensity of transition is represented as [5]

$$\frac{\partial}{\partial t} \mathbf{P}(\tau, t) = \mathbf{P}(\tau, t) \mathbf{\Lambda}(t) \quad (1)$$

and

$$\mathbf{P}(\tau, \tau) = \mathbf{I} \text{ (the identity matrix)} \quad (2)$$

where

$$\mathbf{P}(\tau, t) = \begin{pmatrix} P_{11}(\tau, t) & P_{12}(\tau, t) & \cdots & P_{1N}(\tau, t) \\ P_{21}(\tau, t) & P_{22}(\tau, t) & \cdots & P_{2N}(\tau, t) \\ \vdots & \vdots & \ddots & \vdots \\ P_{N1}(\tau, t) & \cdots & \cdots & P_{NN}(\tau, t) \end{pmatrix} \quad (3)$$

is the transition probability matrix and

$$\mathbf{\Lambda}(t) = \begin{pmatrix} \lambda_{11}(t) & \lambda_{12}(t) & \cdots & \lambda_{1N}(t) \\ \lambda_{21}(t) & \lambda_{22}(t) & \cdots & \lambda_{2N}(t) \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_{N1}(t) & \cdots & \cdots & \lambda_{NN}(t) \end{pmatrix} \quad (4)$$

is the intensity function of transition matrix.

As seen in Eq. (4), in transient system where processes or transition rate of nuclides varies with time, $\mathbf{\Lambda}(t)$ may be no more time homogeneous.

A rock matrix system in groundwater-saturated porous rock of porosity ϕ_p containing a single planar fracture of half width b is considered (Fig. 1). The fracture can be considered as a finite number of N compartments within which complete mixing of nuclides with groundwater takes place instantly. As considered by Tang et al. [4], the permeability of the porous matrix is very low and then transport is dominated in the fracture. In the rock matrix nuclide transport will be done by molecular diffusion in the direction perpendicular to the direction of the axis of the fracture. A decaying nuclide source locates at the inlet of the fracture.

The following processes are to be considered probabilistically to obtain the nuclide distribution in the fracture: (1) transition by the groundwater flow, (2) molecular diffusion from the fracture into the rock matrix, (3) adsorption onto wall of the fracture and within the rock matrix, and (4) radioactive decay. Longitudinal dispersion in the fracture, however, is assumed to be negligible in this study.

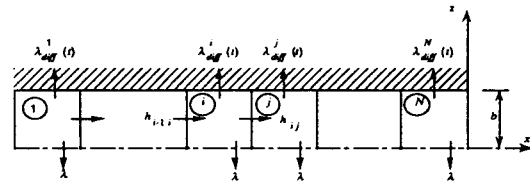


Fig. 1. Schematic Representation of Discretized Compartments of the Rock Matrix System.

Once such geologic system is assumed to have Markov property, since the Markov process requires that only the present value of the time dependent random variable (i. e., time dependent number of nuclides or concentration in certain compartment) be known to determine the future value of the random variable, the nuclide transport in geologic media, which is divided by finite number of geologic compartments N , can then be modeled as a time continuous Markov process, which is continuous in time with respect to the individual transport processes but discrete in medium.

At any time $\tau \in [0, t)$, when nuclides add to the first compartment at rate of $\zeta(\tau)$, that is equal to the volumetric flow rate of nuclides into the first compartment and may be represented as

$$\zeta(\tau) = Q_{in} C_0(\tau) V_1 \quad (5)$$

where

Q_{in} = volumetric flow rate of feeding groundwater into the first compartment ($L^3 T^{-1}$)

$C_0(\tau)$ = source concentration (L^{-3})

V_1 = volume of the first compartment (L^3).

As soon as a freshly fed nuclide enters the system, it may begin to transfer to one of the other compartments at once or may disappear. Here we can assume that all nuclides in the system behave stochastically and independently one another.

The number of new nuclides that enter the compartment in time interval $d\tau$ is $\zeta(\tau) d\tau$. If we consider the number of nuclides that have successfully entered the first compartment, then it has

a respective probability of $P_{ij}(t-\tau)$ that nuclides exist in j at time t , i.e., transition from the first compartment 1 to compartment j during the time interval $(t-\tau)$. Therefore, a binomial distribution can be formed for these new nuclides.

Also for large value of $\zeta(\tau) d\tau$, the binomial distribution is approximated to Poisson distribution.

Then we can get the distribution of $X_j(t)$, as defined in previous paper [1], the number of nuclides remaining in each compartment that have survived as follows:

$$E[X_j(t)] = \sum_{i=1}^N m_i(0) P_{ij}(t) + \int_0^t \zeta(\tau) P_{1j}(t-\tau) d\tau \quad (6)$$

$$\text{Var}[X_j(t)] = \sum_{i=1}^N m_i(0) P_{ij}(t) \{1 - P_{ij}(t)\} + \int_0^t \zeta(\tau) P_{1j}(t-\tau) d\tau \quad (7)$$

Therefore, the expected value and variance of $C_j(t)$, concentration of nuclides in j at time t can be expressed, respectively, as

$$E[C_j(t)] = \frac{E[X_j(t)]}{V_j} \quad (8)$$

$$\text{Var}[C_j(t)] = \frac{\text{Var}[X_j(t)]}{V_j} \quad (9)$$

where

V_j = pore water volume of compartment j of the fracture (L^3).

Specifically let's consider the system of fracture medium through which nuclide transports and which can be regarded as a finite number of N compartments with several processes occurring simultaneously within them.

The transition probability from a compartment i to another compartment j is affected by the intensity of transition. This intensity of transition is related to the process involved. The diffusive

transport of nuclide which is assumed to be negligible compared to advective transport for the media having large Peclet number and another diffusive loss term into the rock matrix is also excluded in this case.

For simplicity, further assumptions may be introduced: the groundwater flow is constant and the groundwater flow and nuclide transport are considered to be made only between adjacent compartments.

Also, on the assumption of the constant feed rate of nuclide, $\zeta(\tau)$ of Eq. (5) can be reduced to constant ζ .

The intensity of transition $\lambda_{ij}(T^{-1})$ for the groundwater flow through some pore volume in porous medium can be written as

$$h_{ij} = \frac{Q_{ij}}{V_i} \quad (10)$$

where

Q_{ij} = volumetric flow rate from compartment i to compartment j ($L^3 T^{-1}$)

V_i = volume of compartment i (L^3).

Assuming that flow is well mixed, the transition probability due to advection can be written as

$$h_{ij} \Delta t + o(\Delta t) = \text{Pr} \{ \text{a nuclide in } i \text{ at time } t \text{ will be in } j \text{ decayed out at time } (t + \Delta t) \} \quad (11)$$

Similarly nuclide may decay out from compartment i at a rate represented by decay constant λ (T^{-1}). Therefore,

$$\lambda \Delta t + o(\Delta t) = \text{Pr} \{ \text{a nuclide in } i \text{ at time } t \text{ will be decayed out at time } (t + \Delta t) \} \quad (12)$$

Under the assumption of linear isotherm sorption of nuclides in the compartment i , h_{ij} can be replaced by h_{ij}/R_p^i , where

$$R_p^i = \left(1 + \frac{\rho_b^i K_d^i}{\phi_p^i} \right) \quad (13)$$

R_p^i = retardation coefficient in compartment i

ρ_b^i = bulk density of compartment i (ML^{-3})

K_a^i =distribution coefficient in compartment i ($L^3 M^{-1}$)

ϕ_p^i =porosity of compartment i .
Then

$$\lambda_{ij} = \sum_{j \neq i} \frac{h_{ij}}{R_i}, \quad i = 1, 2, \dots, N \quad (14)$$

With these the probability that the nuclide will remain at time $t + \Delta t$ in i without making any transition or disappearance is $|1 - (\sum_{j \neq i} \lambda_{ij} \Delta t + \lambda_{ii} \Delta t) + o(\Delta t)|$, from which, if this probability is denoted by $|1 + \lambda_{ii} \Delta t + o(\Delta t)|$ in case of no diffusive loss into the rock matrix,

$$\lambda_{ii} = - \left[\sum_{j \neq i} \frac{h_{ij}}{R_i} + \lambda \right], \quad i = 1, 2, \dots, N \quad (15)$$

where λ_{ii} is interpreted as the negative sum of all probabilities of exit from compartment i .

When the diffusive loss into the rock matrix in the direction perpendicular to the fracture from the fracture is considered in Eq. (15), we should add corresponding intensities of transition for this process. To this end diffusion process can be modeled by Fick's first law and the diffusive loss term can be represented as the mass flux $q(x, t)$ ($ML^{-2} T^{-1}$) across the fracture-rock matrix interface, i.e. at $z=b$ (Fig. 1).

$$q(x, t) = - \phi_p D_p \frac{\partial C_p(x, z, t)}{\partial z} \Big|_{z=b} \quad (16)$$

where

$C_p(x, z, t)$ =nuclide concentration in the rock matrix (L^{-3})

ϕ_p =porosity of the rock matrix ($L^3 L^{-3}$)

From one-dimensional analytical solution to Fick's second law for a homogeneous porous medium with respect to the radioactive-decaying source concentration of C_0 can be written in the orthogonal direction, z to the fracture as

$$\frac{C_p(x, z, t)}{C_0} = e^{-\lambda t} \operatorname{erfc} \left(\frac{z}{\sqrt{4(D_p/R_p)t}} \right) \quad (17)$$

where

D_p =pore diffusion coefficient in the rock matrix ($L^2 T^{-1}$).

Then, the mass rate $m(t)$ (MT^{-1}) through the area occupied by compartment i of the fracture can be derived from Eqs. (16) and (17), under the assumption of constant source concentration $C_0(t)$ in compartment i , as

$$\dot{m}_i(t) = \phi_p A \left\{ \sqrt{\frac{D_p}{\pi R_p t}} \exp \left\{ -\frac{b^2 R_p^i}{4 D_p t} \right\} \right\} C_0^i(t) \quad (18)$$

where

A =area occupied by the fracture wall of the compartment i (L^2).

Therefore, the intensity of transition for diffusive loss $\lambda_{diff}^i(t)$ (T^{-1}) into rock matrix can be expressed as

$$\lambda_{diff}^i(t) = \frac{\phi_p}{b} \left\{ \sqrt{\frac{D_p}{\pi R_p t}} \exp \left\{ -\frac{b^2 R_p^i}{4 D_p t} \right\} \right\} \quad (19)$$

In this case Eqs. (14) and (15) will be changed, under the assumption that the transport is considered to be made only between adjacent compartments, into

$$(\lambda_{ij}(t)) = \begin{cases} - \left[\frac{h_{ij}}{R_j} + \lambda + \lambda_{diff}^i(t) \right], & j = i \\ \frac{h_{ij}}{R_j}, & j = i+1 \\ 0, & \text{otherwise} \end{cases} \quad (20)$$

where

R_f^i =retardation coefficient in the fracture, which is defined as

$$R_f^i = 1 + \frac{K_a^i}{b} \quad (21)$$

where

K_a^i =surface distribution coefficient in the fracture in compartment i (L).

With the time-dependent intensities of transition in Eq. (20), the Eq. (1) is no more time-homogeneous, resulting the situation where analytical solutions for Eq. (1) in closed form as for the time-homogeneous case may not exist. According-

ly a solution scheme, among others, can be considered in similar way to the case of evaluation by discrete time approach of the state variable equations for the time-varying linear system as introduced in Appendix. [6]

3. Numerical Illustration

Since the model presented here must be very sensitive to the number of compartments of the system, in other words, the numerical dispersion phenomena will increase according to decreasing N , some quantitative estimation in the relation between N and the dispersion coefficient must be prerequisite. To this end in Appendix an analysis is made, which gives useful inference for the calibration of the model.

From Fig. 2 for a profile of arbitrary nuclide it is known that some computation results for the system whose parameter values are listed in Table 1 by the present model with varying numbers of compartments of 10, 20, 30, and 50, are agreed well with a deterministic analytical dispersion model (Eq. (A7)) [1,7] with equivalent dispersion coefficients of 50.0, 25.0, 16.7, and 10.0, respectively, which are obtained according to Eq. (A9).

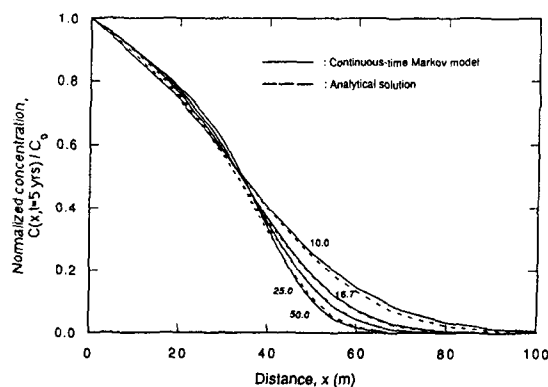


Fig. 2. Comparison of the Numerical Results by Continuous-time Markov Model for Varying Number of Compartments, N , with Corresponding Analytical Solutions for Equivalent Dispersion Coefficients.

Also, in Fig. 3, the concentration profiles by the present model for several different times are shown. It is easily seen that in both cases with and without retardation and radioactive decay, there exists excellent agreement between the results using the present model and the analytical solutions.

To demonstrate the use of the present model and to verify the model by comparing with the deterministic model, a specific illustration was made for single-fractured rock medium with constant groundwater flow rate in the fracture.

For single-fractured rock matrix system with process of diffusive loss into the rock-matrix from the fracture, the parameter values needed are shown in Table 2.

The deterministic differential equation governing the nuclide transport in the fracture with rock matrix diffusion can be given [4]

Table 1. Input Parameters(I)

R	1.0(5.0)
$L(m)$	100
$\lambda(1/yr)$	0.0(0.693/30.2)
$q/\phi(m/yr)$	10.0
$N(\text{for Markov model})$	10, 20, 30 50
$D(=qL/2\phi N \text{ for analytical solution, Eq.(A9)})$	50, 25, 16.7, 10

Table 2. Input Parameters(II)

R_f	1.0(5.0)
R_p	1.0(5.0)
$L(m)(\text{along the fracture})$	100
$\lambda(1/yr)$	0.0(0.693/30.2)
$q_f/\phi_f(m/yr)$	10.0
$D_f(m^2/yr)$	25.0
$N(\text{for Markov model})$	20
$D_p(m^2/yr)$	5×10^{-3}
$b(m)$	1×10^{-3}
$T(yr)$	1.0(2.5, 3.3, 4.2, 5.0)

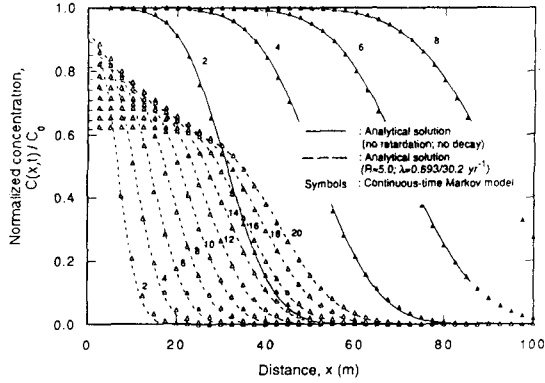


Fig. 3. Concentration Profiles by Continuous-time Markov Model with and Without Retardation and Radioactive Decay Compared to Analytical Solutions for Different Times. The Numbers on the Curves Represent Time.

$$R_f \frac{\partial C_f}{\partial t} - \frac{q_f}{\phi_f} \frac{\partial C_f}{\partial x} - D_f \frac{\partial^2 C_f}{\partial x^2} - \lambda R_f C_f(x, t) + \frac{q(x, t)}{b} = 0 \quad (22)$$

where

$C_f(x, t)$ = nuclide concentration in the fracture (L^{-3})

and $q(x, t)$ is given in Eq. (16), in which $C_p(x, z, t)$ is governed by following Eq. (24).

$$R_f = 1 + \frac{k_a}{b} \quad (23)$$

Similarly, the equation describing the transport of nuclides within the rock matrix is

$$R_p \frac{\partial C_p}{\partial t} - D_p \frac{\partial^2 C_p}{\partial z^2} - \lambda R_p C_p(x, z, t) = 0 \quad (24)$$

where

D_p = molecular diffusion coefficient in the rock matrix ($L^2 T^{-1}$)

and R_p is defined as the same way as Eq. (13).

The solution of Eqs. (22)-(24) subject to following initial and boundary conditions is available [4]

$$C_f(0, t) = C_0 e^{-\lambda t} \quad (25)$$

$$C_f(\infty, t) = 0 \quad (26)$$

$$C_f(x, 0) = 0 \quad (27)$$

$$C_p(x, b, t) = C_f(x, t) \quad (28)$$

$$C_p(x, \infty, t) = 0 \quad (29)$$

$$C_p(x, z, 0) = 0 \quad (30)$$

The expected values of concentration profile predicted by the present model are shown in Fig. 4 as a function of distance along the fracture from the inlet of the rock-matrix system. There, the concentration profile in exact case for no dispersion in the fracture is also shown for reference. In order to evaluate Eq. (1) having inhomogeneous intensity of transition, discrete time approximation scheme represented by Eqs. (A4) and (A5) in Appendix was used.

As for the size of discrete time step T , it is not so effective for the accuracy of the solution even when very small size of T is used as is easily seen in Fig. 5, where two groups of breakthrough curves, each of which is the results at the distance of 20 and 80 m, respectively, are depicted for cases differing in T . In this regard, no special efforts to find out the proper discrete time size was not made to improve the results. Therefore, in this illustration for calculation at time $t=5.0$ yrs,

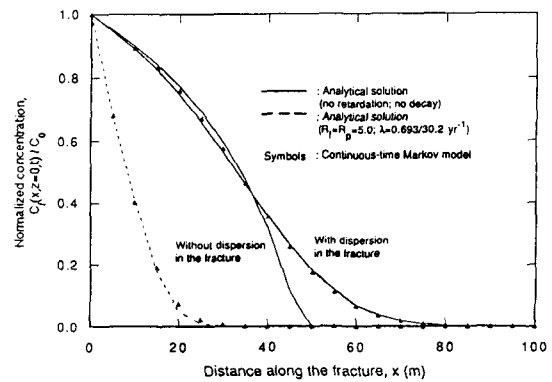


Fig. 4. Concentration Profiles by Continuous-time Markov Model with and Without Retardation (Both in the Fracture and in the Rock Matrix) and Radioactive Decay Compared to Analytical Solutions.

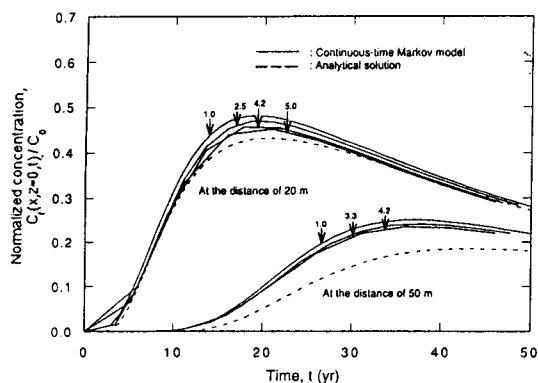


Fig. 5. Breakthrough Curves by Continuous-time Markov Model for Varying Discrete Time, T at the Distances of 20m and 50m Compared to Analytical Solutions. The Numbers Represent Discrete-time Size.

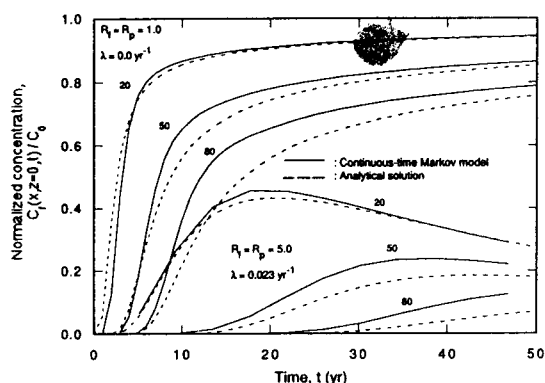


Fig. 6. Comparison of the Numerical Results by Continuous-time Markov Model at the Distance of 20, 50, and 80m Along the Fracture with the Corresponding Analytical Solutions. The Numbers Represent Distances.

5 time steps used resulting each discrete time step of 1.0. To verify the results, an analytical solution developed by Tang et al., to Eqs. (22) through (30) is used with numerical integration using Gaussian quadrature scheme. Fig. 6, which is calculated at the distances of 20, 50, and 80 m for the cases with and without retardation and radioactive decay, exhibits relatively good agreement between

continuous-time Markov process model developed in this work and the analytical solution. However, some discrepancy appears in all breakthrough curves in this figure becoming more severe as much as going far from the inlet, which may be probably due to insufficient discretization of space and time.

4. Conclusions

Through this study a stochastic modeling using a continuous time Markov process for one-dimensional transport of nuclides through the rock matrix around the repository has been made. By calculating the time-dependent transition probability of nuclide from the intensity of transition between, into, and/or from the compartments, the expected value of distribution of nuclide concentration can be obtained as well as its variance.

Since this model is discrete in medium space, physical and geochemical parameters including groundwater velocity, dispersion coefficient, retardation coefficients, and losses due to radioactive decay or diffusion out of the system, which affect nuclide transport, can be easily incorporated for such heterogeneous media as the fractured rock medium having spatially varied parameters.

Even though the Markov process model developed in this study was shown to be sensitive to the number of discretized compartment showing numerical dispersion as the number of compartments are increased, with small compensating of dispersion coefficient, the model agrees well to analytical solution.

Therefore, using this model statistical distribution of the nuclide within the discrete compartments of heterogeneous media around the repository could be well modeled by discretizing the media considering the degree of variation of the parameters when compensating for dispersion coefficient.

Appendix

1) Evaluation of $P_{ij}(t)$ and Nuclide Distribution by Discrete Time Method

If $\lambda_{diff}(t)$ is assumed to be piecewise constant over the small time interval $[t_0, t_1)$ such that

$$\lambda_{diff}(\tau) = \lambda_{diff}(nT) = \text{constant}, \quad \tau \in [nT, (n+1)T), \quad n=1, 2, 3, \dots \quad (A1)$$

where

T = discrete time interval (T).

and t_0 and t_1 are selected as

$$t_0 = nT \quad (A2)$$

$$t_1 = (n+1)T \quad (A3)$$

then the nuclide distribution by Eq. (31) at time t_1 with constant ζ will be expressed as

$$E[X_j[(n+1)T]] = \sum_{i=1}^N m_i(nT) P_{ij}[(n+1)T] + \zeta \int_{nT}^{(n+1)T} P_{ij}[(n+1)T - \tau] d\tau \quad (A4)$$

where $P_{ij}[(n+1)T]$, the transition probabilities can be obtained, from the solution of Eqs. (1) and (2) in case of constant \mathbf{A} [1], as

$$P[(n+1)T] = e^{\mathbf{A}T} P(nT) \quad (A5)$$

Then each term of R. H. S. represents the number of survived nuclides and the number of nuclides newly entered during time interval T , respectively.

2) Derivation of a Correlation Between N and D

For simplicity let's consider the one-dimensional system which is divided into N compartments of equal size with the only one process of advective transport. For such system, the mass balance around the i th compartment gives

$$\begin{aligned} \frac{V}{N} \frac{\partial C_i}{\partial t} &= -Q(C_i - C_{i-1}) \\ &= \frac{Q}{2}(C_{i+1} - 2C_i + C_{i-1}) - \frac{Q}{2}(C_{i+1} - C_{i-1}) \quad (A6) \end{aligned}$$

where

V = total volume of compartments (L^3)

Q = constant flow rate of groundwater from one compartment to another adjacent one ($L^3 T^{-1}$)

C_i = concentration of compartment i (L^{-3}).

A common advection-dispersion model is given in Eq. (A7) for homogeneous porous medium

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \quad (A7)$$

which can be approximated by the centered difference equations by means of Taylor expansion as

$$\frac{\partial C_i}{\partial t} \approx \frac{D}{(\Delta x)^2} (C_{i+1} - 2C_i + C_{i-1}) - \frac{v}{2\Delta x} (C_{i+1} - C_{i-1}) \quad (A8)$$

where

Δx = differential x (L)

v = velocity of groundwater determined by q/ϕ ($L T^{-1}$)

By comparing Eqs. (A6) and (A7) and letting $\Delta x = L/N$ where L is the length of the system, following approximate equivalence will be obtained:

$$D = \frac{vL}{2N} \quad (A9)$$

References

1. Y.M. Lee, C.H. Kang, P.S. Hahn, H.H. Park and K.J. Lee, "A Stochastic Model for the Nuclide Migration in Geologic Media Using a Continuous Time Markov Process," *J. Korean Nucl. Soc.*, **25**, 1, 154 (1993).
2. I. Neretnieks, "Diffusion in the Rock Matrix: An Important Factor in Radionuclide Retardation?" *J. Geophys. Res.*, **85**, B8, 4379 (1980).
3. G.E. Gossal and J.F. Pickens, "Solute Transport Through Fractured Media: 1. The Effect of Matrix Diffusion," *Water Resour. Res.*, **16**, 4, 719 (1980).

4. D.H. Tang, E.O. Frind, and A. Sudicky, "Contaminant Transport in Fractured Porous Media : Analytical solution for a single fracture," *Water Resour. Res.*, **17**, 3, 555 (1981).
5. S. Karlin and H. M. Taylor, *A First Course in Stochastic processes*, Academic Press, New York (1975).
6. W.L. Brogan, *Modern Control Theory*, Prentice-Hall, New Jersey (1991).
7. A.B. Gureghian and G. Jansen, "One-dimensional analytical solutions for the migration of a three-member radionuclide decay chain in a multilayered geologic medium," *Water Resour. Res.*, **21**, 5, 733 (1985).