

Development of Fundamental Technology of Large-Scale Simulation for HLW Repository Design

Project Representative

Hiroshi Okuda The University of Tokyo

Authors

Hiroshi Okuda The University of Tokyo

Keiichi Tsujimoto Mitsubishi Materials Corporation

Joonhong Ahn University of California, Berkeley

Yuji Aoyama Quintessa K.K.

Three simulation codes for HLW (High-Level radioactive waste) repository design have been developed and used for the safety analysis. The first code is a FE large scale groundwater flow and solute transport analysis system. The system is based on the GeoFEM solvers [1], which achieve the high vectorization ratio and the parallel efficiency on the Earth Simulator. The second one is the safety performance assessment code for multiple-canister repository model, VR code [2][3]. An uncertainty analysis was performed by using the VR code. It is shown from the analysis that the uncertainty would decrease with time for the single-canister and the multiple-canister repository model. The third one is the FFDF code, a Monte Carlo code for mass transport in fractured rock with the fracture network. The geo-statistical simulation for the size of rock fracture clusters that connect multiple waste canisters in the same water-flow path is performed, and the mass transport is computed for HLW repository model.

Keywords: HLW repository, finite element method, fracture network, Monte Carlo method, Latin hypercube sampling

1. FE Large scale groundwater flow and solute transport analysis

1.1. Introduction

The governing equations of groundwater flow considered here is given by the non-compressive continuous equation and the Darcy's equation. The governing equation of solute transport is given by the advection-diffusion equation. Finite element solutions of groundwater flow and solute transport are obtained by establishing a weak form of the equations using Galerkin procedure.

A GeoGEM platform[1] has been used in the parallelization, which takes the following strategies:

- 1) Inter-node parallelization,
- 2) Intra-node parallelization and
- 3) Vectorization.

The inter-node parallelization is realized by dividing the analysis model into sub-regions and allocating SMP-nodes. The intra-node parallelization and the vectorization are realized by the optimization of do-loops.

1.2. Performance analysis

The test model used in the performance analysis was a rectangular model as shown in Fig. 1. The model was divided into 8-node cubic elements. The water head on the planes

vertical to the x axis are fixed to 1.0 and 0.0 so that the groundwater flows in the +x direction. The boundary conditions on other planes used in the groundwater flow analysis were non-permeable. The boundary conditions on the planes used in the solute transport analysis were all non-flux.

The performance of the code is shown in Table 1. In the analysis of a model with 500 million-mesh, the vectorization rate is as high as 98.91% using 500 SMP-nodes, and the parallelization efficiency is as high as 99.993%, which is calculated from the execution times of 250 and 500 SMP-nodes.

1.3. Numerical results

A rectangular domain is considered as an analysis model. The permeability and the diffusion coefficient were set to 1.0 and 0.1, respectively in all elements of the model. The concentration at the point of origin was set to 1.0. Figure 1 shows the 2D distribution of concentration originating from one source. The size of the model was 100 x 100 x 100. The model was divided into 100 x 100 x 100 finite elements. Figure 2(a) and (b) show the case where the head gradient is 0.01 and 0.02, respectively. Figure 2 shows the 2D distribution of concentration originating from 1,000 sources as described in Fig. 3. The size of the model was 1,000 x 1,000 x 400. The model was divided into 1,000 x 1,000 x 400 finite elements.

Table 1 Summary of performance analysis

Total mesh	Number of SMP-nodes	Number of PEs	Execution time (s)	Vec. Ratio (%)
16 million	4	32	813	99.15
	8	64	394	99.12
	100	800	54.5	98.30
500 million	250	2,000	399	99.10
	500	4,000	224	98.91

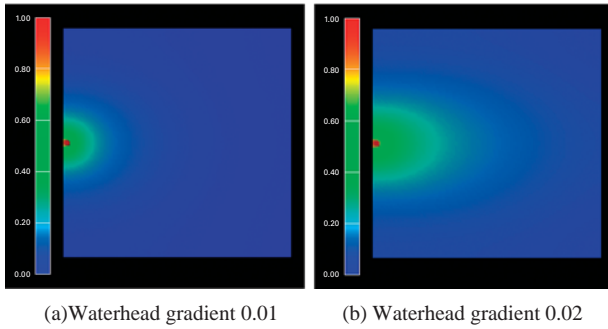
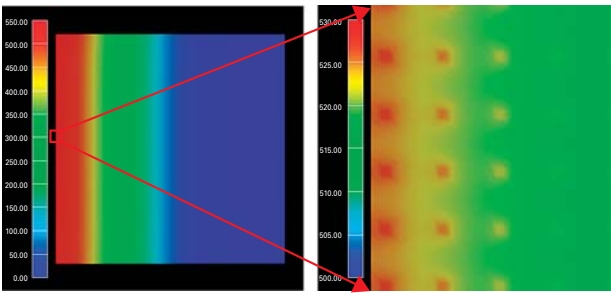
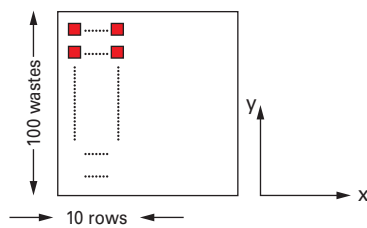
Fig. 1 Concentration distribution ($t = 10,000$) from one radioactive waste containerFig.2 Concentration distribution ($t = 10,000$) from one thousand radioactive waste containers

Fig. 3 Location of radioactive waste

2. Uncertainty Analysis of Multiple Canister Repository Model

2.1. Introduction

In the previous performance assessments [4], the mass transfer and transport were modeled for a single-canister configuration. For example, for a repository with N canisters, results of the single-canister model were simply multiplied by N . Authors have developed the mass transport code VR, which incorporates interference effects of multiple canisters in performance assessment of the repository. By deter-

ministic 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 is significant [2]. In this study, repository performance has been evaluated by using the VR code with its uncertainties resulting from parameter variations. Necessary modification and tuning up of the VR code have been made for transplantation to Earth Simulator.

2.2. Optimization of VR code to Earth Simulator

In the VR code, the repository is considered to 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 (NF) rock. The compartments are positioned in the direction of groundwater flow. Radionuclides are first assumed to be released from the waste canister, diffuse through the buffer, and then released to the NF. The NF rock in a compartment is connected by advection with the neighboring compartments. From the upstream compartment, radionuclides are carried in to the NF of the compartment of interest, and then carried out to the downstream compartment by advection. (Fig. 4)

The code optimized for parallelization and vectorization has attained the vectorization ratio of 98.14% and the parallelization ratio of 99.99% using 512 SMP-nodes.

2.3. Uncertainty Analysis

Variations of input parameters have been determined by literature survey. Parameter values with variations are determined by sampling for each realization. Latin hypercube sampling (LHS) approach has been applied for sampling. The VR code has been coupled with the code for LHS [5] readily available.

Figures 5 and 6 show the numerical results for the case where 50 canisters are included in the repository. Variations have been considered for three input parameters: the glass leach time, the solubility and the retardation factor in the buffer for a radionuclide. Only Neptunium-237 is considered in these figures. The probability distribution functions (pdf's) assumed for these three parameters are as follows [6]: a triangular distribution for the glass leach time with $3.0E+5$ (yr) as the central value and $6.0E+6$ as the range, a discrete distribution for neptunium solubility with 70% probability allocated for the reference value $5.0E-9$ (mol/l), and 15% each for an optimistic $3.0E-9$ and a pessimistic value $1.0E-8$, and a discrete distribution for neptunium retardation factor in the buffer with 70% for $1.8E+5$, 15% each for $1.8E+4$ and $1.8E+6$.

The repository performance is measured by the environmental impact, which is expressed in terms of the mass accumulation of Np-237 in the far field. The far field is defined

in this study the region exterior to the repository region. The present analysis gives the environmental impact and its uncertainty resulting from the uncertainties associated with the aforementioned three parameters.

In Fig. 5, results obtained by a conventional single-canister model are shown. The results of the single-canister model have been obtained first, and then multiplied by 50. The uncertainty associated with the glass leach time has negligible effects on the uncertainty associated with the mass of Np accumulated in the far field.

The result of the uncertainty analysis for the 50-canister repository by VR is shown in Figure 6. These figures show (1) the single-canister model would generate results with a greater uncertainty than the multiple-canister model, and (2) in either case, the uncertainty would decrease with time.

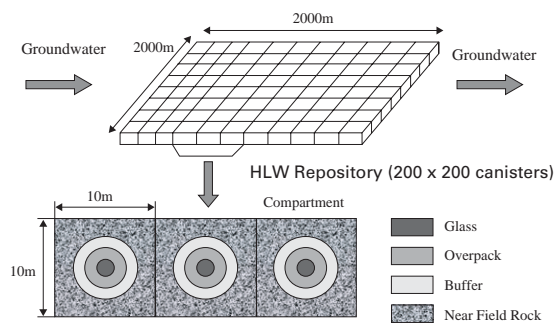


Fig. 4 HLW repository model

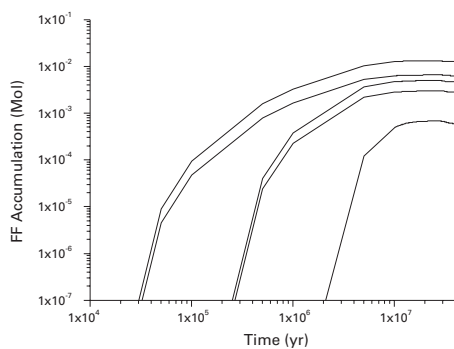


Fig. 5 The Np-237 accumulations in the far field obtained by the single-canister repository model.

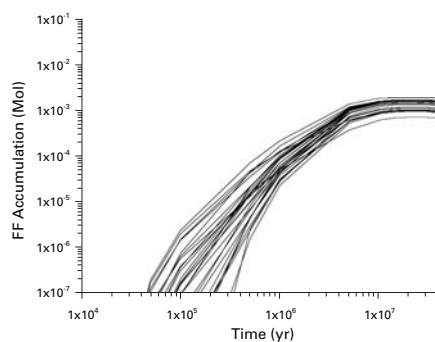


Fig. 6 The Np-237 accumulations in the far field obtained by the 50-canister repository model. (Interference effects by multiple canisters considered)

3. Large-Scale Simulation of Rock Fracture Network for Mass Transport in Geologic Repository

3.1. Introduction

Analyses for groundwater flow and mass transport in fractured rock play a central role in the performance assessment of HLW repository. It is likely that a repository is built in geologic formations where rock fractures are major conduits of groundwater, which is a principal vehicle for radionuclide transport. Rock fractures with finite sizes intersect with each other, forming a cluster, through which groundwater flows. From the viewpoint of repository performance assessment, how large these clusters could be in size and how many waste canisters would be connected by the same cluster need to be known. It was found in the previous theoretical model studies that radionuclides released from a waste canister affect radionuclide release of other canisters within the same water stream [7]. In these previous studies, however, the effects of other canisters in the same cluster were studied by assuming a number of waste canisters in the same water stream, but no discussion was made for how the number of connected canisters can be obtained.

Recently, the FFDF model, a Monte Carlo model for mass transport in fractured rock, was developed [8]. It can calculate groundwater flow and mass transport for a host rock of 10 square meters, with hundreds of fracture segments.

In this study, FFDF code has been transplanted to Earth Simulator 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.

3.2. Calculation Model

In a two-dimensional circular model space considered, a waste canister of interest is located at the center of the model space. In the host rock, fractures are generated based on statistical distribution functions assumed for the orientation angle, the location, the length and the aperture. After a certain number of fractures are generated, inter-connection among the generated fractures is checked, and Flow-Bearing fracture Cluster (FBC) is determined that connects the outer boundary of the circular model space and the inner boundary between the buffer of the central waste canister and the host rock. It is considered that groundwater flows through the FBC, so that radionuclides released from the central waste canister are transported through the FBC. Once a FBC is identified, the number of canisters included in the FBC is counted by overlapping the grid points of the canister array. This procedure has been repeated to obtain a statistical distribution for the total number of the connected canisters by fracture network in the model space. The model space is divided into triangular elements and homogenized parameters for each element are calculated. Groundwater flow

through FBC is calculated by finite element method using homogenized parameters. Mass transport calculation is made based on the Monte Carlo method.

3.3. Numerical Results

The sample realization of a fracture network is shown in Fig. 7. In the figure, the FBC is shown as blue lines, fractures not included in the FBC as green lines, the canisters included in FBC as red circles, and the canisters not included in FBC as yellow circles. A hundred thousand fractures can be handled by one SMP-node of Earth Simulator.

In Fig. 8, the PDF of the number of canisters included in the FBC is shown for three different total numbers of fractures generated in the model space. 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 included in the FBC increases.

It is observed from the calculation results that if the total number of fractures in the model space is over about $3.0E+4$, all the canisters in the model space are included in the FBC. If the total number of fractures is smaller than about $1.0E+4$, a FBC is not generated in the model space. It indicates that the total number of fractures in the repository, which can be evaluated by measuring the number of fractures per unit volume of the host rock, is a key parameter that determines the flow path of groundwater.

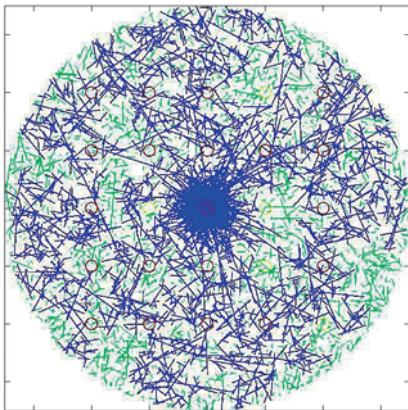


Fig. 7 Fractures generated in the HLW model.

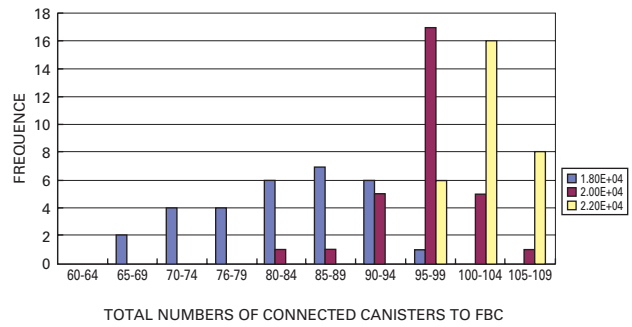


Fig. 8 PDF of the total number of fractures connected to FBC. The PDF is obtained for total number of fractures of $1.8E+4$, $2.0E+4$, and $2.2E+4$. The total number of canisters in the repository model is 109.

References

- [1] Hiroshi Okuda, Kengo Nakajima, Mikio Iizuka, Li Chen, and Hisashi Nakamura, Parallel Finite Element Analysis Platform for the Earth Simulator:GeoFEM, LNCS 2659, Part III, pp.773-780, 2003.
- [2] J.AHN, D.KAWASAKI, and P.L.CHAMBRE, "Relationship Among Performance of Geological Repositories, Canister-array Configuration, and Radioactive Mass in Waste", *Nuclear Technology*, **140**, pp.94-112, 2002.
- [3] K.TSUJIMOTO, and J. AHN, "Development of Object-Oriented Simulation Code for Repository Performance Assessment", *Trans. Am. Nucl. Soc.*, **81**, pp.54-55, Los Angeles, U.S.A., 1999.
- [4] Japan Nuclear Cycle Development Institute, "Second Progress Report on Research and Development for the Geological Disposal of HLW in Japan H12", 2000.
- [5] R. Iman, and M. Shortencarier, "A FORTRAN 77 Program and User's Guide For the Generation of Latin Hypercube and Random Samples for Use With Computer Models", SAND83-2365, 1984.
- [6] NAGRA, "Project Opalinus Clay, Models Codes and Data for Safety Assessment", NTB02-06, 2002.
- [7] J.AHN, D.KAWASAKI, and P.L.CHAMBRE, "Relationship Among Performance of Geological Repositories, Canister-array Configuration, and Radioactive Mass in Waste", *Nuclear Technology*, **140**, pp.94-112, 2002.
- [8] Lim D., "Mass Transport Analysis in the Near Field of Geologic Repository", University of California, UCB-NE-4238, 2003.

HLW処分場設計の為の大規模シミュレーション基盤技術の開発

プロジェクト責任者

奥田 洋司 東京大学

著者

奥田 洋司 東京大学

辻本 恵一 三菱マテリアル株式会社

安俊 弘 カリフォルニア大学バークレイ校

青山 裕司 (株)クインテッサジャパン

本研究ではHLW（高レベル放射性廃棄物）処分場設計のための大規模シミュレーション基盤技術として、(1) 並列有限要素法による地下水流動解析及び物質移動解析コード、(2) 不確実性を考慮した複数廃棄体モデルによるHLW処分場の性能評価コード(VR)、および(3) モンテカルロ法に基づく亀裂性媒体中の物質輸送計算コード(FFDF)を地球シミュレータ向けに開発、最適化し、安全解析に適用した。

「並列有限要素法による地下水流動解析及び物質移動解析システム」はGeoFEMをベースに開発し、地下水流動の支配方程式は非圧縮の連続の式とダルシー則に基づく流れの方程式、物質移動の支配方程式は移流拡散方程式とした。ノード間並列は領域分割に基づき計算領域を複数の部分領域にわけ各ノードに割り当てることで実現した。ノード内並列およびベクトル化は、割り当てられた部分領域内での繰り返し計算(do ループ)に対して行った。その際、オーダリングにより有限要素法のデータ構造に特有の「依存性」を回避した。直方体モデルを用いたパフォーマンスを測定では、 $1,000 \times 1,000 \times 500$ 節点の5億節点モデルを250 ノードおよび500 ノードで計算を行ったとき、ベクトル化率98.91%、並列化率99.993% が得られた。

「複数廃棄体モデルによる不確実性解析」ではHLW処分場の複数廃棄体モデルによる性能評価コードであるVRコードを地球シミュレータに移植して最適化した。VRコードにおいて、利用して入力パラメータを確率密度関数に従って変化させ、試行毎にHLW処分場の物質移行解析を実施した。試行数を低減するためにラテン格子サンプリング適用した。不確実性解析では3種の入力パラメータを変化させた。不確実性解析の結果、不確実性は時間が経過するにつれて減少することが判明した。これは、処分場が一つの廃棄体から構成されるモデル及び複数廃棄体モデルの両方の解析から示された。

「高レベル放射性廃棄物処分場における物質移行の為の亀裂ネットワークの大規模解析」ではモンテカルロ法に基づく亀裂性媒体中の物質輸送計算コードであるFFDFを地球シミュレータに移植して、亀裂ネットワークを連結する亀裂ネットワークのクラスタの大きさを地質統計シミュレーションにより解析した。その結果、処分場中に存在する亀裂数が、亀裂ネットワークによる地下水の流れの挙動を決める主要因であることが判明した。また、モンテカルロ法に基づく物質移行計算をHLW処分場モデルに対して実施した。

キーワード: 大規模シミュレーション, 有限要素法, 不確実性解析, 亀裂ネットワーク, モンテカルロ法, 高レベル放射性廃棄物