Development of Object-Oriented Simulation Code for High-Level Radioactive Waste Repository*

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Abstract

The Object-Oriented technology is applied to mass transport analysis of the high-level radioactive waste repository, and the Virtual RepositoryTM code, a prototype of Object-Oriented simulation code of the repository, has been developed. With the prototype, the feasibility and effectiveness of the computation technology to the repository performance analysis code has been studied. It has been demonstrated that by applying the existing Object-Oriented technology, the repository performance analysis code has been modularized and structured under the unified calculation environment. It is also shown that by utilizing the unified calculation environment, the code can analyze the repository model composed of multiple-canisters with various waste configuration patterns, which has never been performed by the conventional approaches. The present scoping study with the prototype shows that in order to apply the Object-Oriented analysis code to practical high-level radioactive waste repository simulation, the Object-Oriented framework should be optimized for realistic high-level radioactive waste models, especially for highly non-linear phenomena.

Key words: High-Level Radioactive Waste Repository, Performance Assessment, Realistic Model, Multiple-Canister Repository Model, Unified Calculation Environment, Object-Oriented Approach, Framework

I. Introduction

A geologic repository for the high-level radioactive waste (HLW) in which forty thousand canisters are disposed of is planned in Japan ⁽¹⁾. (See **Fig. 1**) The performance assessment of the HLW repository is made in critical stages of the repository development, such as the repository site selection, the repository design optimization, and the license application to a regulatory authority. In the performance assessment of the HLW repository, one of the key tasks is to simulate the transport of radionuclides by modeling various kinds of physical and chemical phenomena occurring in the repository and its vicinity. The simulation result will be utilized to obtain the radionuclide release rate from the region inside the repository, the near-field (NF) region to outside the repository, the far-field (FF) region. The HLW repository consists of tens of thousands of canisters with basically the same size and configuration, implying that the Object-Oriented (OO) modeling is suitable for repository performance assessment models. The

*Received 29 Oct., 2007 (No. 07-0658)
[DOI: 10.1299/jcst.2.281]

models developed previously for this purpose, however, did not apply this approach. Thus, the present study has been motivated to investigate whether the existing OO approach would actually be applicable and useful for repository performance assessment by using a small-scale prototype model. Before we have developed a prototype and made a scoping study, we summarize the technical difficulties that the repository performance assessment had faced, and how the OO approach could be useful to overcome such difficulties.

Fig. 1 The planned HLW repository in Japan

Previous performance assessment models were developed for specific situations. The HLW disposal projects are being carried out in various countries in the world. Because the combination of the engineered-barriers, the host rock and resulting geochemical and geo-hydrological conditions are different, performance assessment codes developed by one country include different features from those developed in other countries. At the same time, those models contain many common features and configurations, such as similar engineered barrier configuration around each waste canister. Efforts of developing performance assessment models and codes have been greatly redundant among various repository programs. By standardization and modularization, i.e., by reusing and sharing sub-system models, we can reduce time and cost for code development and verification. Moreover, with such a common platform, it is possible to compare the effects of different designs and/or site locations on the repository performance on a common basis.

The second point is that many previous performance assessment models were developed for a single waste-canister configuration. (See **Fig. 2**) For example, in Ref. (1), the repository performance was assumed to be linearly proportional to the total numbers of canisters in the repository; the non-linear effects by neighboring canisters had been neglected. Recently, a detailed study revealed that canister multiplicity has important effects on the repository performance⁽²⁾. It has been recognized that the repository as a contaminant source to the far-field region and the biosphere should be modeled by taking into account the canister multiplicity for realistic and reliable assessment. But, this dramatically increases the amount and complexity of computation because of heterogeneity among waste canisters placed in the repository.

Fig. 2 The single-canister repository model⁽¹⁾

Thus, a computation technology is needed, with which a performance assessment model can be constructed flexibly for various designs and conditions with a level of fidelity, i.e., complexity or heterogeneity, higher than that assumed in previous models.

Based on the aforementioned recognition for the necessity of an advanced computation platform for the performance assessment, in this study we have developed a prototype of the unified calculation environment by applying existing Object-Oriented (OO) technology. With the prototype code and model, we have performed a scoping study to identify (1) advantages and disadvantages of this proposed computational approach and (2) necessary technology development for future development of large-scale applications.

An OO approach⁽³⁾ was developed as a bottom-up technique to build a system from the combination of the components. OO approaches satisfy the requirements of modularity and reusability of the program. Applications of OO approaches to scientific calculations were studied in the 1990's.⁽⁴⁾⁽⁵⁾ The research, development, and application of OO simulation (OOS) have rapidly emerged recently.⁽⁶⁾ In an OO approach, codes that are commonly used in a specific problem are collected as a framework.⁽⁷⁾ Numerous frameworks have been developed for various needs, including graphical user interfaces, business applications, and network servers, as well as scientific computations. The examples of OO frameworks to numerically solve partial differential equations are POOMA⁽⁸⁾, PETSc⁽⁹⁾, and OVERTURE⁽¹⁰⁾.

We had previously developed the repository performance assessment code, Virtual RepositoryTM⁽¹¹⁾⁽¹²⁾, by applying OOS technology to the multiple-canister repository model described in Ref. (2). The code was designed for the multiple-canister repository model consisting of various sub models such as the vitrified waste (glass), the buffer, and the NF rock. Only capsulation by OO class was utilized in the code. With the OO framework technology, we can build a calculation code with a unified calculation environment, in which a hierarchical structure of the repository performance assessment models is implemented as the OO framework. We can manage calculation models more easily and efficiently by using the unified calculation environment than by using the capsulation by OO.

In the present study, the prototype of the OOS code has been developed, in which (1) the OO framework technology makes the code possible to construct the calculation model flexibly for various repository designs and conditions, and (2) the canister multiplicity for realistic and reliable performance assessment can be taking into account by applying the multiple-canister repository model described in Ref. (2).

The objective of this study is to demonstrate that the OO technology makes possible the Virtual RepositoryTM code (the VR code) to analyze the mass transport analysis of the repository model composed of multiple-canisters with various waste configuration patterns, which has never been performed by the previous approaches. Then the feasibility and effectiveness of these computational technologies to the HLW repository performance analysis code is evaluated. Future tasks of the technical development including the development for large-scale applications are clarified.

This paper is organized as follows: In chapter two, the mass transport model utilized in the code is described. In chapter three, the development of the unified calculation environment by OO framework is described. In chapter four, the illustrative calculations for the unified calculation environment of the code are described and discussed. Conclusions are described in chapter five.

II. Physical Models

In this study, the code has been developed based on the physical models for multiple-canister repository configuration⁽²⁾. As shown in **Fig. 3**, the HLW repository consists of multiple-canisters of the same size. The repository is divided into compartments, each containing

the vitrified waste, the buffer, and the NF rock. Radionuclides are transported between compartments by groundwater flow in the NF region.

The governing equations of the transport model are written as follows⁽²⁾. For the mass of the radionuclide in the vitrified waste, the governing equation is written as:

$$\frac{dM_k^{n(j)}(t)}{dt} = -\lambda^{n(j)}M_k^{n(j)}(t) + \lambda^{n(j-1)}M_k^{n(j-1)}(t) - q_{b,k}^{n(j)}(t), k = 1, \dots, N, 0 < t < T_k^{n(j)}, \quad (1)$$

where subscript $n(j)$ denotes the j -th member in the decay chain n , $M_k^{n(j)}(t)$ is the mass of radionuclide $n(j)$ in the k -th compartment at time of t , $\lambda^{n(j)}$ is the radioactive decay constant of radionuclide $n(j)$, $q_{b,k}^{n(j)}(t)$ is the release rate of radionuclide $n(j)$ from the vitrified waste to the buffer in the k -th compartment, $T_k^{n(j)}$ is the time when radionuclide $n(j)$ depletes completely from the vitrified waste in the k -th compartment, and N is the total number of compartments.

Fig. 3 The multiple-canister repository model

For the numerical evaluation of radionuclide release from the vitrified waste, the radionuclide concentration at the glass/buffer interface is observed at each time step. Before the interface concentration reaches the solubility, the congruent-release model is applied, where the fractional release rate of radionuclide is the same as that of the waste matrix. If the concentration has reached its solubility, then the solubility-limited release model is applied from that time step and on. In this model, the concentration at the interface is fixed at the radionuclide solubility until radionuclide depletes from the waste-canister region. For more details, see Ref. (2).

The discretization equation of the Eq. (1) is written as:

$$M^{n(j),k,t+1} = M^{n(j),k,t} + \left(\lambda^{n(j-1)}M^{n(j-1),k,t} - \lambda^{n(j)}M^{n(j),k,t} - q_b^{n(j),k,t} \right) \Delta t, \quad (2)$$

where $M^{n(j),k,t}$ is the inventory (mass) of radionuclide $n(j)$ in the vitrified waste in the k -th compartment at time step of t , $q_b^{n(j),k,t}$ is the release rate of radionuclide $n(j)$ from the vitrified waste to the buffer in the k -th compartment at time step of t , and Δt is the length of time step.

For the radionuclide mass in the buffer, the equation is written as:

$$K^{n(j)} \frac{\partial C_k^{n(j)}(x,t)}{\partial t} = D \frac{\partial^2 C_k^{n(j)}(x,t)}{\partial x^2} - K^{n(j)} \lambda^{n(j)} C_k^{n(j)}(x,t) + K^{n(j-1)} \lambda^{n(j-1)} C_k^{n(j-1)}(x,t), k = 1, \dots, N, t > 0, 0 < x < L_b, \quad (3)$$

where $C_k^{n(j)}(x,t)$ is the radionuclide concentration $n(j)$ in the buffer in the k -th compartment at time of t and distance x from the glass/buffer interface, D is the molecular diffusion coefficient,

and $K^{n(j)}$ is the retardation factor of radionuclide $n(j)$ in the buffer, and L_b is the buffer length.

For the radionuclide concentration at waste surface, the equation is written as:

$$C_k^{n(j)}(0, t) = \gamma^{n(j)}(t) C_{e(n(j))}^*, t > 0, \quad (4)$$

where $C_{e(n(j))}^*$ is the solubility of element e in which radionuclide $n(j)$ is included as isotope, $\gamma^{n(j)}(t)$ is the solubility appropriation at time of t for isotope $n(j)$ identified for the entire compartment defined as follows:

$$\gamma^{n(j)}(t) = \frac{M_k^{n(j)}(t)}{\sum_{p=\text{all_isotopes_of_element_e}} M_k^p(t)}, \quad (5)$$

For the radionuclide concentration at buffer/NF rock surface, the boundary condition is defined as:

$$C_k^{n(j)}(L_b, t) = N_k^{n(j)}(t), t > 0, \quad (6)$$

where $N_k^{n(j)}(t)$ is the concentration of radionuclide $n(j)$ in the pore water of the NF rock in the k -th compartment at time step of t .

The discretization equation of the Eq. (3) is written as:

$$\begin{aligned} Ax &= e, \\ e &= By + f, \end{aligned} \quad (7)$$

where

$$A = \begin{bmatrix} q & r & & & \\ p & q & r & & \\ & p & q & r & \\ & & & \ddots & \\ & & & & p & q & r \\ & & & & p & q \end{bmatrix}, B = \begin{bmatrix} t & u & & & \\ s & t & u & & \\ & s & t & u & \\ & & & \ddots & \\ & & & & s & t & u \\ & & & & s & t \end{bmatrix},$$

$$x = [C^{n(j),k,1,t+1}, C^{n(j),k,2,t+1}, \dots, C^{n(j),k,M-1,t+1}]^T,$$

$$y = [C^{n(j),k,1,t}, C^{n(j),k,2,t}, \dots, C^{n(j),k,M-1,t}]^T,$$

$$f = [-pC^{n(j),k,0,t+1} + sC^{n(j),k,0,t}, 0, \dots, 0, -rC^{n(j),k,M,t+1} + uC^{n(j),k,M,t}]^T,$$

$$p = -\frac{\varepsilon V_n D \theta \Delta t}{\left(\frac{\Delta_n + \Delta_{n+1}}{2}\right) \Delta_{n+1}},$$

$$q = K^{n(j)} \varepsilon V_n + 2 \frac{\varepsilon V_n D \theta \Delta t}{\Delta_n \Delta_{n+1}} + \theta \varepsilon V_n \lambda^{n(j)} K^{n(j)} \Delta t,$$

$$r = -\frac{\varepsilon V_n D \theta \Delta t}{\left(\frac{\Delta_n + \Delta_{n+1}}{2}\right) \Delta_n},$$

$$s = (1 - \theta) \frac{\varepsilon V_n D \Delta t}{\left(\frac{\Delta_n + \Delta_{n+1}}{2}\right) \Delta_{n+1}},$$

$$t = K^{n(j)} \varepsilon V_n - 2(1 - \theta) \frac{\varepsilon V_n D \Delta t}{\Delta_n \Delta_{n+1}} + (1 - \theta) \theta \varepsilon V_n \lambda^{n(j)} K^{n(j)} \Delta t,$$

$$u = (1 - \theta) \frac{\varepsilon V_n D \Delta t}{\left(\frac{\Delta_n + \Delta_{n+1}}{2} \right) \Delta_n},$$

where $C^{n(j),k,n,t}$ is the concentration of radionuclide $n(j)$ of the n -th mesh in the buffer in the k -th compartment at time step of t , ε is the porosity of the buffer, V_n is the volume of the n -th mesh, Δ_n is the length of the n -th mesh, M is the total number of meshes in the buffer, and θ is the weight factor of the discretization scheme. If θ is 1, Eq. (7) corresponds to the implicit difference scheme, and if θ is 0, it corresponds to the explicit difference scheme.

The radionuclide concentration is obtained by solving Eq. (7) by inverting tri-diagonal matrix, A , which is performed by LU decomposition method.

For the radionuclide mass in the NF rock, the equation is written as:

$$\begin{aligned} \varepsilon_p R^{n(j)} V \frac{dN_k^{n(j)}(t)}{dt} = & -\lambda_k^{n(j)} \varepsilon_p R^{n(j)} V N_k^{n(j)}(t) + \lambda_k^{n(j-1)} \varepsilon_p R^{n(j-1)} V N_k^{n(j-1)}(t) \\ & + F N_{k-1}^{n(j)}(t) - F N_k^{n(j)}(t) + q_{r,k}^{n(j)}(t), k = 1, \dots, N, t > 0, \end{aligned} \quad (8)$$

where ε_p is the porosity of the NF rock, V is the volume of the NF rock in a compartment, $R^{n(j)}$ is the retardation factor of radionuclide $n(j)$ in the NF rock, F is the volumetric flow rate of water through the interface between two adjacent compartments, and $q_{r,k}^{n(j)}(t)$ is the release rate of radionuclide $n(j)$ from the buffer to the NF rock in the k -th compartment at time of t . Since the complete mixed tank model is utilized in the NF rock calculation, $N_k^{n(j)}(t)$ has a uniform distribution in all the area of the pore water of the NF rock.

The discretization equation of the Eq. (8) is written as:

$$\begin{aligned} N^{n(j),k,t+1} = & N^{n(j),k,t} \\ & + \frac{\Delta t}{\varepsilon_p V R^{n(j)}} \{ F N^{n(j),k-1,t} - F N^{n(j),k,t} + q_{r,k}^{n(j),t} \\ & + \varepsilon_p V (R^{n(j-1)} \lambda^{n(j-1)} N^{n(j-1),k,t} - R^{n(j)} \lambda^{n(j)} N^{n(j),k,t}) \}, \end{aligned} \quad (9)$$

where $N^{n(j),k,t}$ is the concentration of radionuclide $n(j)$ in the pore water of the NF rock in the k -th compartment at time step of t , and $q_{r,k}^{n(j),t}$ is the release rate of radionuclide $n(j)$ from the buffer to the NF rock in the k -th compartment at time step of t .

The radionuclide profile in the buffer and the radionuclide concentration in the NF rock is calculated by the coupling calculations: the radionuclide profile in the buffer is obtained by using the NF rock concentration as the boundary condition defined by Eq. (6), and the NF rock concentration is obtained by Eq. (8) by using the radionuclide release rate from the buffer to the NF rock, $q_{r,k}^{n(j)}$ in Eq. (8), calculated from the radionuclide profile in the buffer.

The radionuclide is released from the repository region to the FF region, exterior to the repository region, for which the equation is written as:

$$\frac{dM_f^{n(j)}(t)}{dt} = -\lambda^{n(j)} M_f^{n(j)}(t) + \lambda^{n(j-1)} M_f^{n(j-1)}(t) + F N_N^{n(j)}(t), t > 0, \quad (10)$$

where $M_f^{n(j)}(t)$ is the mass of radionuclide $n(j)$ existing in the FF region at time of t , and $N_N^{n(j)}(t)$ is the concentration of radionuclide $n(j)$ of water leaving the most downstream compartment N .

The discretization equation of the Eq. (10) is written as:

$$M_f^{n(j),t+1} = M_f^{n(j),t} + (F N_N^{n(j),t} - \lambda^{n(j)} M_f^{n(j),t} + \lambda^{n(j-1)} M_f^{n(j-1),t}) \Delta t, \quad (11)$$

where $M_f^{n(j),t}$ is the mass of radionuclide $n(j)$ in the FF region at time step of t .

The flow of mass transport calculations is based on the multiple-canister repository model ⁽²⁾. The radionuclide release from the vitrified waste is calculated by the radionuclide

release model. The transient diffusion of radionuclide in the buffer with a radioactive decay chain is numerically solved by the implicit or explicit method. A complete mixing tank model is applied for the mass transport from one compartment to another through the NF rock. The radionuclide accumulation in the FF region is calculated. The coupling calculation between the buffer and NR rock is performed to incorporate the non-linear canister interference effect.

The difference between the present transport model and the multiple-canister repository model described in Ref. (2) is that the present transport model can assign different initial inventory in each vitrified waste by utilizing the unified calculation environment, for which the equation is written as:

$$M_k^{n(j)}(0) = M_k^{0,n(j)}, \quad (12)$$

where $M_k^{0,n(j)}$ is the inventory of radionuclide $n(j)$ in the vitrified waste in the k -th compartment at time step of 0.

In the multiple-canister repository model described in Ref. (2), the calculation model and data are set to be identical for the entire vitrified wastes.

III. Development of the Unified Calculation Environment

We have developed the unified calculation environment implemented as the OO framework for the multiple-canister repository model ⁽²⁾ shown in Fig. 4. The framework is composed of two layers, the application layer and component layer. The application layer consists of classes that are direct abstraction of the physical model, so that the layer includes the simulation control and abstract classes corresponding with the frozen spots of the framework. The component layer consists of solvers corresponding with the hot spots of the framework, which are application dependent. The framework makes possible the management of the solvers by modifying the component layer without changing the application layer.

Fig. 4 The framework structure

The C++ language ⁽¹³⁾, an OO language, is utilized in the program implementation. UML ⁽¹⁴⁾, a graphical language, is utilized in the OO model expression in this study.

The framework has been developed by using a design pattern (Factory Method) ⁽¹⁵⁾. In case of inventory calculation, s_sdif calls $s_glasscalcbase$, whose implementation is contained in its subclasses $s_glasscalc_solcon$ and $s_glasscalc_sol$. Objects are created by $s_objectcreator$. The component layer contains $s_glasscalc_solcon$, $s_glasscalc_sol$, and $s_objectcreator$. Due to the abstraction of calculation model, a suitable calculation model is selected and executed if s_sdif calls $s_glasscalcbase$ whether which of $s_glasscalc_solcon$ and $s_glasscalc_sol$ is selected as

the inventory calculation model.

IV. Calculation Results and Discussions

(1) The flexibility and reusability of the code

The first set of illustrative calculations has been prepared for demonstrating the flexibility and reusability of the code that is implemented by the unified calculation environment, i.e., that the calculation models can be changed by using the developed framework.

In this example, two numerical schemes for evaluation of the concentration profile of Np-237 in the buffer, the adaptive and uniform mesh generation functions, have been implemented in the buffer solver of the framework. The radionuclide concentration profile in the buffer is obtained with the condition of uniform mesh with 12, 100, and 1,000 partitions, and adaptive mesh with 12 partitions. Only a single compartment is considered in the example. The calculation model is shown in Fig. 5. Parameter values, referred from Ref. (16), are summarized in Table 1.

Fig. 5 The single-canister repository model

The Np-237 concentration profiles in the buffer at 100 years are shown in Fig. 6. A uniform mesh with 1,000 partitions is considered as the reference. The figure shows that the adaptive mesh calculation result is closer to the reference than other uniform mesh results (12 and 100 partitions) in spite of the small numbers of meshes. This is because the concentration profile at the glass/buffer boundary is calculated precisely in the adaptive mesh calculation in which the mesh size adjacent to the waste is smaller than the diffusion characteristics length.

Table 1 The input data for mass transport analysis

(a) Property Data

Description	Parameters	Units
Areal extent of the compartment	10×10	m
Surface area of the waste glass	2.1	m ²
Thickness of the bentonite buffer	0.98	m
Diffusion coefficient in the bentonite	0.03	m ² /yr
Glass leach time	1,000.0	yr
Distance between canisters	10.0	m
Buffer porosity	0.3	-
Rock porosity	0.5	-
Groundwater velocity	1.0	m/yr

(b) Element data

Element	Solubility (mol/m ³)	Retardation factor in buffer (-)	Retardation factor in rock (-)
Curium	1.0×10 ⁻⁴	42,600	27
Americium	1.0×10 ⁻⁴	42,600	27
Plutonium	1.0×10 ⁻⁵	42,600	66
Neptunium	1.0×10 ⁻⁵	427	3.6
Uranium	1.0×10 ⁻⁵	427	1.3

(c) Radionuclide data

Chain number	Nuclide	Half life (yr)	Initial inventory (mol)
1	Pu240	6.57×10^3	0.1
	U236	2.34×10^7	0.028
2	Cm245	9.30×10^3	0.003783
	Am241	4.58×10^2	0.141
	Np237	2.14×10^6	2.01
	U233	1.62×10^5	0.000615
3	Pu242	3.76×10^5	0.009
	U238	4.46×10^9	2.92
	U234	2.45×10^5	0.00555
4	Am243	7.37×10^3	0.243
	Pu239	2.44×10^4	0.127
	U235	7.04×10^8	0.035

Fig. 6 The comparison of the buffer concentration profile

(2) Canister interference effect with uniform waste composition

The second set of calculations has been prepared for demonstrating the non-linear canister interference effect of the multiple-canister repository model ⁽²⁾. In this example, mass transport calculations for the repository model with 128-canisters and single-canister with a simulation time of 10^6 years have been performed by the prototype. The calculation model and data including waste compositions are set to be identical for the entire wastes. The same repository model, in which waste calculation model and data are identical, was utilized in Ref. (2). The repository model depicted in **Fig. 7**, and the input data shown in **Table 1** are utilized in the calculation.

The numerical result is shown in **Fig. 8**. It is shown from the figure that the radionuclide release rate obtained from the 128-canister repository model is nearly 10 times smaller than those from the single-canister repository model for every nuclide. The non-linear effect of the repository performance observed in Ref. (2) has been confirmed by this example.

Fig.7 The 128-canisters repository model

Fig.8 The radionuclide release rate distribution from the NF to FF region

(3) Canister interference effect with heterogeneous waste composition

The third set of illustrative calculations has been prepared for demonstrating the flexibility and reusability of the code and the non-linear canister interference effect considering the heterogeneous waste compositions.

In the HLW repository, it is likely that the variations of the fuel type and burn-up of spent nuclear fuels, from which high-level radioactive wastes are generated, forms the heterogeneous waste compositions. However the analysis of the repository model composed of multiple-canisters considering the heterogeneous waste composition was not performed in the previous approaches. For example, the waste compositions are set to be identical for the entire wastes in the multiple-canister repository model ⁽²⁾, and most of the previous HLW safety performance codes utilized the single-canister repository model. By utilizing the unified calculation environment to assign different inventory data to waste objects in the repository model, the VR code is able to analyze the repository model composed of multiple-canisters considering the heterogeneous waste composition without major modifications of the code.

In this calculation, as an example of OO framework application, the repository model composed of 205 wastes considering canister interference effect and various waste configuration patterns occurring from heterogeneous waste composition is analyzed by the prototype, which has never been performed by the previous approaches.

In this study, it is assumed that, as a radionuclide, only Np-237 is contained in the glass. The glass compositions, classified on the basis of burn-up and type of spent fuel, are summarized in Table 2.

Table 2 Parameter values for glass composition ⁽¹⁷⁾

Waste type number	Waste type name	Type of spent fuel	Burn-up (MWD/t) of spent fuel	Np-237 concentration of waste (mol/waste)
1	PWR-1	PWR	32,000	2.386
2	BWR-1	BWR	29,500	2.499
3	BWR-2	BWR	33,000	2.533
4	PWR-2	PWR	43,000	2.686
5	BWR-3	BWR	39,500	2.700
6	BWR-4	BWR	45,000	2.803
7	PWR-3	PWR	48,000	2.906

*PWR stands for Pressurized-Water Reactors. BWR stands for Boiling-Water Reactors.

Based on the heterogeneous waste composition, eight kinds of waste configuration patterns, patterns 1 to 8, are set for repository calculation. Furthermore, two fictitious waste configuration patterns, patterns 9 and 10, are added to the waste configuration patterns, in which the entire compartments are composed of only one waste type whose Np-237 concentration is the highest or the lowest among eight waste types. The waste configuration patterns, the distribution patterns of the initial inventory of the vitrified waste, used in the repository calculation are shown in Fig. 9. The repository model consisting of 200 rows each containing 205 compartments is considered. Each compartment row contains seven or one waste types in ten different configuration patterns.

For more details, see Ref. (17).

Fig. 9 The full-scale repository model and waste configuration patterns

The resultant accumulations of Np-237 in the FF region with various configuration patterns are shown in **Fig. 10**. It is observed that eight patterns considering the heterogeneous waste composition are within the range set by the two bounding cases, patterns 9 and 10.

The numerical demonstration shows that by applying the OO framework optimized for the multiple-canister repository model ⁽²⁾, the prototype code is able to analyze the realistic performance assessment model for HLW repository composed of multiple-canisters considering (1) the non-linear canister interference effect and (2) the various waste configuration patterns without modifying the code, which has never been performed by the conventional approaches. It is also shown that the OO technology is a promising method for the simulation of the realistic HLW repository model in which the calculation models can be constructed flexibly for various repository designs and conditions.

Fig. 10 The accumulation distributions of radionuclides in the FF region for various waste configuration patterns

In this study, we have considered application of the OO technology to the radionuclide transport model based on the compartment model approach, which is utilized in the multiple-canister repository model ⁽²⁾. In the compartment model approach, physical models are connected in a linear manner except for the canister interference effect. In more realistic performance assessment models, we need to deal with a hierarchical model structure, and coupled phenomena, which are in many cases highly non-linear than the canister interference effect which is taken into account in the VR code in the present study. For example, waste dissolution changes surrounding chemical conditions and hydrological conditions, which in return affects waste dissolution. For such coupled phenomena, we need to develop an optimized OO framework.

V. Conclusions

We have developed the Virtual RepositoryTM code, a prototype of the Object-Oriented calculation code for the performance assessment of the high-level radioactive waste repository composed of multiple-canisters. The feasibility and effectiveness of the Object-Oriented technology to the repository performance analysis code has been studied by the prototype.

By applying the existing Object-Oriented technology, the repository performance analysis code has been modularized and structured under the unified calculation environment developed in this study. It is shown that the Virtual RepositoryTM code can analyze more realistic performance assessment models for the repository than the conventional approaches by utilizing the unified calculation environment without major modifications of the code: the prototype can analyze the repository model composed of multiple-canisters with various waste configuration patterns, which has never been performed by the conventional approaches of the high-level radioactive waste repository analysis.

It is also shown that the Object-Oriented technology is a promising method for the simulation of the realistic repository model in which the calculation models can be constructed flexibly for various repository designs and conditions.

As the present study has been performed with the prototype, we still need to make substantial technology development for a realistic large-scale repository performance analysis models. Those items for future technology development identified in the present scoping study is the development of the Object-Oriented framework optimized for the more realistic performance assessment models for the high-level radioactive waste repository, especially for coupled highly non-linear phenomena.

Acknowledgement

Authors are grateful to Professor Hiroshi Okuda of the University of Tokyo for his valuable suggestion on this study.

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