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Uncertainty Analysis of Multiple Canister Repository Model by Earth Simulator

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Abstract An uncertainty analysis considering the heterogeneity of host rock has been made by using the multiple-canister radionuclide transport code, the VR code, for performance assessment for the high-level radioactive waste (HLW) repository. By the previous studies with the VR code, it was found that where water flows in parallel to the repository plane, the effects of neighboring canisters on the release of radionuclides from the canister of interest are significant. However in the previous VR calculations, the number of connected canisters in the same water stream was determined arbitrary. In this study, the number of connected canisters in the same water-flow stream has been determined statistically by counting the number of canisters included in the same fracture network by using the FFDF code. The uncertainty resulting from fracture networks in host rock has been taken into account by applying the probability distribution function (PDF) of the numbers of connected canisters by a fracture cluster obtained by the FFDF code. The release rate of ^{237}Np from a hypothetical repository model containing 500 canisters has been evaluated by using the VR code with uncertainties associated with the ^{237}Np release rate resulting from variations of the number of connected canisters. The VR code and the FFDF code had been ported to the Earth Simulator by authors to perform large-scale computations. The Latin Hypercube Sampling has been utilized to reduce the number of samplings in Monte-Carlo calculation utilized in the VR code.

Keywords: uncertainty analysis, multiple canister repository model, high-level radioactive waste, fracture network, mass transport

1. Introduction

An uncertainty analysis considering heterogeneity of the host rock has been made by using the multiple-canister radionuclide transport code, the VR code [1][2][1], for performance assessment of the High-level radioactive waste (HLW) repository.

In the VR code, the repository is modeled as an array of compartments, each containing a waste canister, the buffer, and the near-field rock modeled as slabs. The compartments are assumed to be positioned in the direction of groundwater flow and radionuclides are first assumed to be released from the waste canister, to diffuse through the buffer, and then to be released to the near-field rock. The radionuclide release rate from the buffer to the near-field rock is used as the boundary condition of the buffer and the near-field rock interface, which is obtained by the coupling calculation of radionuclide release from the buffer to the near-field rock, and the near-field rock concentration. The canister interaction effect caused by the solubility limit of a radionuclide, is modeled in the VR code.

An uncertainty analysis plays an important role in the safety performance assessment of HLW repository due to the fact that uncertainty is inherently included in parameters and models of the repository, mainly resulting from the heterogeneity of geological environments and a very long time-frame for performance assessment.

In the previous performance assessments [3], the mass transport was modeled for a single-canister configuration. For example, for a repository with *n* canisters, results for a single canister were simply multiplied by *n*. Authors devel-

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[1] The VR code is the property of the University of California

oped the mass transport code, the VR code, which incorporates interference effects of multiple canisters. By deterministic studies with the VR code, it was found that, especially for a water-saturated repository where water flows in parallel to the repository plane, the effects of neighboring canisters on the release of radionuclides from the canister of interest are significant [1]. In the previous deterministic VR calculations, however, the number of connected canisters in the same water stream was determined arbitrary.

In reality, groundwater flows through fracture clusters that connect waste canisters in the repository and the regional groundwater flow field in the region exterior to the repository. The number of connected canisters in the same water-flow stream is an important parameter because the radionuclides are released from the only canisters in the water-flow stream, and transported via the groundwater flow. The number of connected canisters in the same water-flow stream could be determined statistically by counting the number of canisters hedrologically-connected in a fracture network.

Recently, the FFDF model, a Monte-Carlo model for mass transport in fractured rock, was developed. [4] In FFDF model, the connectivity of the fracture network is evaluated and the existence of a water-flow path via the fracture network between two points is judged. The local area of fracture clusters is converted to equivalent continuous model for groundwater flow calculation.

Monte-Carlo method is one of the promising methods to calculate mass transport via complicated fracture path. As the groundwater flow data is necessary in the radionuclide transport calculation, fracture clusters must be converted to equivalent continuous model to calculate groundwater flow.

In the FFDF code[2], a two-dimensional circular model space considered as the repository in which a waste canister of interest is located at the center of the model space. The central waste canister is surrounded by the buffer and the host rock. In the host rock, fractures are generated based on statistical distribution functions assumed for the geological parameters like the orientation angle, location, length and aperture. After a certain number of fractures are generated, inter-connection among the generated fractures is checked, and Flow-Bearing fracture Cluster (FBC), which connects the outer boundary of the circular model space and the outer boundary of the buffer in the central waste canister, is determined. The radionuclides released from the central waste canister are transported through the FBC.

The FFDF code was developed originally for personal computers (PC). It can calculate groundwater flow and mass transport for a host rock within a region of 10 square meters, with hundreds of fracture segments.

The FFDF code has been ported to the Earth Simulator [5] for a large-scale simulation of the fracture network in a circular domain with a radius of 60 m with more than a hundred thousand fractures. This scale of calculation has never been made in the previous calculations by PCs. The probabilistic distribution functions of the total numbers of connected canisters by the same fracture cluster are obtained by the code.

Probability distribution function (PDF) for the number of waste canisters included in a FBC is obtained by the FFDF code and parameters significantly affecting the distribution are investigated.

The release rate of ^{237}Np from a hypothetical repository containing 500 canisters has been evaluated by using the VR code as a surrogate measure for repository performance. Uncertainties associated with the release rate resulting from parameter variations including the number of connected canisters by a fracture network have been evaluated. In the uncertainty analysis, the PDF for the number of connected waste canisters by fracture network obtained by the FFDF code is used.

From the viewpoint of computational workload, we needed to solve the issue of a vast amount of calculation to obtain statistical convergence if a standard Monte-Carlo approach is applied. While the original VR code adopts parallel computing technology for a PC cluster, it still requires significant computation time even for one deterministic realization.

To overcome this difficulty, we have tried two things. One is utilization of the Earth Simulator. Necessary modification and optimization for the VR code have been made upon porting to the Earth Simulator [6]. We executed the VR code with the full node utilization of the Earth Simulator. The other is application of the Latin Hypercube Sampling (LHS) [7] to reduce the number of samplings. The computer code for LHS [7] has been coupled with the VR code in this study.

2. FFDF Code

2.1 Governing Equations

The basic model has been developed by Lim [4], and reported in detail elsewhere. We summarize the model here for the reader's convenience.

2.1.1 Fracture Generation

In this study, a model space is defined as two-dimensional circle shown in Figure 1. The black-filled circle represents the central waste canister, while the outer circle represents the outer boundary of the model space. We

[2] The FEDF code is the property of the University of California

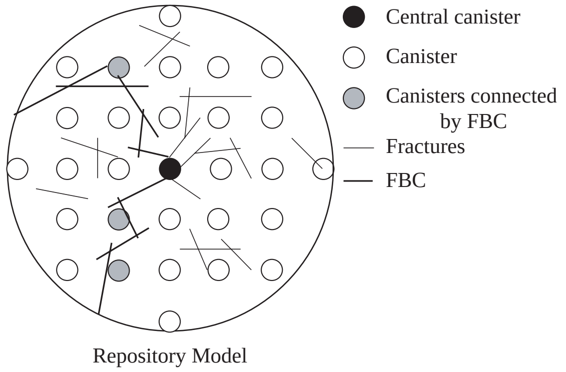

Fig. 1 Identification of FBC.

call this model space the near-field. A non-black circle represents the wastes other than central waste, which are positioned in the grid form. Each canister is assumed to be surrounded by a bentonite buffer region, where molecular diffusion is dominant and water flow is neglected.

A fracture is represented as a line element in the repository model. Fracture elements are generated randomly based on statistic parameter of fracture geometry.

The fracture interconnections are identified after the fractures are generated. The fracture clusters that connect the near-filed boundary and the buffer region of the central waste canister are identified as Flow Bearing Clusters (FBC). They are groundwater paths between the central waste canister and the outer boundary.

2.1.2 Homogenization

The FBC is partitioned into triangular elements. Within each element, fractures included in the FBC are homogenized to obtain the equivalent porosity and hydraulic conductivity.

The equivalent porosity for an element is calculated by the following equation.

$$\varepsilon_e = \frac{\sum_{j=1}^{Ni}(l_{e,j}\, b_{e,j})}{\Delta_e}, \tag{1}$$

where Δ_e is the area of the triangular element e, $l_{e,j}$ is the length of the fracture j, which is included in the element, and the $b_{e,j}$ is the aperture of the fracture j.

The equivalent permeability is obtained by the Kozeny-Carman equation.[4]

$$k_e = C\frac{\varepsilon_e^2}{(1-\varepsilon_e)_2 M_{s,e}^2}, \tag{2}$$

where C is constant, ε_e is the equivalent porosity, and $M_{s,e}$ is the pore surface area wet by groundwater per porous media unit volume.

The hydraulic conductivity of an element e is obtained by the following equation.

$$K_e = \frac{k_e \rho g}{\mu_w}, \tag{3}$$

where ρ is water density, g is gravity constant, and μ_w is water viscosity.

2.1.3 Groundwater Flow Calculation

The governing equation of the water flow is obtained by the conservation of mass. [4]

$$\frac{\partial(\varepsilon\rho)}{\partial t} + div(\rho\vec{q}) = 0, \tag{4}$$

where $\vec{q}$ is the Darcy velocity, and ε is the porosity.

In this study ρ is assumed to be constant for incompressible water flow.

The governing equation of the steady state groundwater flow is as follows.

$$\frac{\partial}{\partial x}\left[K_x(x,y)\frac{\partial\phi}{\partial x}\right] + \frac{\partial}{\partial y}\left[K_y(x,y)\frac{\partial\phi}{\partial y}\right] = 0, \tag{5}$$

where ϕ is the potential head, K_x, and K_y are the hydraulic conductivity.

2.1.4 Mass Transport Calculation

The solute transport model for large three-dimensional heterogeneous flow system is developed by Tompson. [8] The step equation for time and space dependent water velocity and constant molecular diffusion for two-dimensional water saturated system is as follows.

$$x(t+\tau) = x(t) + v_x(\vec{X}(t))\tau + Z_x\sqrt{2D\tau}, \tag{6}$$

$$y(t+\tau) = y(t) + v_y(\vec{X}(t))\tau + Z_y\sqrt{2D\tau}, \tag{7}$$

where x, and y are random variables, $\vec{X}(t)$ the position vector at time t, $v_x(\vec{X}(t))$ and $v_y(\vec{X}(t))$ x and y components of pore water velocity vector at time t, respectively, D the diffusion coefficient constant with time and space. Z_x and Z_y are independent random numbers which satisfy the following condition,

$$<Z_x>=0, <Z_x^2>=1, <Z_y>=0, <Z_y^2>=1. \tag{8}$$

2.2 Estimation of Total Numbers of Fractures in the Repository

In this study, the total number of fractures existing in the model space is estimated based on the geological survey data at JNC Horonobe site [9], where the linear frequency distribution of fractures is obtained. The average and maximum values of the linear frequency obtained from the literature data are 2.95 (average) and 19 (maximum). The number density of fractures is obtained from the linear frequency of fractures using the following equation [10] as

$$\lambda_A = \frac{\pi\lambda}{2l_\alpha}, \tag{9}$$

where λ_A is the number density, λ the linear frequency, and l_α the average length of fractures. In this study l_α is set to be 1.0 [m]. The total number of fractures existing in the model space is calculated by multiplying the model-space area to the number density of fractures.

For a repository with the areal extent of 2000 m by 2000 m, the resultant total number of fractures is 2.0E+7 (linear frequency of 2.95) and 1.0E+8 (linear frequency of 19).

2.3 FFDF Code Conversion to Earth Simulator

As the FFDF code was originally developed for PC in C++ language, the code has been converted to Fortran-90 language. The code has also been modified to treat a greater model space with multiple canisters. The new function to judge and count waste canisters that are interconnected by the FBC has been newly added to the code.

2.4 Parameter Values and Computation

For the two-dimensional circular model space shown in Figure 1, the input parameters for the FFDF code are set as shown in Table 1. The calculation scheme of the FFDF code is shown in Figure 2.

Table 1 Input parameters for the FFDF code.

Group	Parameters	Input data	Unit
Geometry	Radius of the near-field outer boundary	60	m
	Radius of the surface of the buffer of the central waste	1	m
	Radius of the surface of the canister of the central waste	0.35	m
Fracture	Ratio of total number of secondary fractures to that of primary fractures	0.3	-
	β_L of aperture	7.068E-5	m
	α_L of aperture	0.832555	-
	β_L of length of the primary fractures	1.0	m
	α_L of length of the primary fractures	1.0	-
	β_L of length of the secondary fractures	1.0	m
	α_L of length of the secondary fractures	1.0	-
Elements	Number of nodes along the circular boundary	10	-
	Number of nodes between R_0 and R_2 in radial direction	10	-
	Number of nodes between R_1 and R_0 in radial direction	1	-
Transport	Number of particle	10	-
	Maximum time	1.0E+7	y
Property	Porosity for the buffer region	0.3	-
	Hydraulic conductivity for the buffer	2.3e-14	m/y
	Derivative of hydraulic head (dh/dx)	0.1	-
	Diffusion coefficient in the buffer	3.2E-3	m2/y
	Diffusion coefficient in the FBC	3.2E-2	m2/y
	Diffusion coefficient in the Non-FBC	2.1E-4	m2/y

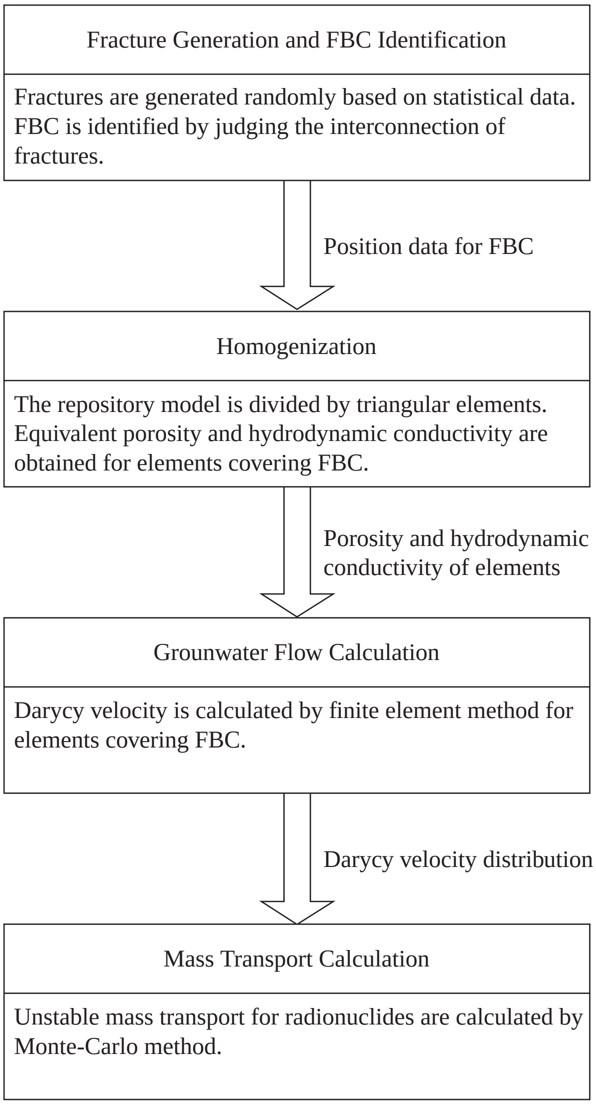

Fig. 2 Calculation scheme of FFDF code.

2.5 Calculation Results

A simulation of fracture networks in a circular model space with a radius of 60 m with more than a hundred thousand fractures have been executed by the Earth Simulator.

2.5.1 Evaluation of Number of FBC-connected Canisters

Cases have been set for various total numbers of fractures in a circular model with a radius of 60 m with 109 canisters. For each case, the number of connected canisters by FBC has been evaluated. The total number of fracture is set to range from 10000 to 32000 with a 2000 interval. 10 trials for fracture generation are performed for each total number of fractures.

The averaged numbers of connected canisters by FBC are plotted to the total number of fractures in Figure 3. It is observed that the number of canisters connected by FBC increases as the total number of fractures increases, while leveling off with the total number of fractures greater than 25,000, where all canisters in the model space are included in the FBC.

Figures 4 and 5 show fracture networks for the total numbers of fractures of 12000 and 20000. In the figures, the FBC are shown as blue lines, fractures not included in

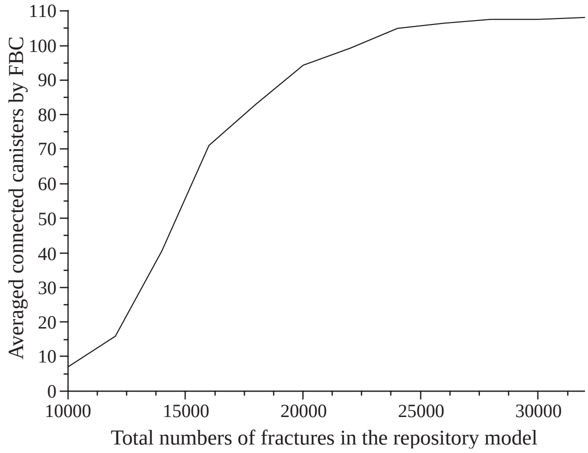

Fig. 3 Connected canister number to fracture number.

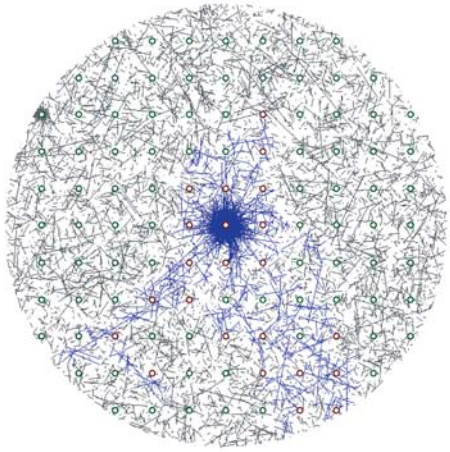

Fig. 4 FBC for 12000 fractures.

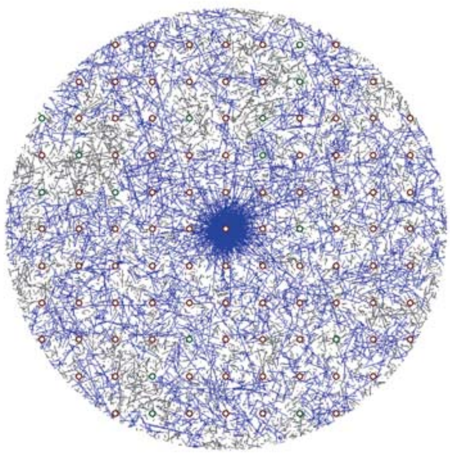

Fig. 5 FBC for 20000 fractures.

the FBC as gray lines, the canisters included in FBC as red circles, and the canisters not included in FBC as green circles. As the total number of fractures in the model space increases, the FBC becomes larger in size, and more canisters are connected by FBC.

100 trials for fracture generation have been performed for each of total numbers of fractures of 8000 to 28000 with a 4000 interval, to obtain the PDF of the total numbers of fractures connected by FBC. The result is shown in Figure 6. As shown in Figure 6, each PDF has a bell-shape with its peak. The PDF strongly depends on the total number of fractures in the model space. As the total number of fractures increases, the distribution becomes narrower, and the median value for the number of canisters connected by the FBC increases.

The statistical data of PDF of the total numbers of canisters connected by FBC for various total numbers of fractures are summarized in the Table 2. It is observed from Table 2 that as the total numbers of fractures increases, the averaged number of canisters connected by FBC increases, and standard deviation of canisters connected by FBC decreases. Also observed is that the standard deviation increases as the total numbers of fractures increases from 8000 to 14000.

We observe that if the total number of fractures in the model space is over 28000, almost all of the canisters in the model space are included in the FBC. If the total number of fractures is smaller than 8000, a FBC is not generated in the model space. It indicates that the total number of fractures in the repository model space is a key parameter that determines the flow path of groundwater.

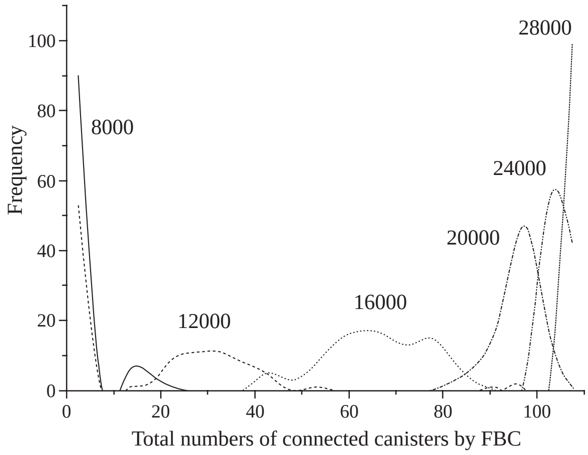

Fig. 6 The frequency of total numbers of canisters connected by FBC for various number of fractures in the repository model.

Mass transport calculations in a circular model space with a radius of 60 m with 109 canisters have also been performed. The results are shown in Table 3.

The average residence time of 10000 particles used in Monte-Carlo calculation is shown to compare the results of mass transport calculation. It is observed that as the total numbers of fractures increases, the averaged residence time increases. This is because the transport path

Table 2 Statistical data of PDF of the total numbers of canisters connected by FBC.

Total numbers of Fractures	Averaged number of canisters connected by FBC	Standard deviation of number of canisters connected by FBC
8000	1.43	4.39
10000	10.1	14.1
12000	14.3	16.0
14000	38.3	16.7
16000	65.5	11.0
18000	82.4	7.7
20000	95.6	4.5
22000	101.1	3.3
24000	103.9	2.3
26000	106.4	1.5
28000	107.5	1.2
30000	108.2	0.9
32000	108.6	0.7

Table 3 The results of mass transport calculation by the FFDF code.

Items	Measured data			
The total numbers of fractures	12000	18000	22000	26000
The total numbers of fractures that compose FBC	4730	10872	17326	23595
The total numbers of canisters connected by FBC	34	79	100	105
Element number (Radial and radius direction)	40 × 10			
Total numbers of particles	10000			
The averaged residence time of particles	279	226	213	161

becomes less tortuous as the total number of fractures increase. The FBC tends to cover the entire model space, and approaches a continuum as more fractures are added to the model space.

3. Uncertainty Analysis

Uncertainty analysis is performed by the VR code, a mass transport calculation code for multiple-canister repository model.

3.1 VR Model

In the VR model, the repository consist of multiple compartments, each containing a waste canister, the buffer that backfills the space between the waste canister and the disposal tunnel surface, and the near-field rock. The compartments are positioned in the direction of groundwater flow. Radionuclides are first assumed to be released from the waste canister, to diffuse through the buffer, and then to be released to the near-field. The near-field rock in a compartment is connected by advection with the neighboring compartments. From the upstream compartment, radionuclides are carried in to the near-field of the compartment of interest, and then carried out to the downstream compartment by advection.

When the radionuclide concentration at the interface between the waste canister and the buffer reaches the solubility, the release of the radionuclides is assumed to be limited by the solubility.

The waste canister, the buffer, and the near-field rock are modeled as slabs in the compartment model in the VR code (Figure 7).

3.2 Uncertainty Analysis

The PDF for the maximum value of the ^{237}Np release rate to the far-field has been obtained by the uncertainty

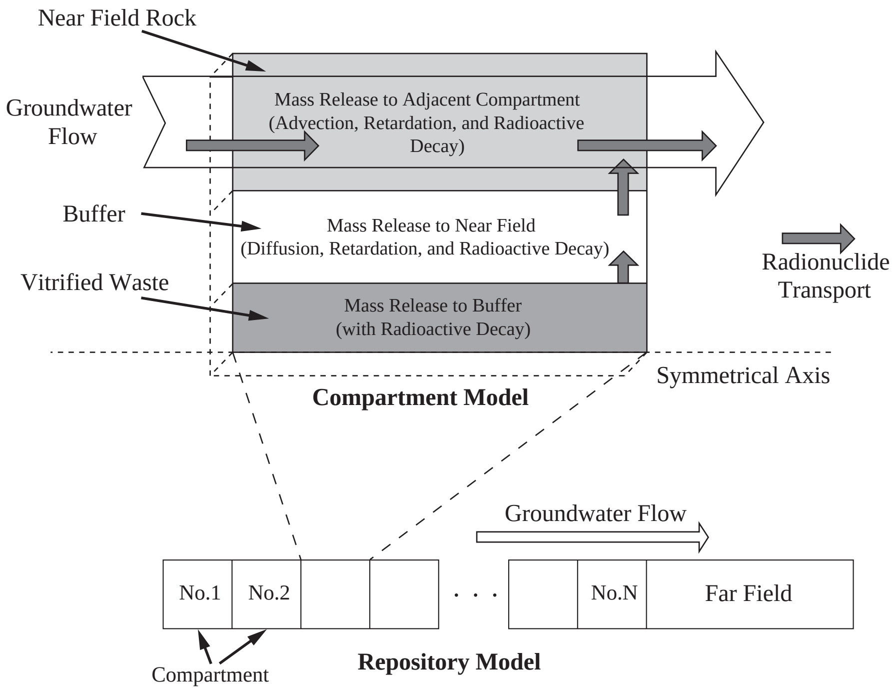

Fig. 7 Compartment model for the repository.

analysis. In this study, the ^{237}Np release rate to the far-field is used as a surrogate performance measure of the repository.

3.2.1 Method

We assume that the following input parameters for the VR model are associated with uncertainties: the solubility, the sorption coefficients of the radionuclide, and the number of connected canisters in a row.

We consider that among the canisters in the repository only n canisters are included in the fracture cluster that is connected with the groundwater flow field in the region exterior to the repository, or the far-field (Figure 8). The probability for the event that a row of n compartments occurs is given by the PDF determined in [5].

Input parameter values have been sampled for each realization based on the PDF for the solubility and the sorption coefficients of the radionuclide. The sampling has been made for each of n compartments in a row. It means that different values have been assigned for n compartments in a row for these two parameters.

The VR code has been performed for each trial calculation, and the maximum value of the ^{237}Np release rate has been obtained and recorded to obtain the PDF for the release rate. The release rate to the far-field has been calculated by

$$F(t) = \sum_{j=1}^{N} P_j R_j(t), \tag{10}$$

where $F(t)$ is the release rate from the repository to the far-field at time of t, P_j the probability for the number of connected canisters by a fracture cluster to be j, $R_j(t)$ the release rate from a row of j compartments at time of t obtained by the VR model, and N the total number of canisters in the repository model, set to be 500 in this study.

3.2.2 Input Parameters

1) Solubility

The uncertainty associated with the solubility results from the uncertainty of more fundamental parameters, such as pH and temperature. Because these fundamental parameters vary with time as the in-canister chemistry evolves with time, and because we do not have complete knowledge about the fundamental parameters, the solubility becomes uncertain. The PDF of the solubility for ^{237}Np reported in [11] has been utilized. The PDF is assumed to be a discrete distribution as shown in Table 4.

2) Sorption coefficient

The PDF of the sorption coefficient reported in [11] has also been utilized in the uncertainty analysis. The PDF is assumed to be a discrete distribution as shown in Table 4.

The retardation factor R is defined as

$$R = 1 + \frac{(1-\varepsilon)}{\varepsilon} \rho Kd, \tag{11}$$

where, ε and ρ (kg/m^3) are the porosity and the density of buffer, and Kd (m^3/kg) is the sorption distribution coefficient.

For the bentonite buffer, we fix the porosity at 0.36 [11] and the density at 1.6 Mg/m^3 [3].

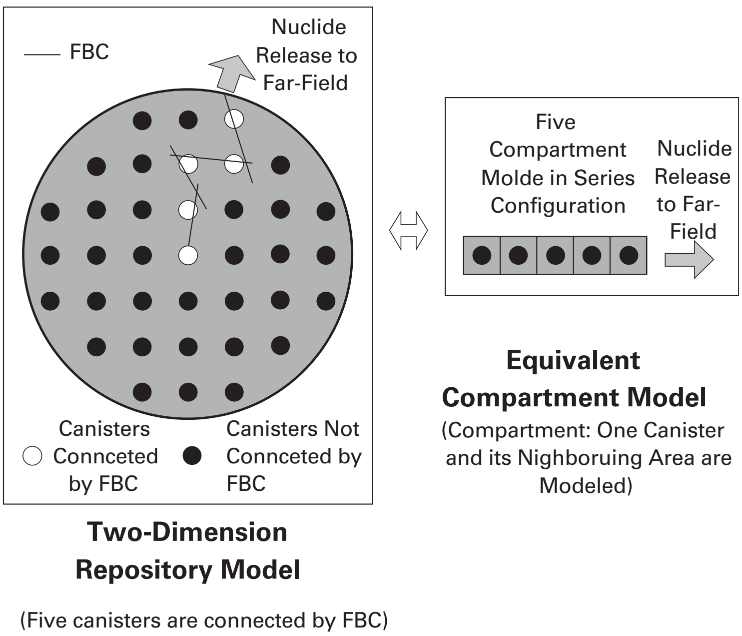

Fig. 8 Correspondence between two-dimensional mass transport model with the one-dimensional compartment model.

Table 4 Distributions for input parameters of uncertainty analysis for Np-237.

Parameter	Probability and value	Unit
Solubility	70% probability for 5.0E-6 (reference) 15% probability for 3.0E-6 (optimistic) 15% probability for 1.0E-5 (pessimistic)	mol/m^3
Sorption coefficient	70% probability for 60 (reference) 15% probability for 600 (optimistic) 15% probability for 6 (pessimistic)	m^3/kg

3) Total number of connected canisters

The PDF for the total number of connected canisters by fracture cluster have been obtained in [5] for the total numbers of fractures of 8000, 10000, 12000, 16000, and 18000. The PDF are shown in Figure 9. We observe from the figure that as the number of fractures increases, the distribution shifts to the right. This means that with more fractures included in the repository model space, a greater number of canisters are connected in the FBC. The figure also shows that with 8000 fractures, a few canisters are likely to be connected, while with 18,000 fractures, about 80% of the canisters in the repository are likely to be connected.

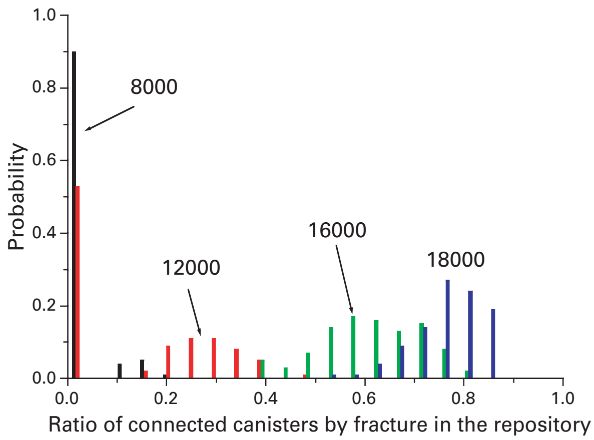

Fig. 9 PDFs for the numbers of connected canisters for various numbers fractures.

3.2.3 Cases for Uncertainty Evaluation

We have included uncertainty of one parameter at a time to see its effects in the ^{237}Np release rate distribution. The combination of input parameters is shown in Table 5. For each of these cases, 100 realizations have been calculated.

Table 5 Statistical data of PDF of the maximum of the release rate of ^{237}Np.

Cases	Input parameters with uncertainty	Statistical Data	Number of fractures			
			8000	12000	16000	18000
1	Sorption coefficient only	Standard Deviation	1.8E-08	1.7E-08	1.8E-08	2.1E-08
		Average	2.1E-07	2.7E-07	2.9E-07	2.9E-07
2	Solubility only	Standard Deviation	1.1E-08	1.0E-08	1.1E-08	1.3E-08
		Average	2.7E-07	3.6E-07	3.8E-07	3.8E-07
3	Sorption coefficient and Solubility	Standard Deviation	2.9E-08	2.6E-08	2.1E-08	2.6E-08
		Average	2.2E-07	2.9E-07	3.0E-07	3.0E-07

3.2.4 Calculation Results

Figure 10 shows the result with 500 canisters (fixed) with variations for the solubility and the sorption coefficient.

Figure 11 shows the ^{237}Np release rate with the PDF for the numbers of connected canister for 8000 and 18000 fractures for Case 3. Thus, variations of the solubility and the sorption coefficient are also considered in the ^{237}Np release rate for 8000 and 18000 fractures. The primary interest is the peaks of the release rate. We observe that the peak value for 8000 is smaller than that for 18000. This is because with more fractures, more canisters are connected by the fracture cluster, so that greater mass of the radionuclide is released from the repository.

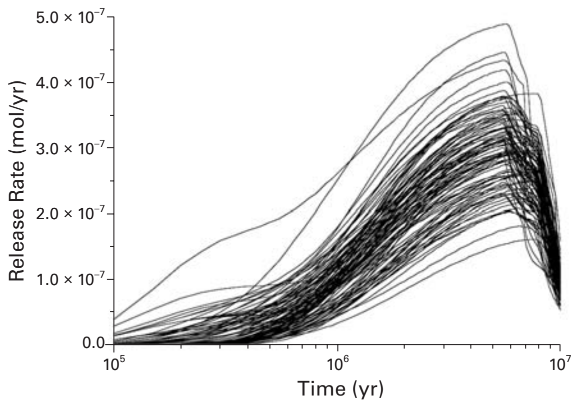

Fig. 10 ^{237}Np release rate with 500 canisters for case 3.

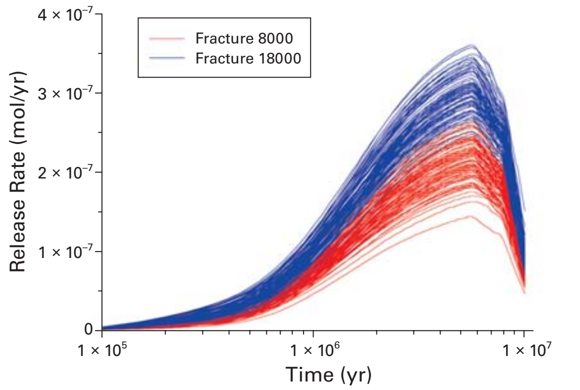

Fig. 11 ^{237}Np release rate with the PDF for the number of connected canister for 8000 and 18000 fractures in the repository for case 3.

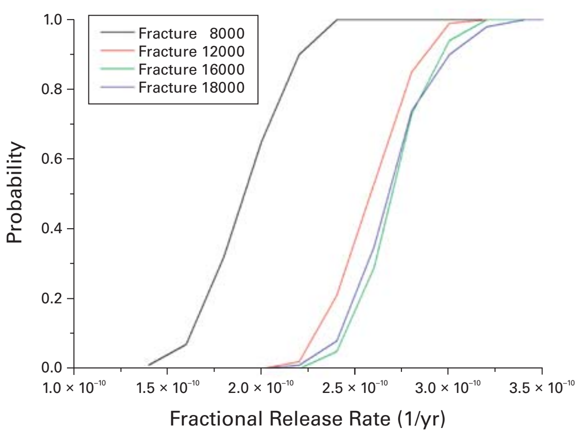

Fig. 12 The cumulative distribution function for the peak fractional release rate of ^{237}Np for Case 3.

Based on these results, we have obtained the cumulative distribution function (CDF) for the maximum fractional release rate for various numbers of fractures. Figure 12 shows the results for various fracture numbers. The fractional release rate is obtained by dividing the release rate by the total mass of the radionuclide initially included in the *n* canisters in the repository, and has been taken as the horizontal axis because the release rate is related with the total inventory of the radionuclide in the *n* canisters; the more canisters are included, the greater the release rate is. Thus, to compare the results for various numbers of canisters connected, the fractional release rate is appropriate index.

From Figure 12, it is observed that with a fewer fractures, the fractional release rate tends to be smaller. With the fracture number 12000 or greater, the fractional release rate distributes around the same range.

For a small number of fracture, such as for the case with 8000 fractures, the number of realizations, in which no fracture cluster connecting to the outer boundary of the repository model exists and ^{237}Np release rate is 0, is large. This gives the small median value of the distribution of the maximum of ^{237}Np release rate.

The characteristics of the PDF of the ^{237}Np maximum fractional release rate are summarized in Table 5.

We observe from Table 5 that

- (effects of number of fractures on the median) The median value for 8000 fractures is the smallest, and those for other fracture numbers are almost the same.
- (effects of number of fractures on the standard deviation) Among the four different values of fracture numbers, the difference in standard deviation is small.
- (effects of parameter variations on the median) For the same fracture number, case 2 resulted in the largest.
- (effects of parameter variations on the standard deviation) For the same fracture number, the standard deviation for case 3 is the largest.

4. Discussions

4.1 Effects of Rock Porosity in the Near-field

In the present study, no statistical variation has been assumed for the porosity of the rock in the near-field.

However, in the two-dimension repository model used in the calculation of the PDF of the numbers of connected canisters by fracture cluster, it is assumed that canisters are connected by the transport via groundwater flow through the fractures in the same fracture cluster. Hence, uncertainty in the porosity would result in significant uncertainty in the release rate. It is desirable that the PDF should have also been assumed for the porosity in near-field rock, which can be evaluated by the fracture generation calculation in the repository model [5].

The porosity in the near-field rock could have a significant effect on radionuclide transport in near-field rock. The incorporation of the PDF of the porosity in the near-field rock in the uncertainty analysis is the future task.

4.2 Sampling for Number of Canisters

In this study, as the method to apply the PDF for the number of the connected canisters to the compartment model, Eq. (10) has been used, in which radionuclides release rate for various numbers of canisters in the compartment model are weighted by the probability. In this method, we have implicitly assumed that the numbers of fracture is small, so that there is only one groundwater path, fracture cluster, through which groundwater flows to the far-field (Figure 8); canisters only connected in this cluster are assumed to contribute to the radionuclide release. Other canisters *not* included in the cluster are assumed not to release radionuclides to the far-field.

In contrast, if the number of fractures is so large that most of the canisters in the repository are connected by fracture clusters, the above assumption that only one row of canister exists is inapplicable. In this case, the assumption that there are several groundwater paths (fracture clusters) in the repository model and the radionuclides release rate to the far-field is the sum of the release rate for each groundwater path (fracture cluster) is realistic. In this study, this approach has not been tested.

Comparison of these two methods is the future task.

4.3 Computational Performance of the FFDF Code

We have measured the computational performance of the FFDF code with the repository model with a radius of 20 m containing 10 canisters. The CPU time and the amount of memory consumption for fracture calculation part of the code are measured by varying parameters of the numbers of fractures.

The measured computational performance is as follows:

The total numbers of fractures in the repository dominates the CPU time for fracture calculation. The CPU time is approximately proportional to the total numbers of fractures raised to the second power.

Since the total numbers of canisters in the HLW repository is 40,000, from the viewpoint of the numbers of fractures, the FFDF code with the present calculation models and the optimization condition can not calculate the fracture generation and interconnection judgment for the full-scale HLW repository model with more than 1.0E+6 fractures by using the Earth Simulator with full nodes.

To overcome this difficulty, the more efficient optimization of the FFDF code, the development of a new fracture calculation algorithm, and the improvement of the calculation model of HLW repository are needed. For example, the development of the homogenization model of the canister and its surrounding materials is the promising method to improve the HLW repository calculation model to reduce the CPU time without severely decreasing the precision of the mass transport calculation. We should study further to decide which solutions is the most promising and has the highest priority to overcome the difficulty.

5. Conclusions

We have successfully ported the FFDF code, a fracture network generation, water flow, and mass transport code based on Monte-Carlo approach, on the Earth Simulator and executed for a model space containing 109 waste canisters.

We have also successfully ported the VR code on the Earth Simulator, and combined with the Latin Hypercube Sampling code for the uncertainty analysis.

For the PDF for the number of connected canisters, we have utilized the results of the FFDF code analysis, where fracture network is generated statistically and connection of canisters by fracture clusters is quantitatively analyzed. We have made numerical exploration for the peak release rate of ^{237}Np from the hypothetical repository consisting of 500 canisters.

With the codes we have made numerical exploration, and reached the following observations.

The fracture network generation, water flow, and mass transport calculation results obtained by the FFDF code:

- Simulation of fracture networks in a circular model of a repository with a radius of 60 m with more than a hundred thousand fractures has been executed by the Earth Simulator.
- The key parameter that determines the PDF of the total numbers of canisters connected by Flow Bearing Cluster is the total number of fractures in the model space. As the total number of fractures increases, the distribution becomes narrower, and the average value for the number of canisters included in the FBC increases.
- The key parameter that determines the residence time of the particles used in Monte-Carlo calculation is also the total number of fractures in the model space. As the total number of fractures increases, the average residence time decreases.
- Considering that the total numbers of canisters in the

HLW repository is 40,000 and CPU time of the FFDF code is approximately proportional to the total numbers of fractures raised to the second power, from the viewpoint of the numbers of fractures, the present FFDF code can not handle the fracture calculation of the full-scale HLW repository model with more than 1.0E+6 fractures by using the Earth Simulator with full nodes. To overcome this difficulty, the more efficient optimization of the FFDF code, the development of new fracture calculation algorithm, and the improvement of the calculation model of HLW repository, are needed. We should study further to decide which solutions is the most promising and has the highest priority to overcome the difficulty.

The uncertainty calculation results of radionuclide transport in multiple-canister repository model obtained by the VR code:

- As the number of fractures included in the repository increases, the average for the peak release rate of the radionuclide increases. For sufficiently large number of fractures, the average peak release rate becomes unchanging, because in such a case most of the canisters in the repository are connected by the fracture cluster, and additional fractures does not change the number of connected canisters.
- However, for such large numbers of connected canisters, there would be multiple conduits of water in fracture clusters that connect to the far-field. In such a case, the sampling method applied in this study is not applicable.
- While a fixed value has been assumed for the near-field rock porosity in the present study, a PDF should be assumed based on the fracture distributions obtained by the FFDF code [5].

(This article is reviewed by Dr. Horst D. Simon.)

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