Activation Calculation and Verification in BESNA for Reactor Problems

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1. Introduction

Recently, the depletion code BESNA [1] has been developed by Hanyang University through the supports from NRF and KINS with the capabilities to estimate the nuclide compositions during burnup as well as to evaluate the radiation source terms, such as neutron and photon spectra. However, the verification of BESNA was only focused on fuel depletion problem with the cross section library generated by MCNP6.

In this work, the verification of BESNA activation calculation is performed by comparing the activity, in unit of Curies, with the reference result from ORIGEN module in SCALE 6.2 [2]. The JEFF-3.1/A [3] activation files, which consists of cross section data for 774 target nuclides in ENDF-6 format, are used to create multi-group cross section library for BESNA activation calculations. The rest of this paper shortly introduces the BESNA code, as well as the auxiliary program used to generate activation library for BESNA, and the verification results of an activation problem.

2. Calculation Methods

2.1 Depletion calculation with BESNA for activation problems

This section shortly presents the method on activation calculation with BESNA. Unlike the depletion calculation for the spent fuel problem, the activation calculation uses fixed cross section library for all the depletion steps. Therefore, the straight forward calculations are performed without the predictor – corrector scheme, where the nuclide concentration vector at the end of each step can be expressed by

$$\vec{N}_t = e^{t(A^d + A^r\phi)}\vec{N}_0. \quad (1)$$

where $\vec{N}_0$ represents the concentration vector at the beginning of each step, A^d and A^r are the decay and reaction matrix, respectively, and ϕ is the neutron flux, which should be specified in the user's input.

Eq. (1) is solved by the CRAM method with the order of 16 in BESNA.

2.2 Cross section library for BESNA activation calculations

The activation calculation with BESNA uses the one-group cross section library created from JEFF-3.1/A neutron activation files. The JEFF-3.1/A activation files contain the point-wise neutron-induced cross section data of 23 reaction types for 774 target nuclides. These reaction types are listed in **Table 1**, where each reaction type can be further divided based on the metastable states of the residual nuclide. These cross section data are formatted as the ENDF-6 format, with the cross sections presents in File 3, multiplicities in File 10, and branching ratio to different metastable states in File 9.

Table 1. Reaction types in JEFF-3.1/A activation files

Reaction	MT number	Description
1	4	(n, n')
2	16	$(n, 2n)$
3	17	$(n, 3n)$
4	18	(n, f)
5	22	$(n, n\alpha)$
6	24	$(n, 2n\alpha)$
7	25	$(n, 3n\alpha)$
8	28	(n, np)
9	29	$(n, n2\alpha)$
10	32	(n, nd)
11	33	(n, nt)
12	34	(n, n^3_2He)
13	37	$(n, 4n)$
14	41	$(n, 2np)$
15	102	(n, γ)
16	103	(n, p)
17	104	(n, d)
18	105	(n, t)
19	106	$(n, ^3_2He)$
20	107	(n, α)
21	108	$(n, 2\alpha)$

22	111	$(n, 2p)$
23	112	$(n, p\alpha)$

At first, a multi-group cross section library is created from the JEFF-3.1/A activation files with the use of NJOY code and a C++ auxiliary program. In the NJOY execution, the point-wise cross section data are Doppler broadened to 900K, and collapsed using a thermal Maxwellian-1/E-fission weighting spectrum to provide infinite dilution multi-group cross sections. The coefficients used in the weighting spectrum can be determined by the user, and will be presented later in this paper. In our work, a 49-group cross section library, which is a collapsed version of the 238-group structure, is created with the energy group structure given in **Table 2**.

Table 2. 49-energy group structure used in the cross section library

#G	Upper bound (eV)	Lower bound (eV)	#G	Upper bound (eV)	Lower bound (eV)
1	2.000E+07	8.187E+06	26	1.250E+00	1.150E+00
2	8.187E+06	6.434E+06	27	1.150E+00	1.100E+00
3	6.434E+06	4.800E+06	28	1.100E+00	1.050E+00
4	4.800E+06	3.000E+06	29	1.050E+00	1.000E+00
5	3.000E+06	2.479E+06	30	1.000E+00	6.250E-01
6	2.479E+06	2.354E+06	31	6.250E-01	4.000E-01
7	2.354E+06	1.850E+06	32	4.000E-01	3.750E-01
8	1.850E+06	1.400E+06	33	3.750E-01	3.500E-01
9	1.400E+06	9.000E+05	34	3.500E-01	3.250E-01
10	9.000E+05	4.000E+05	35	3.250E-01	2.750E-01
11	4.000E+05	1.000E+05	36	2.750E-01	2.500E-01
12	1.000E+05	2.500E+04	37	2.500E-01	2.250E-01
13	2.500E+04	1.700E+04	38	2.250E-01	2.000E-01
14	1.700E+04	3.000E+03	39	2.000E-01	1.500E-01
15	3.000E+03	5.500E+02	40	1.500E-01	1.000E-01
16	5.500E+02	1.000E+02	41	1.000E-01	7.000E-02
17	1.000E+02	3.000E+01	42	7.000E-02	5.000E-02
18	3.000E+01	1.000E+01	43	5.000E-02	4.000E-02
19	1.000E+01	8.100E+00	44	4.000E-02	3.000E-02
20	8.100E+00	6.000E+00	45	3.000E-02	2.530E-02
21	6.000E+00	4.750E+00	46	2.530E-02	1.000E-02
22	4.750E+00	3.000E+00	47	1.000E-02	7.500E-03
23	3.000E+00	1.770E+00	48	7.500E-03	3.000E-03
24	1.770E+00	1.500E+00	49	3.000E-03	1.000E-05
25	1.500E+00	1.250E+00			

Even though the JEFF-3.1/A activation files contain the cross section data for 774 target nuclides, the multi-group cross section library considers only 762 target nuclides where these decay data are available. Furthermore, for each target nuclide, the reactions which result a residual nuclide that not exists in the decay data file will be discarded from the multi-group library. The process to generate multi-group library is presented in **Figure 1**, where the NJOY executions are omitted for simplicity.

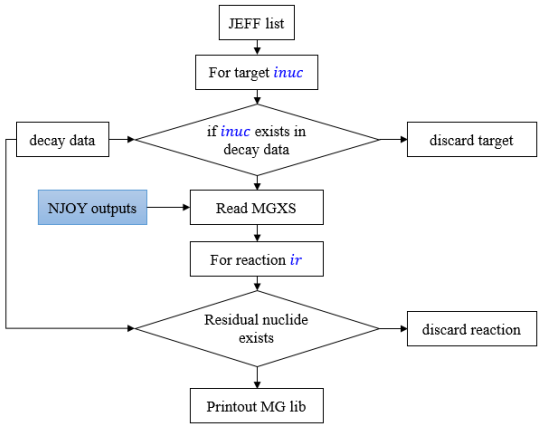

Figure 1. Procedure to generate multi-group cross section library for activation calculation

Finally, the one-group cross section library, which can be used directly in BESNA activation calculation, is created by collapsing the multi-group cross section library with the 49-group flux provided in user's input.

3. Verification Problem and Results

3.1 Problem description

In this section, a test problem is considered with to estimate the nuclide inventories after neutron activation in the PWR reactor vessel. For this problem, the transport calculations with STRAUM [4] were performed to estimate the multi-group neutron fluxes in the vessel, which are used in the activation calculations with BESNA.

In the transport calculation, a quarter PWR model is considered with the reflective boundaries are applied. The axial and radial layouts of the calculation model are presented in **Figures 2a** and **2b**, respectively. As can be seen from **Figure 2a**, only and octant of the PWR core was considered in the calculation with the reflective boundary condition. On the other hand, at the top of the core region, the reflector materials are

modeled with the vacuum boundary condition. The total axial height of the calculation model is 215 cm, with 190 cm of the active core region. In the calculation model, the structure regions outside the active core are modeled with the baffle, barrel, and reactor vessel, where the baffle and barrel region have the same thickness of 5 cm. The structure regions in this problem were modeled by stainless steel SS304, where the detailed nuclide compositions are given in **Table 3**.

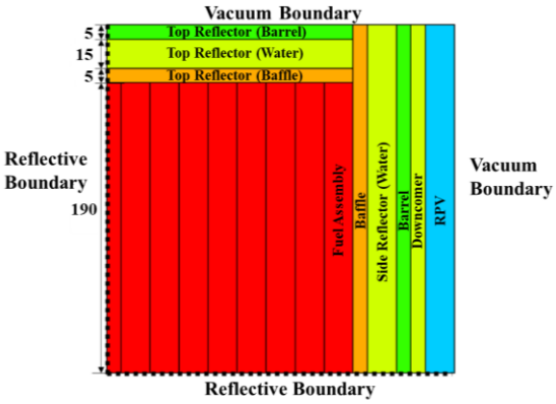

Figure 2a. Axial layout of the PWR model in the test problem (all dimensions are in cm)

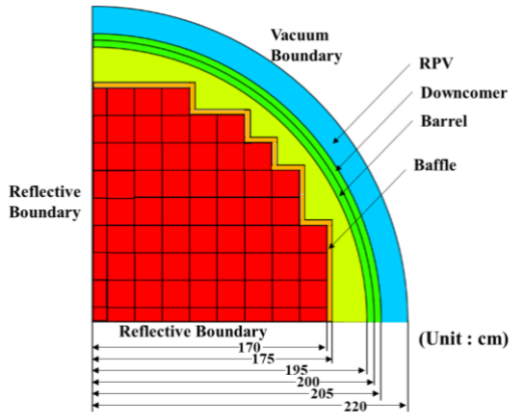

Figure 2b. Radial layout of the PWR model in the test problem (all dimensions are in cm)

Table 3. Nuclide compositions of structure material

Isotope	Atomic number density (atom/barn.cm)
^{12}C	3.184871e-04
^{28}Si	1.570105e-03
^{29}Si	7.976252e-05
^{30}Si	5.264156e-05
^{31}P	6.946885e-05
^{50}Cr	7.591782e-04
^{52}Cr	1.464000e-02
^{53}Cr	1.660058e-03
^{54}Cr	4.132236e-04
^{55}Mn	1.740717e-03
^{54}Fe	3.421905e-03
^{56}Fe	5.371659e-02
^{57}Fe	1.240550e-03
^{58}Fe	1.650944e-04
^{58}Ni	5.268730e-03
^{60}Ni	2.029506e-03
^{61}Ni	8.822120e-05
^{62}Ni	2.812878e-04
^{64}Ni	7.163571e-05

The PWR model was modeled by Gmsh [5] as shown in **Figure 3**, where 177,575 tetrahedral meshes are generated for STRAUM transport calculation. The transport calculation in STRAUM performed using Gauss-Chebyshev angular quadrature of 6 azimuthal and 6 polar directions per octant for this problem. In the depletion calculation with BESNA, we assumed that the reactor vessel was irradiated in three operation cycles each has the length of 300 days and the cooling time between each cycle is 100 days. The multi-group fluxes obtained by STRAUM calculation, which are used in both generating one-group cross section and activation calculation with BESNA, are presented in **Figure 4**.

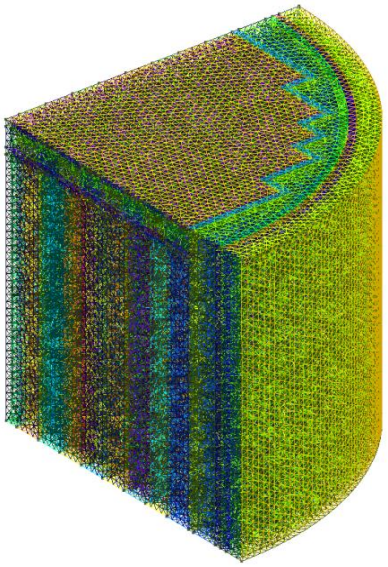

Figure 3. Geometry modeling for transport calculation with STRAUM

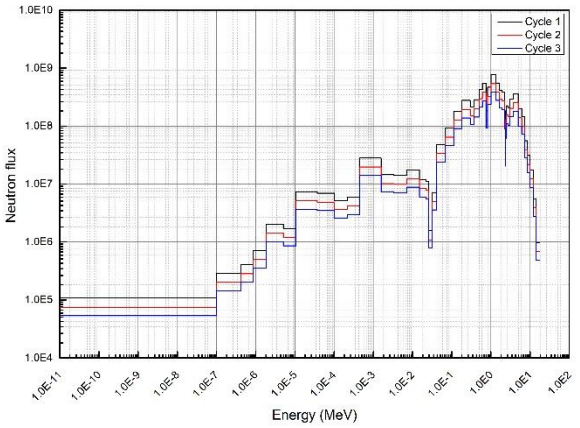

Figure 4. Multi-group flux during operation cycles calculated by STRAUM

3.2 Verification results

For the verification purpose, firstly, the activation calculations with BESNA was conducted by using the cross section data printed out from the COUPLE module in SCALE, which are based on the JEFF-3.0/A activation files. It is aimed to verify the accuracy of the solver implemented in BESNA. The activation results in unit of Curies are presented in **Figure 5**, where the activity calculated by BESNA show the good consistency with the SCALE calculations.

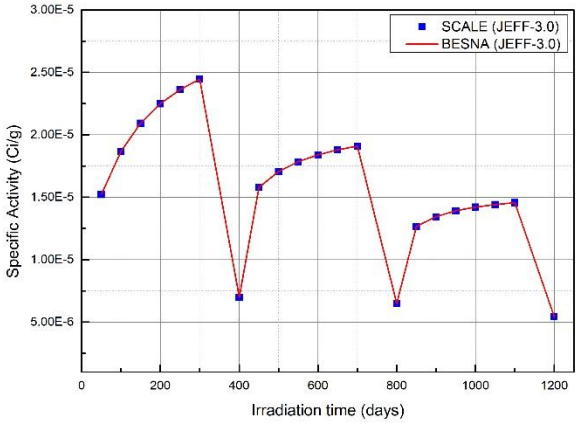

Figure 5. Activity calculation with BESNA and SCALE/COUPLE using JEFF-3.0/A library

In the second step, the activation calculations with BESNA are performed with JEFF-3.1/A activation files. As mentioned earlier in this paper, the weighting spectrum parameters can be chosen by the user. However, these coefficients may lead to a large discrepancy in the activity results. In this paper, 2,000 sets of fission energy and fission cut-off coefficients are randomly generated, and the multi-group cross section libraries are generated for each set of coefficients. From these multi-group libraries, the one-group activation libraries are created by collapsing with multi-group fluxes from STRAUM for direct use in activation calculation with BESNA. The activity results at the last time step then are compared with the reference result from SCALE calculation using JEFF-3.0/A activation files, as presented in **Figure 6**.

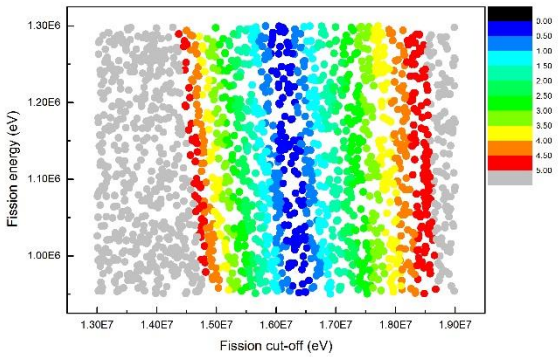

Figure 6. Relative discrepancy (%) in activity of BESNA compared to SCALE/COUPLE

As can be seen in **Figure 6**, there is a region where the activity results in the last step from BESNA show a very good consistency with the result from SCALE/ORIGEN, which corresponds to the fission cut-off of about 16 MeV.

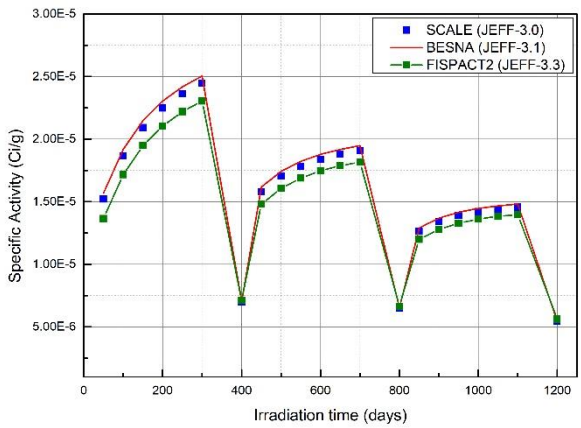

Figure 7. Activity calculation with BESNA using JEFF 3.1/A library compared to other codes

In **Figure 7**, the activation results calculated by BESNA and FISPACT-II [6] are presented, with the reference result from SCALE/ORIGEN. The JEFF-3.3 library is used for the FISPACT-II calculations, where the result show the discrepancies of about less than 10% for the irradiation steps, and about 3% for the cooling steps, compared to the reference result from SCALE/ORIGEN. On the other hand, the results from BESNA with JEFF-3.1/A library show the

discrepancies of about 3% for the irradiation steps. These results indicated that the differences in cross section source are remarkable, and a discrepancy about 3% of BESNA compared to SCALE/ORIGEN is acceptable for activation calculations.

4. Conclusions

This paper presents the procedure to generate one-group cross section library for BESNA activation calculation from the JEFF-3.1/A activation files. The multi-group cross section files consist of 49-group cross section data for 23 type of reactions for 762 target nuclides. These multi-group cross section libraries can be used to create one-group library for BESNA with various collapsing flux spectra given by user. In this paper, the activation results from BESNA were verified with the reference data calculated by ORIGEN module in SCALE. The results indicated that the activation results from BESNA are about 3% in difference compared to SCALE, which may resulted from the differences in data sources, as well as the weighting flux used in generating multi-group library. However, the final activation result after cooling time show good agreement between two codes, which leads to a conclusion that the BESNA activation results are comparable with SCALE.

Acknowledgments

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REFERENCES

[1]. D.L. Ta, S.G. Hong, D.S. Yook, “A spent nuclear fuel source term calculation code BESNA with a new modified predictor-corrector scheme”, Nuclear Engineering and Technology, 4722-4730, 2022.
[2]. B.T. Rearden, M.A. Jessee (Eds.), SCALE Code System, ORNL/TM-2005/39, Version 6.2.1, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 2016.
[3]. OECD/NEA Data Bank Home Page, URL: Nuclear Energy Agency (NEA) - Data Bank (oecd-nea.org).
[4]. M.H. Woo and S.G. Hong, “STRAUM-MATXST: A code system for multi-group neutron-gamma coupled transport calculation with unstructured tetrahedral meshes”, Nuclear Engineering and Technology, 4280-4295, 2022 (54).
[5]. C. Geuzaine and J-F. Remacle, “Gmsh: a three-dimensional finite element mesh generator with built-in pre- and post-processing facilities”, International Journal for Numerical Methods in Engineering 79(11), pp. 1309-1331, 2009.
[6]. M. Fleming, T. Stainer, M. Gilbert, The FISPACT-II User Manual, UK Atomic Energy Authority, 2018.