Development of PENECA-F for equilibrium cycle analysis in a fast neutron environment

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1. Introduction

FNC is developing PENECA-F (Program for Equilibrium and Non-Equilibrium Cycle Analysis - Fast Reactor), a computer program for equilibrium cycle analysis in a fast neutron environment, and has linked it with NeuMOCA(Neutron transport solver using the Method of Characteristics Analysis), a neutron transport equation analysis code being developed at KAERI, to obtain a neutron flux for burnup calculations.

Nuclear cycle analysis is classified into two types incore cycle analysis, which considers burnup within the reactor, and ex-core cycle analysis, which simulates a series of processes in which nuclear fuel is withdrawn and loaded into the reactor via reprocessing, refabrication, etc. The PENECA-F code has an ex-core cycle analysis module, an in-core nuclear fuel burnup calculation module, and a charged fuel enrichment search module, all of which ensure that the end-of-cycle criticality is set by the user.

Although the main modules of PENECA-F have been developed, the module that can be verified at the current stage is the module that analyzes the matrix exponential linear system, which is firstly detailed in Chapter 2. Other contents are described in Chapter 3.

2. Matrix Exponential Analysis Module Verification

In order to determine the inventory of each nuclide over time after constructing a radioactive decay matrix or burnup matrix, a module capable of obtaining a solution from the matrix exponential function is needed. This was accomplished in PENECA-F by using the Series Expansion Method, and in order to confirm this, the results were compared with the differential equation solution that was determined by hand calculation.

2.1 Simple Decay Chain

The case shown in Eq. (1) was assumed as a simple burnup chain problem.

$$A \xrightarrow{\lambda_A} B \xrightarrow{\lambda_B} C \tag{1}$$

The solution to Eq. (2) to (4) can be derived by analytically solving this equation with the assumption that the initial inventory of nuclides B and C is 0.0.

$$N_A = N_{A0} e^{-\lambda_A t} \tag{2}$$

$$N_{B} = \frac{\lambda_{A}}{\lambda_{B} - \lambda_{A}} N_{A0} \left(e^{-\lambda_{A}t} - e^{-\lambda_{B}t} \right)$$
(3)

$$N_{C} = -\frac{\lambda_{B}}{\lambda_{B} - \lambda_{A}} N_{A0} e^{-\lambda_{A}t} + \frac{\lambda_{A}}{\lambda_{B} - \lambda_{A}} N_{A0} e^{-\lambda_{B}t} + N_{A0} \quad (4)$$

Table I: Calculation Condition for Verification

N _{A0}	N_{B0}	N _{C0}
100.0	0.0	0.0
$\lambda_{\rm A} [\rm s^{-1}]$	$\lambda_{\rm B} [\rm s^{-1}]$	t _{elapse}
1.0	2.0	1.0
N _A	N _B	N _C
36.788	23.254	39.958

If the computation is performed under the same conditions as Table I, the number density of nuclides A, B, and C can be obtained, which is confirmed to be the same as the code's result.

2.2 Decay Chain with Independent Source

Additionally, verification was performed for cases such as Eq. (5) when there is an external, independent source of nuclides.

$$A \xrightarrow{\lambda_{A}} B \xrightarrow{\lambda_{B}} C$$

$$\uparrow \qquad \uparrow \qquad \uparrow \qquad (5)$$

$$S_{A} \qquad S_{B} \qquad S_{C}$$

By assuming that the initial inventory of nuclides C is 0.0, the solutions to Eq. (6) to (8) can be obtained by solving.

$$N_A = N_{A0} e^{-\lambda_A t} + \frac{1}{\lambda_A} \left(1 - e^{-\lambda_A t} \right) S_A \tag{6}$$

$$N_{B} = N_{B0}e^{-\lambda_{B}t} + \frac{\lambda_{A}}{\lambda_{B} - \lambda_{A}}N_{A0}\left(e^{-\lambda_{A}t} - e^{-\lambda_{B}t}\right) + \frac{S_{A}}{\lambda_{B}}\left(1 - e^{-\lambda_{B}t}\right) - \frac{S_{A}}{\lambda_{B} - \lambda_{A}}\left(e^{-\lambda_{A}t} - e^{-\lambda_{B}t}\right) + \frac{S_{B}}{\lambda_{B}}\left(1 - e^{-\lambda_{B}t}\right)$$
(7)

$$\begin{split} N_{C} &= N_{B0} \left(1 - e^{-\lambda_{gl}} \right) + \frac{\lambda_{A} \lambda_{B}}{\lambda_{B} - \lambda_{A}} N_{A0} \left(\frac{1}{\lambda_{A}} \left(1 - e^{-\lambda_{al}} \right) - \frac{1}{\lambda_{B}} \left(1 - e^{-\lambda_{gl}} \right) \right) \\ &+ \frac{S_{A} \lambda_{B}}{\lambda_{B}} \left(1 - \frac{1}{\lambda_{B}} \left(1 - e^{-\lambda_{gl}} \right) \right) - \frac{S_{A} \lambda_{B}}{\lambda_{B} - \lambda_{A}} \left(\frac{1}{\lambda_{A}} \left(1 - e^{-\lambda_{gl}} \right) - \frac{1}{\lambda_{B}} \left(1 - e^{-\lambda_{gl}} \right) \right) \end{split}$$
(8)
$$&+ \frac{S_{B} \lambda_{B}}{\lambda_{A}} \left(1 - \frac{1}{\lambda_{A}} \left(1 - e^{-\lambda_{gl}} \right) \right) + S_{C} t \end{split}$$

Table I	II:	Calcula	tion (Condition	ı for	Vei	rifica	ation
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N _{A0}	N _{B0}	N _{C0}		
100.0	50.0	0.0		
$\lambda_{\rm A} [{\rm s}^{-1}]$	$\lambda_{\rm B} [s^{-1}]$	t _{elapse}		
1.0	2.0	1.0		
S _A	S _B	S _C		
0.1	0.2	0.3		
N _A	N _B	N _C		
36.851	30.128	83.621		

For Eq. (5), the matrix exponential formula can be set as Eq. (9). The decay matrix M and the nuclide inventory vector V are given as Eq. (10).

$$\frac{d\mathbf{V}}{dt} = \mathbf{M} \cdot \mathbf{V} \to \mathbf{V} = \mathbf{V}_0 e^{\mathbf{M}t}$$
(9)

$$\mathbf{M} = \begin{pmatrix} -1 & 0 & 0 & 0.1 \\ 1 & -2 & 0 & 0.2 \\ 0 & 2 & 0 & 0.3 \\ 0 & 0 & 0 & 0 \end{pmatrix} \mathbf{V} = \begin{pmatrix} N_A \\ N_B \\ N_C \\ 1 \end{pmatrix}$$
(10)

If the calculation is performed under the same conditions as in Table II, the number density of nuclides A, B, and C can be obtained, which is confirmed to be the same as the result calculated in the code. The above verification approach proved that the currently designed matrix exponential solver produces accurate results.

3. PENECA-F Main Modules

The main analysis modules of PENECA-F are the excore cycle analysis module, the cyclic analysis module, the nuclear fuel enrichment search module, and the neutron transport analysis execution module. The overall calculation flow is shown in Fig. 1.



Fig. 1. Equilibrium cycle flow chart.

EOC criticality, cycle length, enrichment search factor and other parameters are set as input, and the delivery factor Q_f from the independent nuclear fuel source supply facility is calculated in the ex-core cycle module to set the initial number density of nuclear fuel. The burnup stage and region number density are then calculated in the cyclic analysis module. And although it is not currently implemented, if a specific nuclide's burnup limit is specified, the cycle length will be updated accordingly. Finally, after adjusting the nuclear fuel enrichment based on the EOC criticality value, the delivery factors Q_r and Q_f at the reprocessing facility and nuclear fuel source supply facility are calculated in the ex-core cycle module and repeated cycle analysis is performed.

3.1 Ex-core Cycle Analysis Module

This module, as shown in Fig. 2, takes into account radiation decay during the cooling and reprocessing periods. In addition to nuclear fuel reshaping and processing, radiation decay during this period is estimated. Finally, radiation decay prior to the nuclear fuel reloading is reflected. This module calculates and updates the number density of each nuclide that makes up nuclear fuel.



Fig. 2. Flow chart in ex-core module.

3.2 Cyclic Analysis Module

The cyclic analysis module consists of three major subroutines. The first is the CalRegionDensity subroutine, which runs in the innermost loop, and calculates the region number density at specific burnup stages and specific burnup time nodes for all nuclear fuel types, as well as the transformation matrix B or Bhat for the subregions. The flow chart is shown in Fig. 3. This subroutine is called within the RunRegionDensityIteration subroutine.



Fig. 3. CalRegionDensity subroutine flowchart.

The second key subroutine is RunRegionDensity-Iteration subroutine, which repeats the region number density calculation for one burnup cycle in the specific burnup stage and calculates the accumulated transformation matrix Bhat for all time nodes in that burnup stage. Fig. 4 depicts its flow chart.



Fig. 4. RunRegionDensityIteration subroutine flowchart.

The final key subroutine is RunStageDensityIteration subroutine, which determines region number density calculations for all burnup stages as well as stage number density.



Fig. 5. RunStageDensityIteration subroutine flowchart.

3.3 Nuclear Fuel Enrichment Search Module

The enrichment is determined utilizing the enrichment search factor x, and the composition ratio of the loaded fuel is calculated. At this time, enrichment is determined by the initial value e_0 and scaling factor δ given by the user via the input statement shown below.

$$e = e_0 \left(1 + (x - 1)\delta \right) \tag{10}$$

The enrichment search factor x is adjusted in the nuclear fuel enrichment search module by interpolating a linear or quadratic function based on the EOC criticality value.

3.4 Neutron Transport Analysis Execution Module

This module runs the NeuMOCA code with burnup stage and region number density data as inputs. It is called in the cyclic module. Data linkage was implemented by reading the output file of the NeuMOCA code.

4. Conclusions and Future Works

PENECA-F is in development, and the algorithms and functions of its main module have been detailed. Additionally, the matrix exponential analysis module was verified. However, since verification of major modules has not yet been completed, further verification calculations will be performed using similar programs such as REBUS3.

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