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ARTICLE

Scenario analysis of future nuclear energy use in Japan: (1) Methodology of Nuclear fuel cycle simulator: NMB4.0

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The realization of nuclear fuel cycle is expected to contribute significantly to achieving net-zero greenhouse gas emissions. Since the nuclear fuel cycle is a complex system, comprehensive and quantitative discussions involving various stakeholders are necessary to evaluate new technologies and new nuclear energy utilization strategies. Therefore, the NMB4.0 was developed. NMB4.0 is a calculation code that quantitatively simulates the material flow in all stages of the nuclear fuel cycle, from the front end, such as the amount of mined uranium, to the back end, such as the number of waste packages and the area of geological repository. NMB4.0 is an open source code that runs on Microsoft Excel®, so it can be easily used by many people regardless of their specialties and backgrounds. This paper describes the methodology of NMB4.0 in detail.

Keywords: nuclear fuel cycle simulation; NMB4.0; materila balance calculation

Nomenclature

A_i	Heat generation of the nuclide i in waste unit [W/body]	Q	Heat generation density of waste [W/m^3]
a	A constant of 0, 0.5, or 1	q_i	Time distribution of decay heat of nuclide i
c	Specific thermal power [MWt/t]	rawU	Raw U
D	Decay chain matrix	r	position
depU	Depleted U	T	The time in which a fuel spent in the reactor [year]
e	Enrichment [-]	t	Time
enrU	Enriched U	u_i	Contribution of the nuclide i to all heat source [K/W]
$\vec{F}$	Vector of microscopic fission cross section [barn]	u	Temperature [K]
i	Nuclide	W_{SWU}	Separative work [SWU]
k_∞	Infinite multiplication factor [-]	w	Weight of material [t]
$\vec{N}$	Nuclide quantity vector	x_i	Weight of isotope i *in material* [t]
m	Material tag	ϵ_{op}	Operation efficiency [-]
M_i	Relative atomic mass of nuclide i	ϵ_t	Thermal efficiency [-]
n	Mass number of nuclide [-]	κ	Thermal conductivity [W/K/m]
P_e	Power generation [GWe]	ν	Number of neutrons per fission [-]
P_t	Reactor power [Wt]	ρ	Mass density [kg/m^3]
$\overrightarrow{P_F}$	Vector of power per fission [Wt]	σ_c	Microscopic capture cross section [barn]
P_e	Generation capacity [TWh]	σ_f	Microscopic fission cross section [barn]
p_i	Special distribution of decay heat of nuclide i normalized to 1 W/body	σ	Specific heat [J/kg/K]

1. Introduction

The nuclear fuel cycle is a complex system consisting of multiple processes: the front-end like uranium (U) mining process, burnup in nuclear reactor and the back-end like waste management process. Currently, research on new technologies for the nuclear fuel cycle including fast reactor and partitioning technology are being conducted around the world. In order to evaluate the usefulness of these technologies and to develop their introduction strategies, it is desirable to hold discussions involving many stakeholders. In addition, many countries that use nuclear energy as an energy source have important issues regarding high level radioactive waste (HLW) disposal.

In order to discuss the nuclear fuel cycle and solve the issues, stakeholders need to have a common understanding of the components of nuclear fuel cycle and to assess the

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technologies and implementation strategies of the nuclear fuel cycle quantitively. Several countries have developed codes to simulate the nuclear fuel cycle [1-3]. These codes focus on the burnup of nuclear fuel material in the front-end and in the reactor and are primarily aimed at tracking actinide nuclides. On the other hand, most of them do not track fission products (FPs), which limits the analysis related to waste.

NMB4.0 has been developed in collaboration between Japan Atomic Energy Agency (JAEA) and Tokyo Institute of Technology (Tokyo Tech) [4]. This code simulates the entire nuclear fuel cycle by calculating the amount of 26 actinides and 153 FPs from the front-end to the back-end. Unlike other nuclear fuel cycle simulators, the nuclides to be analyzed have been selected for the calculation about waste management and a repository heat transfer analysis model is implemented in this code. Therefore, it is capable of calculating the number of HLW packages and the area of repository. NMB4.0 is an open source code, which runs on Microsoft Excel®, and makes it possible to easily conduct nuclear fuel cycle studies by a variety of stakeholders. NMB4.0 simulates the nuclear fuel cycle by dividing the entire nuclear fuel cycle into six "plants" and calculating the logistics between each plant. [4] provided the limited discussion of the function of NMB4.0. Therefore, the objective of this paper is unified description of the methodology and explicit statement of the calculation model to simulate all plants in NMB4.0. In particular, the repository heat transfer analysis model and data of the repository temperature compiled in a database of NMB4.0 are discussed based on a concrete example of a calculation.

2. Methodology

2.1. Material

The fundamental function of NMB4.0 is to calculate the weight $x_i(m,t)$ of material processed at each plant in the nuclear fuel cycle. Where i, isotope; m,material tag; t, year. i contains 26 actinides with a half-life of more than 2 days, as well as 153 FPs selected to perform precise back-end analysis. FPs were selected from the species treated in ORIGEN2 [5] to construct a burnup chain that reproduces the calculated mass, decay heat, radioactivity, and radio-toxicity with an accuracy of 99.9% [6]. m denotes the name of each material and is used to distinguish them at each plant. Three types of material tags exist: fresh fuel (FF), spent fuel (SF), and raw materials like recovered U, plutonium (Pu), and minor actinide (MA). They change throughout each plant as shown in **Figure 1 (a)**.

2.2. Models of six fuel cycle plants

Figure 1 (b) shows a conceptual diagram of the nuclear fuel cycle analyzed in NMB4.0. Among the plants in the figure, only nuclear power plant and reprocessing plant allow the user to specify the throughput and the start-up year. The throughputs and the timing of operation of other plants are determined subordinately from these two plants. Inside the NMB4.0 simulation, the operation of reprocessing plant, dismantling and decommissioning of reactor plant, fuel exchange, and construction of reactor plant are sequentially performed as time t progresses. Other plant operations are performed in conjunction with these operations.

In the front-end, the amount and timing of material for fresh fuel corresponding to the user-specified nuclear power plant throughput is calculated at the mining plant, the enrichment plant, and the fuel fabrication plant. In these three plants, calculations are performed at the moment that the demands from their downstream power plants occur. In addition, their total throughput is supposed to be unlimited. In other words, NMB4.0 displays the various quantities in an ideal front-end plant operation that correspond to the fuel demand of the user's assumed reactor operation plan.

In the back-end, the amount of raw material separated from SF and the throughput of solidification, storage, and disposal processes in the waste management plant are calculated based on the throughput and the operation period of the reprocessing plant. Only wastes from SF are calculated; activation products are not included. In this calculation, as with the front end, the storage capacity of the raw materials and the amount of material treated in

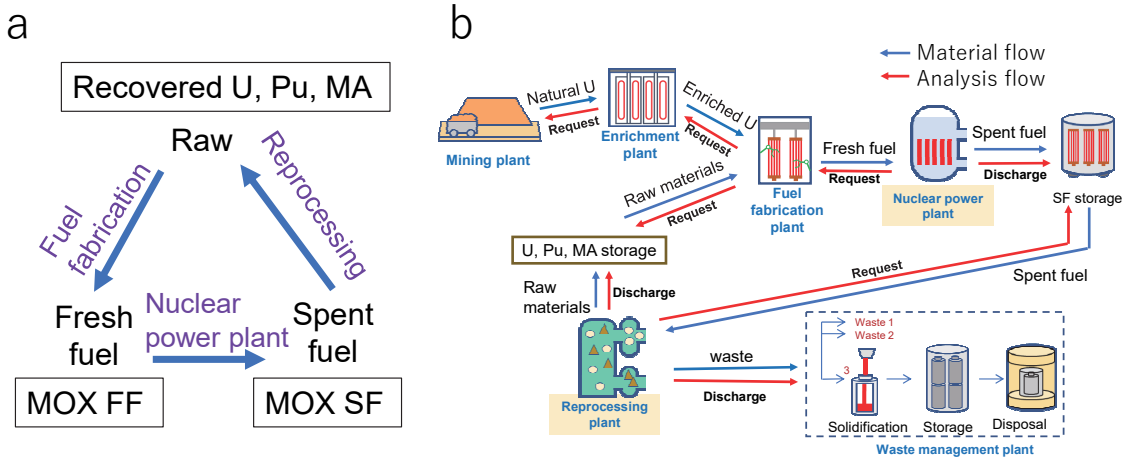

Figure 1. (a) Change of material tags through the plants. (example: mixed oxide (MOX) fuel), (b) Material and analysis flow of NMB4.0.

each process of the waste management plant are treated as unlimited.

If it is desired to impose a limit on the amount of processing at each subordinal plant, the throughput of the nuclear power plant and the reprocessing plant must be adjusted by user to meet that limit.

2.3. Mining plant

The amount of natural U mined to produce the required amount of enriched U is determined by Eq. (1).

$$w_{\mathrm{natU}} = \frac{e_{\mathrm{enrU},235} - e_{\mathrm{depU},235}}{e_{\mathrm{natU},235} - e_{\mathrm{depU},235}} w_{\mathrm{enrU}} \tag{1}$$

All e can be specified by the user to any value. w_{enrU} and $e_{\mathrm{enrU},235}$ can be automatically calculated within NMB4.0 to the appropriate value corresponding to the fuel of the specified reactor using Eqs. (8) and Eq. (9), respectively, as described in chap. 2.5. The throughput of the mining plant is defined as the amount of natural U mined, w_{natU}.

2.4. Enrichment plant

In the enrichment plant, the amount of depleted U generated during the production of enriched U is calculated and the enrichments of U nuclides in the enriched U and depleted U are determined.

First, the amount of depleted U and the amount of required raw U are determined. The amount of depleted U is obtained from Eq. (2), where rawU represents raw U, which can be natural U, depleted U, or recovered U. the amount of required raw U are determined in the same way as in Eq. (1)

$$w_{\mathrm{depU}} = \frac{e_{\mathrm{enrU},235} - e_{\mathrm{rawU},235}}{e_{\mathrm{rawU},235} - e_{\mathrm{depU},235}} w_{\mathrm{enrU}} \tag{2}$$

Next, the enrichment of U isotopes from ^{232}U to ^{238}U are calculated. Each U nuclide except ^{235}U and ^{238}U is treated approximately as a ternary system with ^{235}U and ^{238}U, and the enrichment of each nuclide is calculated separately by solving the simultaneous equations of Eq. (3) and Eq. (4) [7]. k in Eq.4 is defined by Eq.5.

$$w_{\mathrm{enrU}} \times e_{\mathrm{enrU},i} + w_{\mathrm{depU}} \times e_{\mathrm{depU},i} - w_{\mathrm{rawU}} \times e_{\mathrm{rawU},i} = 0 \tag{3}$$

$$\frac{w_{\mathrm{enrU}} \times e_{\mathrm{enrU},i}}{\left\{\frac{e_{\mathrm{enrU},235}}{1 - e_{\mathrm{enrU},235} - e_{\mathrm{enrU},i}}\right\}^{2k-1}} + \frac{w_{\mathrm{depU}} \times e_{\mathrm{depU},i}}{\left\{\frac{e_{\mathrm{depU},235}}{1 - e_{\mathrm{depU},235} - e_{\mathrm{depU},i}}\right\}^{2k-1}} - \frac{w_{\mathrm{rawU}} \times e_{\mathrm{rawU},i}}{\left\{\frac{e_{\mathrm{rawU},235}}{1 - e_{\mathrm{rawU},235} - e_{\mathrm{rawU},i}}\right\}^{2k-1}} = 0 \tag{4}$$

$$k = \frac{238 - n_i}{238 - 235} \tag{5}$$

The throughput of enrichment plant is expressed in w_{rawU} or separative work W_{SWU} calculated from Eq. (6) and Eq. (7) [7].

$$W_{SWU} = w_{\mathrm{enrU}} V(e_{enrU}) + w_{\mathrm{depU}} V(e_{\mathrm{depU}}) - w_{\mathrm{rawU}} V(e_{\mathrm{rawU}}) \tag{6}$$

$$V(e) = \left(\sum_{i \neq 238} \frac{2k_i}{2k_i - 1} e_i - 1\right) \ln \frac{e_{235}}{e_{238}} \tag{7}$$

2.5. Fuel fabrication plant

In addition to calculating the weight of FF, the fuel fabrication plant determines the composition of the FF based on the amount and isotopic vector of Pu and other stored raw materials.

First, the FF weight w that satisfies the throughput of the nuclear power plant specified by the user is obtained from Eq. (8).

$$w = \frac{P_e}{\epsilon_t \times c \times 10^3} \tag{8}$$

In UO_2 FF, this w is equal to w_{enrU} used in the mining and enrichment plants. Since the enrichment of ^{235}U in UO_2 fuel and the Pu fraction in MOX fuel depend on the type of fuel and the compositions of the stored raw materials, NMB4.0 determines these values using the infinite multiplication factor k_∞ shown in Eq. (9). The user can specify the value of k_∞ in the beginning, middle, and end of burnup period.

$$k_\infty = \frac{\sum_i \nu_i \sigma_{\mathrm{f},i}\, x_i(\mathrm{FF}, t+aT)/M_i}{\sum_i (\sigma_{\mathrm{c},i} + \sigma_{\mathrm{f},i})\, x_i(\mathrm{FF}, t+aT)/M_i} \tag{9}$$

NMB4.0 performs preliminary burnup calculations during t and $t + aT$ and adjusts the fuel composition using the false position method so that k_∞ matches the user-specified value. Non-actinide elements mixed in the raw materials are also taken into account when calculating the infinite multiplication factor.

The throughput of the fuel fabrication plant is defined as weight w of FF.

2.6. Nuclear power plant

The user can specify the type of nuclear plant, year of construction, throughput (i.e., electricity capacity), and operating period (i.e., reactor life). The plants belonging to the front-end are estimated based on these specifications as mentioned above. NMB4.0 supports batch operation, and when the time comes for a fuel change, a part of the core fuel is taken out as SF and loaded with FF.

The composition of the SF is obtained by solving the burnup equations Eq. (10) and Eq. (11).

$$\frac{d\vec{N}(T)}{dt} = \boldsymbol{A}\vec{N}(T) \tag{10}$$

$$A = D + \frac{P_t}{\vec{P}_F \cdot \vec{F} \cdot \vec{N}} \left(C_{fission} + C_{capture} + C_{n,2n} \ldots\right) \tag{11}$$

When a FF is loaded at time t_0 and burned up until time t_1, the boundary condition is Eq. (12) and composition at time t_1 is Eq. (13).

$$\vec{N}(T)\big|_{T=t_0} = x_i(\mathrm{FF}, t_0) \quad (12)$$

$$x_i(\mathrm{SF}, t_1) = \vec{N}(T)\big|_{T=t_1-t_0} \quad (13)$$

In the 179 nuclides considered in NMB4.0, the shortest half-life is 9.14 hours of ^{135}Xe. When using the conventional matrix exponential method, it is necessary to use small time step or higher expansion order to avoid divergence of the solution, which is computationally expensive. To reduce the computational cost, Okamura explicit method (OEM) [8] was developed and implemented. NMB4.0 adopts the solutions of the second-order transpose OEM (Eq. (14) and Eq. (15)), which is superior in both computational cost and accuracy.

$$N_i^{(2)} = N_i^{(1)} + \frac{1}{2}\widetilde{\Delta t_i}\sum_{j\neq i} A_{ij}N_j^{(1)} \quad (14)$$

$$N_i^{(1)} = N_i + \widetilde{\Delta t_i}\sum_j A_{ij}N_i^{(0)} \quad (15)$$

The throughput of a nuclear plant is the generation capacity P_e, which is obtained by Eq.16.

$$P_e = P_t \times 365.25 \times 24 \times 10^{-6} \times \epsilon_{op} \quad (16)$$

2.7. Reprocessing plant

The user can specify the annual throughput of each reprocessing plant, and NMB4.0 selects SF from the storage until that capacity is reached. NMB4.0 retains information of the year in which SF is stored, so the user can select how to take SF out from first-in-first-out (FIFO) and last-in-first-out (LIFO). Then, based on the distribution ratio specified by the user, the selected SF is divided into raw material such as Pu and recovered U and waste containing other elements. The distribution ratio for the raw materials and waste can be specified for each element. At this time, the waste is not divided into more detailed materials. The raw materials are stored in storage for each material, and the waste is processed in a waste management plant.

2.8. Waste management plant

First, the waste management plant divides the whole waste from the reprocessing plant into several types of waste. For example, waste generated from UO_2 SF is divided into noble gas, silver iodide waste, and HLW in a typical PUREX process. The distribution ratio used in this process can be user-specified for each element as in a reprocessing plant.

Next, solidification, storage, and disposal are performed on each divided wastes to meet user-defined limits. In the HLW solidification, the main limitation is the weight of radioactive nuclides per vitrified waste unit. However, if the waste to be solidified contains nuclides such as ^{90}Sr and ^{137}Cs, which cause high heat generation due to decay, the heat generation per solidified waste unit can be a limitation. In this case, if the waste is to be disposed in a geological repository, other parameters such as the storage period of the solidified waste and the emplacement pitch of waste package in the repository must be taken into account to find the maximum waste loading that will satisfy the repository temperature limit. This is because it is most important to ensure that the maximum temperature of the buffer material does not exceed the upper temperature limit to design repository. **Table 1** shows the limitations of solidification that can be considered in NMB4.0. These limits can be combined arbitrarily, and the maximum waste loading that satisfies all specified limits is automatically determined.

In the storage process, it is assumed that the waste is stored for a user-specified number of years, and decay calculations are performed for the nuclides contained in the waste.

In the disposal process, emplacement method of the waste, such as the repository layout, is determined. There are two ways to determine it. One is to specify a particular method. The other is to automatically select the optimal one from candidate methods to meet the temperature limit of the repository. In this method, the repository temperature is evaluated in order from the emplacement method with the shortest waste package pitch, considering the waste that meets the solidification conditions. Then, those that satisfy the temperature limit of the repository are adopted.

To perform the repository temperature evaluation, a

Table 1. Limitations of solidification.

Item	Unit	Description
Waste element loading	%	Oxide or element weight percentage in waste
Heat at solidification	W/waste	Heat generation of a waste after solidification process
Maximum temperature of buffer material	℃	Maximum temperature of buffer material in repository when disposed of by specified emplacement method after specified storage period
Heat at disposal	W/waste	Heat generation of a waste after storage
MoO_3 loading	%	Weight percentage of molybdenum oxide
PGM loading	%	Weight percentage of platinum group element oxides

temperature evaluation model is implemented in NMB4.0. The heat conduction equation to be solved is Eq. (17).

$$\sigma\rho\frac{d}{dt}u(r,t) = \kappa\nabla^2 u(r,t) + Q(r,t) \quad (17)$$

Assuming that each property value has no temperature dependence, $Q(r,t)$ can be divided into each nuclide i that constitutes the heat source as shown in Eq. (18) because Eq. (17) has linearity. ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{241}Am, ^{242m}Am, ^{243}Am, ^{244}Cm, ^{90}Sr, and ^{137}Cs, were selected as nuclide i. Because of their very short half-lives, the decay heat of ^{242}Cm, ^{242}Am, ^{90}Y, and ^{137m}Ba are added to the decay heat of their parent nuclides.

$$Q(r,t) = \sum_i Q_i(r,t) = \sum_i A_i p_i(r) q_i(t) \quad (18)$$

Therefore, assuming that $p_i(r)$ is uniform within the waste unit, we can solve Eq. (17) for each heat source nuclide i and sum up the product of A_i and the obtained repository temperature increase $u_i(r,t)$ to obtain the solution of Eq. (17).

$$\sigma\rho\frac{d}{dt}u_i(r,t) = \kappa\nabla^2 u_i(r,t) + p_i(r) q_i(t) \quad (19)$$

$q_i(t)$ is calculated in advance with ORIGEN2 for the case where the waste body has heat generation of 1 W for a number of heat source nuclides, and the temperature change $u_i(r_{peak},t)$ at the point where the buffer material temperature is the highest is obtained for several disposal methods using finite element method (FEM). The data are compiled into a database. In NMB4.0, this database is used to obtain the buffer material temperature by the following Eq. (20).

$$u(r_{peak},t) = \sum_i A_i u_i(r_{peak},t) \quad (20)$$

The validity of this method is demonstrated by comparing the left-hand side with the right-hand of Eq. (20) using FEM analysis code and compiled data in NMB4.0. The comparison is based on the case of a pressurized water reactor (PWR) MOX SF with burnup of 50 GWd/t at discharge, which is directly disposed after 75 years of cooling. SF composition and heat generation were determined by ORIGEN2. The waste unit was a 1.24 m diameter canister containing only one SF assembly, and the buffer surrounding the waste unit was 70 cm thick. The waste unit pitch was 18 m and the disposal tunnel pitch was 20 m. The disposal depth was 600 m. The location of r_{peak} is center in height along inner surface of the hollow cylinder of the buffer material.

Figure 2 shows results of $q_i(t)$ and the corresponding $u_i(r_{peak},t)$ for ^{241}Pu, ^{241}Am and ^{137}Cs. The $q_i(t)$ of ^{241}Pu increased rapidly and then decreased exponentially, because the decay heat of ^{241}Am was added to the heat generated by ^{241}Pu. Most of ^{241}Pu decay into ^{241}Am in a short time because it has a half-life of 14 years. The decay mode of ^{241}Pu is β-decay, which generates little heat, while that of ^{241}Am is α-decay, which generates a great deal of heat. Therefore, as shown in Figure 2, $q_i(t)$ and $u_i(r_{peak},t)$ of ^{241}Pu with an initial heat value of 1 W shows the same change as that of ^{241}Am after 100 years. And each $u_i(r_{peak},t)$ reflects the change in each $q_i(t)$,

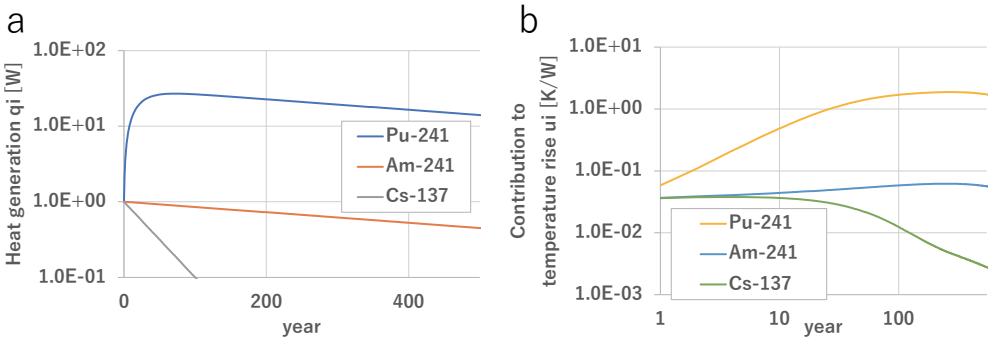

Figure 2. (a) Examples of $q_i(t)$; (b) Examples of $u_i(r_{peak},t)$.

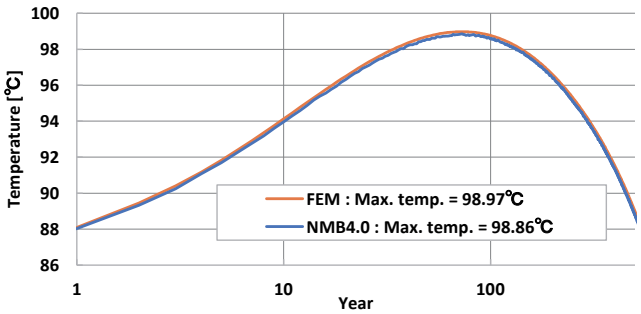

Figure 3. Comparison of the temperature evolution of buffer material for NMB4.0 and FEM.

indicating the contribution of nuclide i to the buffer material temperature. **Figure 3** shows a comparison of the time evolution of $u(r_{peak}, t)$ calculated by the NMB4.0 method and FEM, which are labeled "NMB4.0" and "FEM" respectively. Both results agree very well, and the difference in maximum temperature rise is about 0.2%. Therefore, the temperature analysis method implemented in NMB4.0 is sufficiently sophisticated and contributes to the study of repository scale. Since this method includes a database of pre-computed FEM results, the computational cost in running NMB is very low.

3. Summary

This paper provides the unified description of the methodology of the nuclear fuel cycle simulator NMB4.0. NMB4.0 performs calculations on six modeled plants based on inputs about reactor plants and reprocessing plants, and the calculation models in each plant are showed. In order to analyze the back-end analysis fast and precisely, NMB4.0 implements OEM, which is a burnup calculation method with low computational cost even when considering a very large number of FPs, and an original repository temperature evaluation model that uses the results of FEM analysis in a database.

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