Prediction of Plutonium-239 Production by using AnyLogic System Dynamics Platform

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1. Introduction

The Korea Institute of Nuclear Nonproliferation And Control (KINAC) is developing an analysis model that can simulate the entire nuclear fuel cycle. It focuses on the development of a visualized analysis model to be easily accessed by general policy makers who do not have in-depth knowledge of nuclear fuel cycle. To simulate the nuclear fuel cycle, one of system dynamics platforms, AnyLogic, has been selected. It is noted that the system dynamics is an approach to understanding the nonlinear behavior of complex systems over time using stocks, flows and internal feedback loops [1].

In this paper, research contents on the development of nuclear fuel depletion and breeding model to predict plutonium-239 production with AnyLogic are described. To simulate the isotopic changes in a reactor due to neutron-induced reactions and radioactive decay, burn-up chain characterized by the Bateman depletion equation is built. Neutron fluxes are obtained from the two-group representation of the point kinetics equations. The model implementation on AnyLogic platform is validated by comparing the calculation results from the developed AnyLogic model with the counterparts of an independent Java program on Pu-239 production.

2. Governing Equations

In order to perform nuclear fuel burn-up (depletion and breeding) calculation by using the AnyLogic, it is necessary to define the governing equations that describe the actual physical phenomenon mathematically. The Bateman equation is a mathematical model describing abundances and activities in a decay chain as a function of time, based on the decay rates and initial abundances [2]. The neutron flux required to calculate the nuclear reaction must be updated periodically. Since the neutron flux to be obtained is limited to the average neutron flux in space, the neutron flux can be updated using the steady-state solution of the point kinetics equations.

2.1 Bateman Equation

The number density vector of nuclides consisting of the number densities of the total I nuclides at time t is given by Eq. (1).

$$\mathbf{n}(t)=\left[n_1(t),n_2(t),\cdots,n_i(t),\cdots,n_I(t)\right]^T. \tag{1}$$

In Eq. (1), $n_i(t)$ denotes the number density of the i^{th} nuclide at time t. The change in nuclide number density at time t is calculated by the nuclide transformation equation as known as the Bateman Equation. It can be expressed as Eq. (2).

$$\begin{aligned}&\frac{d}{dt}n_i(t)=\\&\sum_{j=1}^{I}\left[\sum_x \gamma_{jx}^i\left(\sigma_{jx}^F\phi^F(t)+\sigma_{jx}^T\phi^T(t)\right)+\gamma_{jd}^i\lambda_j\right]n_j(t)\\&-\left[\left(\sigma_{ia}^F\phi^F(t)+\sigma_{ia}^T\phi^T(t)\right)+\lambda_i\right]n_i(t),\end{aligned} \tag{2}$$

where σ_{jx}^F and σ_{jx}^T mean microscopic cross-sections of reaction type x and nuclide j in fast neutron energy region and thermal energy region, respectively. γ_{jx}^i represents the production rate of nuclide i due to the x type nuclear reaction of nuclide j. γ_{jd}^i represents the production rate of nuclide i due to the radioactive decay of nuclide j. λ_i and λ_j denote the decay constants of nuclide i and j, respectively. In order to obtain the number density, $n_i(t)$ of the nuclide i at time t, production terms and loss terms of nuclide i should be properly calculated. The linear system which is constructed with above equation for all nuclides can be written as follows.

$$\frac{\partial}{\partial t}\mathbf{n}(t)=\mathbf{A}(\phi,\sigma,\lambda)\cdot\mathbf{n}(t). \tag{3}$$

In Eq. (3), the operator on the RHS is a so-called transmutation matrix, and the elements are expressed as Eqs. (4) and (5).

$$a_{ij}(t)=\sum_x \gamma_{jx}^i\left(\sigma_{jx}^F\phi^F(t)+\sigma_{jx}^T\phi^T(t)\right)+\gamma_{jd}^i\lambda_j \quad (i\neq j), \tag{4}$$

and

$$a_{ii}(t)=\left(\sigma_{ia}^F\phi^F(t)+\sigma_{ia}^T\phi^T(t)\right)+\lambda_i. \tag{5}$$

2.2 Point Kinetics Equations

The deterministic time-dependent equations by the neutron number density and the delayed neutron precursors can be described by the two energy groups prompt neutron number density equations with 6 groups of delayed neutron precursors [3].

$$\frac{dn_1(t)}{dt} = \left(\frac{(\rho_1(t) - \beta)}{\Lambda_1} - \Sigma_{s12} v_1 \right) n_1(t) + \frac{1}{\Lambda_2}(1-\beta) n_2(t) + \sum_{i=1}^{6} \lambda_i C_i(t), \tag{6}$$

$$\frac{dn_2(t)}{dt} = \frac{(\rho_2(t) - 1)}{\Lambda_2} n_2(t) + \Sigma_{s12} v_1 n_1(t), \tag{7}$$

$$\frac{dC_i(t)}{dt} = \beta_i \left(\frac{1}{\Lambda_1} n_1(t) + \frac{1}{\Lambda_2} n_2(t) \right) - \lambda_i C_i(t), \tag{8}$$

$$\beta = \sum_{i=1}^{6} \beta_i, \tag{9}$$

where $n_1(t)$ and $n_2(t)$ are the fast and thermal neutron number densities, respectively, while $C_i(t)$ is the precursor concentration density of i^{th} group delayed neutrons. $\rho_1(t)$ and $\rho_2(t)$ are the reactivities induced by fast and thermal neutrons, respectively. β_i is the fraction of i^{th} group delayed neutrons. Λ_1 and Λ_2 are the fast and thermal neutron generation times, respectively. Σ_{s12} is the macroscopic scattering cross-section from fast group to thermal group and v_1 is the fast neutron average velocity. λ_i is the decay constant of i^{th} group delayed neutrons.

In order to obtain the ratio of thermal neutron flux and fast neutron flux in the steady state, following conditions are substituted in Eq. (7), and the relation between the number densities of thermal neutrons with fast neutrons is assumed as Eq. (11).

$$\frac{dn_2(t)}{dt} = 0, \quad \rho_2(t) = 0, \tag{10}$$

and

$$n_2(t) = \Lambda_2 \Sigma_{s12} v_1 n_1(t). \tag{11}$$

In Eq. (11), each variable satisfies the conditions as Eq. (12), so by substituting it into Eq. (11), Eq. (13) is obtained.

$$\Lambda_2 = \frac{1}{\nu\Sigma_{f2} v_2}, \quad \phi_1(t) = v_1 n_1(t), \quad \phi_2(t) = v_2 n_2(t), \tag{12}$$

and

$$\phi_2(t) = \frac{\Sigma_{s12}}{\nu\Sigma_{f2}} \phi_1(t), \tag{13}$$

where $\nu\Sigma_{f2}$ is the macroscopic nu-fission cross-section in the thermal region.

It can be assumed that the amount of moderator hardly changes while the reactor is operating. The macroscopic scattering cross-section, Σ_{s12} can also be assumed that it is constant. In this way, the ratio of the thermal neutron flux to the fast neutron flux depends only on the macroscopic nu-fission cross-section, $\nu\Sigma_{f2}$.

3. AnyLogic Analysis Model

The initial screen of the developed model by using AnyLogic was configured to input information on reactor power, nuclear fuel loading, nuclear fuel enrichment, and neutron flux ratio and so on as shown in Fig. 1.

Fig. 1. AnyLogic initial input configuration.

3.1 Burn-up Chain

In AnyLogic simulation, number density of the i^{th} nuclide at time t, $n_i(t)$ is implemented as stock, and the reaction(transmutation) rate in $n_i(t)$ is implemented as flow. The neutron fluxes representing the neutron spectrum as a reactor environment are implemented as parameters. If the initial neutron fluxes are determined, Σ_{s12} value which is considered as constant can be obtained from Eq. (13). The (n,γ) reaction occurs when the parent nuclide absorbs neutron and then emits gamma ray. In Fig. 2, the (n,γ) reaction rate was modeled as a yellow flow. The $(n,2n)$ reaction occurs when the parent nuclide absorbs neutron and then emits two neutrons. The $(n,2n)$ reaction rate was modeled as a green flow. The (n,f) reaction occurs when the parent nuclide absorbs neutron and then emits two fission fragments. Since fission products were excluded when constituting the burn-up chain, this reaction acts as a loss term for the nuclides constituting the burn-up chain. The α - decay occurs when the parent nuclide emits an alpha particle,

He_2^4. The α decay rate was modeled as a red flow. β decay occurs when the parent nuclide emits an electron. The β decay rate was modeled as a blue flow. If the target of the reaction does not exist in the burn-up chain, such as fission products generated when fission occurs, these loss terms are included in the white flow.

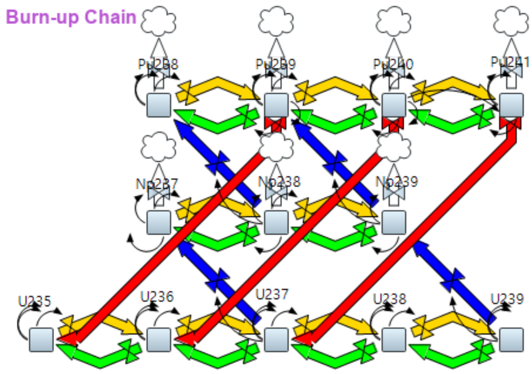

Fig. 2. AnyLogic burn-up chain configuration.

3.2 Flux Update

During burn-up calculations, the inventory of nuclear fuel changes over time, so as to ensure that the reactor power maintains a certain power, it is necessary to update the neutron flux. The neutron fluxes are updated using the relationship in Eq. (13). Assuming that the amount of coolant in the reactor is constant; it can be assumed that the value of Σ_{s12} does not changed. This assumption can be used to update the neutron flux by calculating $\nu\Sigma_{f2}$ which changes with changes in the nuclear fuel inventory. In this way, the ratio of thermal neutron flux to fast neutron flux was updated. The magnitude of these two neutron fluxes is corrected by calculating the kappa-fission rate. There is a kappa-fission rate value corresponding to the reactor power given as an input, and the magnitude of the neutron flux is determined by comparing calculated value with the setting value. The procedure of burn-up calculation to predict Pu-239 production during the operation time with neutron flux update is shown in Fig. 3.

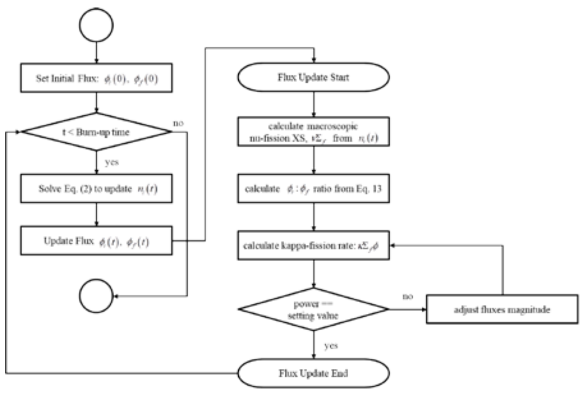

Fig. 3. AnyLogic burn-up calculation procedure.

3.3 AnyLogic Analysis Model Executions

A screen as shown in Fig. 4 is presented when AnyLogic burn-up calculation model is executed. Variations in mass of major nuclides and Pu quality over time can be checked.

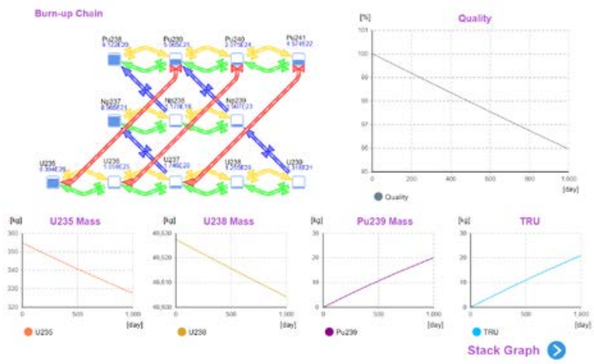

Fig. 4. Main execution screen.

3.4 Validation of AnyLogic Analysis Model

In order to validate the AnyLogic analysis model, an independent Java code was written that applied the same 4th order RungeKutta method to solve the first-order differential equation. A Magnox type nuclear reactor is selected to define the problem for this burn-up benchmark calculation [4]. The thermal power of the reactor was assumed to be 25 MW, and the amount of uranium loaded in the reactor was assumed to be 50 MT. The enrichment of uranium used as nuclear fuel was assumed to be 0.71. The ratio of thermal neutron flux to fast neutron flux was assumed to be 1.69. These conditions are shown in Table I. The burn-up calculation was performed for 800 days, and the results calculated by AnyLogic model were compared with the results obtained from the independent Java code.

Table I: Validation Calculation Conditions

Thermal Power [MWth]	Uranium Mass [MT]
25	50
Enrichment [%]	$\phi_2(0)/\phi_1(0)$
0.71	1.69

Fig. 5 shows the mass change of Pu-239 over time. It can be seen that there is no significant difference between the Pu-239 production in AnyLogic and the Pu-239 production in the Java code. The relative error at the beginning of the calculation occurred up to 1.711%, but it continued to decrease, and it was confirmed that the relative error at the end of the calculation decreased to 8.493e-3%.

Fig. 6 shows the quality change of Pu over time. Quality means the mass fraction of Pu-239 among the Pu, and the higher the Quality, the higher the possibility of mineralization of Pu. It can be seen that the Pu

Quality result in AnyLogic and the Pu Quality result in the Java code are almost identical. The maximum relative error of the two results was calculated to be 3.544e-3 %.

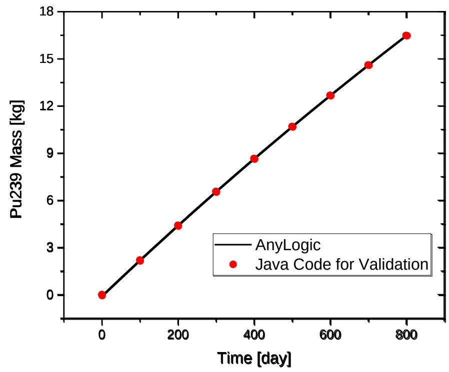

Fig. 5. Pu-239 production over operation times.

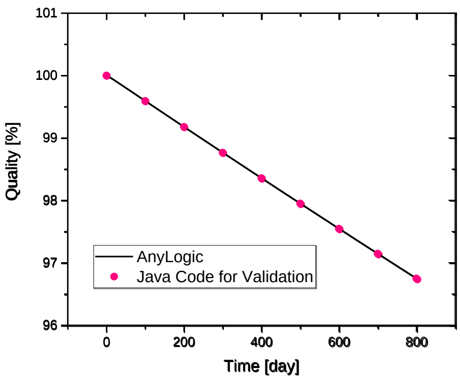

Fig. 6. Pu quality changing over operation times.

4. Conclusions

As part of the nuclear fuel cycle simulation package at KINAC, a nuclear fuel depletion and breeding model to predict the Pu-239 production during the service period was developed by employing AnyLogic which is one of system dynamics platforms. The burn-up chain, a key element of the nuclear fuel depletion and breeding model, was constructed with simplification such that it predicts the production of concerned material in reasonable accuracy. In addition, a method to update the neutron flux during burn-up calculation was suggested. Results obtained from the validity test of the developed AnyLogic model show good agreement with the results by the reference solution model. In spite of the limitations of the simplified model and its applicability, the developed nuclear fuel depletion and breeding model on AnyLogic platform can be a useful, user-friendly tool to estimate the production of specific strategic material from a reactor with limited information.

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