Test Calculations of a new spent fuel source term calculation code BESNA

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1. Introduction

The accurate prediction of the nuclide compositions during burnup or irradiation including decay is important in many nuclear engineering problems such as the source term estimation for criticality and shielding calculations and neutron activation. In addition, the depletion calculation module can be used in fuel assembly calculations. Among the methods used in depletion calculation, the transmutation trajectory analysis (TTA) method and matrix exponential method are most popular. In the matrix exponential method, the solution is obtained by the approximation of the matrix exponential with various approaches such as using Taylor series (ORIGEN code) or with the Chebyshev rational approximation method (CRAM).

In this work, we introduce our new depletion code BESNA (Bateman Equation Solver for Nuclear Applications) which uses CRAM as the depletion solver and can evaluate the source terms including neutron and gamma emission spectra from spent fuels. For a preliminary validation, we applied BESNA to a simple test problem and compared the results with those of the other codes (i.e., MCNP and TRITON and ORIGEN-S in SCALE 6.2).

2. Theory and Methods

2.1 Calculation theory

In this section, the method for solving depletion equation implemented in our code is described. In depletion calculation with a mixture of nuclides, a system of depletion equations are written in the matrix form where the diagonal terms represent the loss of nuclide over time and the off-diagonal terms represent the production of a nuclide from other nuclides. The change of a nuclide can be written in the differential equation as follows:

$$\frac{dn_i}{dt} = (-\lambda_i - \sigma_i\phi)n_i + \sum_{j=1, j\neq i}^{N} (\lambda_j b_{j,i} + \sigma_{j,i}\phi)n_j, \quad (1)$$

where λ_i is the decay constant of nuclide i, $b_{j,i}$ is the decay branching of nuclide j which results nuclide i, ϕ is the one group neutron flux, σ_i is the total microscopic one-group removal cross-section of nuclide i, and $\sigma_{j,i}$ is the microscopic one-group cross-section of the reactions of nuclide j which results nuclide i.

In our depletion code, the Chebyshev rational approximation method [1, 2] was used to solve the depletion matrix, where the solution can be approximated by

$$N(t) = e^{At}N_0 = \alpha_0 N_0 - 2Re\sum_{i=1}^{k/2}(\theta_i I - At)^{-1}\alpha_i N_{0,} \quad (2)$$

where k is the order of the approximation, α_0 is the limit at the infinity and α_i is the residues at the poles θ_i.

The approximation order $k = 14$ was used in our calculation with the approximation coefficients taken from a literature [3]. The BESNA code includes two calculation modes: 1) Irradiation calculation with the constant flux given in each step and 2) the burnup calculation with the fixed power was used in each step. In the burnup calculation mode, a prediction scheme is applied to estimate the average neutron flux of each step. The prediction calculation in each step starts with the beginning of step (BOS) flux and the BOS composition to obtain the end of step (EOS) compositions. Then, the EOS flux is calculated using the EOS composition and the desired power. The step-average flux is estimated as the average value of the beginning and end of step fluxes. The depletion calculation in each step then starts with the step-average flux and the cross-sections at the mid-point of the burnup step for the final results of each step. The depletion scheme also includes an option to select the number of sub-steps which can be used in each burnup step, where the neutron flux can be calculated for each sub-step based on a normalization coefficient [4].

The neutron and photon spectra calculation are implemented in BESNA where the neutron source calculation includes neutrons from (α, n) reactions, spontaneous fission and delayed neutron. The calculation methods are based on the method presented in the SOURCES 4B code [5, 6] for the homogeneous medium. The continuous spontaneous fission neutron spectra are approximated by a Watt's fission spectra as follows:

$$\chi_i(E) = R_i^{SF} e^{-E/a} sinh\sqrt{bE}. \quad (3)$$

where R_i^{SF} is the average number of spontaneous fission neutrons emitted per decay of nuclide i, a and b are the parameters given for each spontaneous fission source nuclide. For the photon source calculation, the method using in the ORIGEN-S code of SCALE [7] is implemented in our code, which includes the photon sources from decays (gamma and X-ray), spontaneous fission and bremsstrahlung in UO_2 or water medium.

2.2 Data library

In this part we describe the data libraries used in our depletion calculation, which include the decay data, one-group cross-sections and fission yield library. The decay data consists of general information such as nuclide type (activation, actinide and fission product group nuclide), decay constant, decay heat recoverable and branching ratios for 11 decay modes which are considered in SCALE/ORIGEN library for 2237 nuclides.

The one-group cross-sections used in our depletion calculation are generated by using MCNP6 [8] reaction rate and flux tallies for a simple pin cell model, which will be improved using fuel assembly models. The one-group cross-sections were calculated for 430 nuclides that exist in ENDF-B/VII.1 cross-section data of MCNP6. At present, we considered the following eight reactions in the one-group cross section library : (n,γ), $(n,2n)$ to ground or isomer state, (n,α), (n,p), (n,d), (n,t), $(n,3n)$ and fission. The one-group cross-section library includes one-group cross-sections for these reactions at 42 burnup points over 60 GWd/MTU. During the depletion calculation, the one-group cross-sections at a desired burnup are produced by using a linear interpolation between two consecutive available data points.

The fission yield library used in BESNA is prepared based on fission yield data in SCALE code system, which is based on ENDF/B-VII.1. The yield data from SCALE includes fission yields of 1151 fission products for 30 fissionable actinide nuclides at energies of 0.0253 eV, 2 MeV and 14 MeV. The list of the fissionable actinide nuclides is given in Table. 1. To obtain one-group fission yield data, the linear interpolation with 51 neutron group fluxes obtained from MCNP6 pin cell calculation is applied to the SCALE fission yield data. The neutron group structure used for calculating fission yield is presented in Table. 2.

Table.1. List of fission source nuclides

^{227}Th	^{229}Th	^{232}Th	^{231}Pa	^{232}U	^{233}U
^{234}U	^{235}U	^{236}U	^{237}U	^{238}U	^{237}Np
^{238}Np	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu
^{241}Am	^{242m}Am	^{243}Am	^{242}Cm	^{243}Cm	^{244}Cm
^{245}Cm	^{246}Cm	^{248}Cm	^{249}Cf	^{251}Cf	^{254}Es

Table.2. The 51 groups neutron structure

Group	Upper bound (MeV)	Group	Upper bound (MeV)
1	1.00E-08	27	5.40E-06
2	3.00E-08	28	6.25E-06
3	4.00E-08	29	7.15E-06
4	6.00E-08	30	8.10E-06
5	8.00E-08	31	1.19E-05
6	1.00E-07	32	1.44E-05
7	1.50E-07	33	3.00E-05
8	2.00E-07	34	4.83E-05
9	2.75E-07	35	7.60E-05
10	3.50E-07	36	1.43E-04
11	5.00E-07	37	3.05E-04
12	6.25E-07	38	9.50E-04
13	7.50E-07	39	2.25E-03
14	9.25E-07	40	9.50E-03
15	9.75E-07	41	2.00E-02
16	1.01E-06	42	5.00E-02
17	1.08E-06	43	7.30E-02
18	1.13E-06	44	2.00E-01
19	1.18E-06	45	4.92E-01
20	1.25E-06	46	8.20E-01
21	1.45E-06	47	1.36E+00
22	1.86E-06	48	2.35E+00
23	2.47E-06	49	4.30E+00
24	3.73E-06	50	6.43E+00
25	4.70E-06	51	2.00E+01
26	5.00E-06		

3. Numerical Test and Discussion

3.1. Comparison problem

In this section, we considered a depletion problem with pin-cell model to verify our depletion calculations. The depletion calculation is performed with the constant power of 0.06739 MWt up to 1200 days, divided into 24 steps where each step has the length of 50 days. The considered pin-cell model has the size of 1.292 cm x 1.292 cm, where the pellet and cladding outer radius are 0.413 cm and 0.4215 cm, respectively. The height of the pin-cell is 381 cm and the volume of the fuel region is 204.162 cm^3. The initial composition information of the model is given in Table. 3. The additional depletion calculations using MCNP6 and SCALE/TRITON were also performed for comparison.

Table. 3. Initial composition information

	Nuclide	Concentration (atom/barn.cm)
Fuel	^{235}U	1.05056E-03
	^{238}U	2.33403E-02
	^{16}O	4.89084E-02
Clad	Zr-alloy	4.32489E-02
Moderator	Water	1.00284E-01

3.2. Depletion results

The relative differences (not percent difference) for representative actinide nuclides including ^{235}U and ^{239}Pu of our calculation results were compared with MCNP6 results in Fig. 1. The calculation results show that the relative difference of ^{235}U increases over time, up to about 3% at the last calculation step, while the relative difference of ^{239}Pu is much smaller than those of ^{235}U. Fig. 2 presents the relative errors of our calculation and TRITON compared to MCNP for several important actinides at the last burnup step. The maximum differences is about 5% for ^{242}Pu. For the actinide nuclides, the differences of TRITON to MCNP6 is higher than BESNA, which may come from the differences in one group cross-section library.

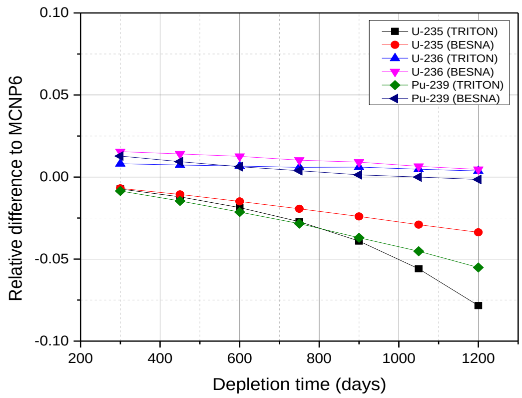

Fig. 1. Relative difference compared to MCNP6 of ^{235}U and ^{239}Pu

The relative differences for several fission product nuclides at the last burnup step is given in Fig. 3. The relative differences from TRITON to MCNP6 are less than 10% for all the nuclides considered while our results showed the higher differences for ^{109}Ag and ^{155}Gd. The relative differences of ^{109}Ag and ^{155}Gd are about 11% and 22%, respectively while the other nuclides showed the differences are less than 5%. The higher differences of these nuclides may come from the lack of cross-section data and will be considered in our future work.

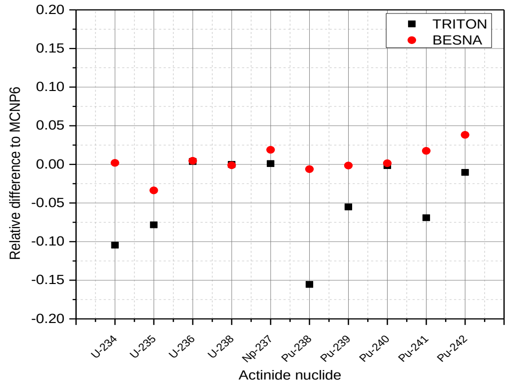

Fig. 2. Relative difference of several actinides at last burnup step

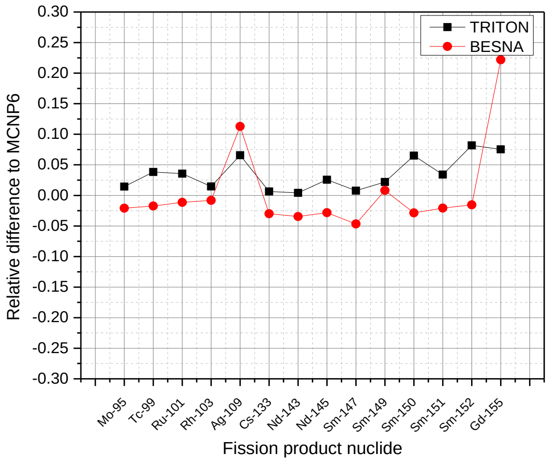

Fig. 3. Relative difference of Fission products at last burnup step

3.3. Neutron and Photon Spectra

This part presents the neutron and photon emission spectra calculated with the nuclide compositions at 150 days. Neutron spectra from (α, n) reaction and spontaneous fission calculated by our code is shown in Fig. 4. Fig. 5 compares the results of photon spectra calculated by BESNA and ORIGEN-S. The calculations for photon spectrum consider the contribution of photon from gamma and X-ray decay, spontaneous fission and bremsstrahlung in UO_2 mixture. From Fig. 5, it was shown that the photon emission spectra from BESNA give very good agreements with those from ORIGEN-S. The relative differences of BESNA for neutron and photon emission spectra compared to the results from SCALE/ORIGEN is given in Fig. 6, where the differences are less than 2% in all energy groups.

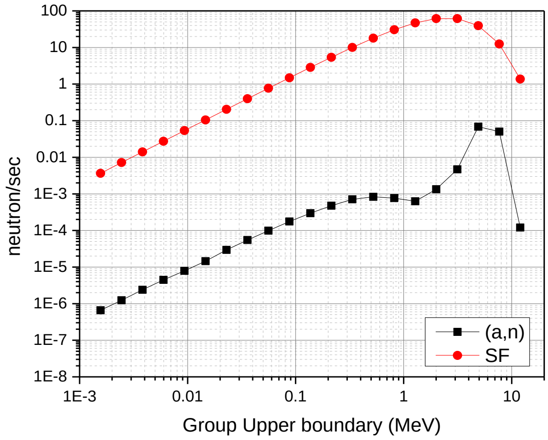

Fig. 4. Neutron spectrum from (α, n) reaction and spontaneous fission for BESNA

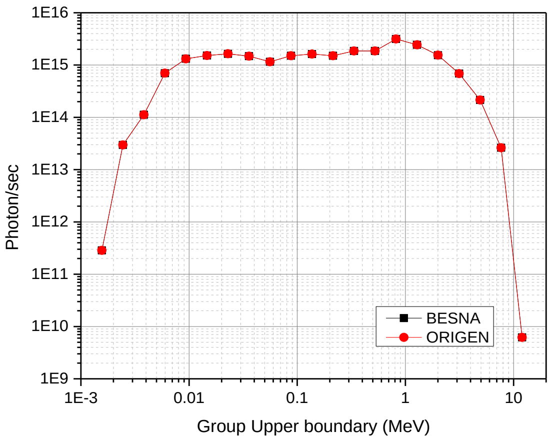

Fig. 5. Comparison of photon emission spectra obtained with BESNA and ORIGEN-S

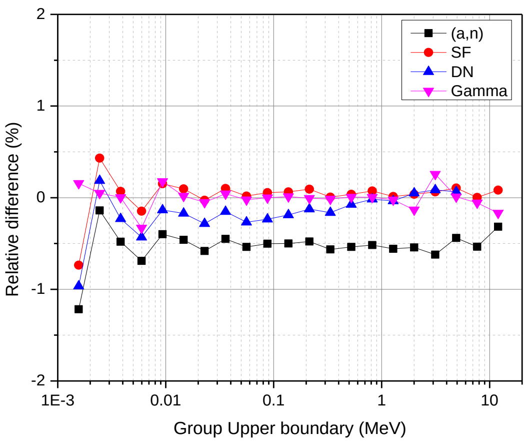

Fig. 6. Relative percent differences (%) in neutron and photon spectra between BESNA and ORIGEN-S

3. Conclusions

In this paper, we introduced our depletion code called BESNA, which is developed for estimating spent fuel compositions as well as calculating neutron and photon spectra. A test calculation was conducted for a simple problem with the use of one-group cross-section generated by MCNP6 and the depletion results were compared with those from MCNP6 and SCALE/TRITON, while the neutron and photon spectra were compared with the results of SCALE/ORIGEN-S. The comparisons showed that our depletion results have good agreements for the actinides and most of fission product nuclides, and that the emission spectra by BESNA gave small differences compared to SCALE/ORIGEN. However, our calculation results showed larger errors compared to MCNP6 and TRITON results for several fission products. These relatively large difference may come from the lack of cross-section file in ENDF library. In future work, we will consider the TENDL library for the nuclides which the ENDF cross-section data is not available, and verify our code with available experimental depletion data.

Acknowledgments

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