Verification of Activation Calculation using STRAUM-BESNA through Comparison with MCNP6-FISPACT-II and MONACO/MAVRIC-ORIGEN

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1. Introduction

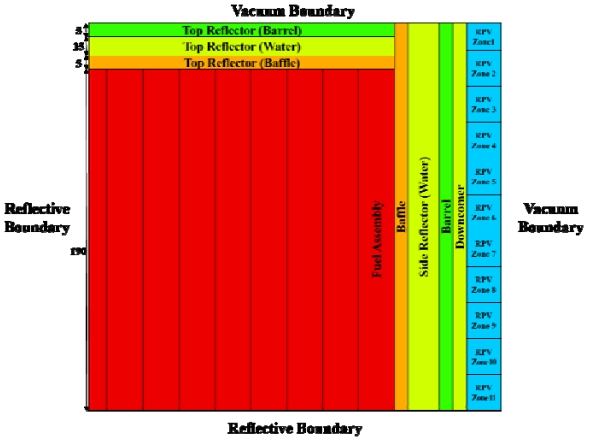
It is very important to figure out the radioactivity of the structural material inside reactor related with the decommissioning of nuclear power plant. The estimation of radioactivity in the structure materials is comprised of the neutron flux calculation and the solution of the Bateman equation with the given composition and neutron flux. In particular, a precise neutron flux calculation is crucial for accurate activation calculation. The STRAUM code [1], a deterministic transport code using the S_N method, is capable of solving the multi-group forward and adjoint transport equations for complicated geometry by using unstructured meshes. Recently, STRAUM has employed the Krylov subspace method [1] to accelerate the source iteration. Also, Hanyang University has developed a point depletion code BESNA [2] for source term evaluation. BESNA which can estimate the neutron and gamma emission spectra and rates from spent fuels or activated materials [3].

The objective of this work is to provide a benchmark problem for activation and to verify the capability of STRAUM-BESNA combination for the benchmark problem. For this purpose, the activation calculation results using STRAUM-BESNA was compared with those of the MCNP6 [4]-FISPACT-II [5] and Monaco/MAVRIC-ORIGEN in SCALE 6.2 [6].

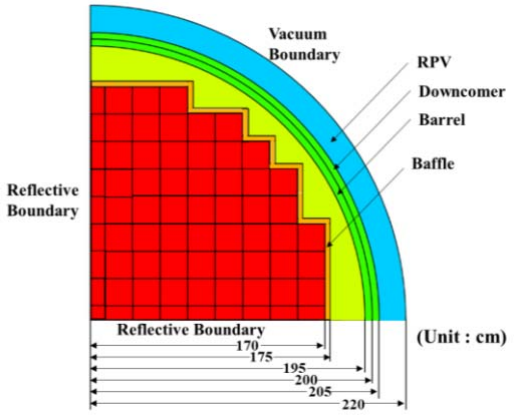
2. Methods

2.1 Reactor pressure vessel problem

For the purpose of code verification in activation calculation, a reactor pressure vessel [7] problem was considered. Fig. 1 depicts the layout of an octant of a PWR core. This problem is comprised of the fuel assemblies, baffle, reflector, barrel and reactor pressure vessel. The fuel assembly is represented by a square homogenized material region modeling 16x16 fuel pins array and coolant The side length of a fuel assembly is 20.0 cm and the composition of the fuel assembly region is a homogeneous mixture of fresh UO_2 pellet (4.5% uranium enrichment, 10.96 g/cm^3 density), Zircaloy-4 (6.56 g/cm^3), and water coolant (1.0 g/cm^3 density) with their volume fractions of 30%, 11% and 59%, respectively. All the structure regions (i.e., baffle, barrel and reactor pressure vessel) are 100% SS304. The thicknesses of these structural regions are 5 cm, 5 cm, and 15 cm, respectively. The water reflector is located between baffle and barrel. The downcomer region between barrel and vessel is also water. The density of water for all the regions is 1.0 g/cm^3. The composition of SS304 is presented in Table 1. The reactor pressure vessel region is axially divided into 11 zones to show the distribution of activity, as indicated in Fig. 1. Each of the reactor vessel zones has the same height of 20 cm, with exception of zone 1 (i.e., top region) which has a height is 15 cm. Consequently, the zone 11 represent the axially central region of the reactor model. A reflective boundary condition is applied within the core internal faces.



a. Axial layout



b. Radial layout

Fig. 1. Configuration of the reactor vessel benchmark problem

Table 1. Nuclide composition of SS304

Isotope	Atomic number density (atom/barn.cm)	Isotope	Atomic number density (atom/barn.cm)
^{12}C	1.57552E-04	^{53}Cr	1.65811E-03
^{13}C	1.68794E-06	^{54}Cr	4.12739E-04
^{28}Si	7.84438E-04	^{55}Mn	8.69349E-04
^{29}Si	3.97194E-05	^{54}Fe	3.51071E-03
^{30}Si	2.63662E-05	^{56}Fe	5.50611E-02
^{31}P	3.54751E-05	^{57}Fe	1.27226E-03
^{32}S	2.12354E-05	^{58}Fe	1.68034E-04
^{33}S	1.67612E-07	^{58}Ni	5.12408E-03
^{34}S	9.40864E-07	^{60}Ni	1.97378E-03
^{36}S	4.46966E-09	^{61}Ni	8.58065E-05
^{50}Cr	7.58288E-04	^{62}Ni	2.73602E-04
^{52}Cr	1.46228E-02	^{64}Ni	6.96990E-05

2.2 Transport calculation

The neutron transport calculations were conducted using three different codes: MCNP6, Monaco/MAVRIC, and STRAUM. The reactor power was set to 3983.0 MWt and fuel assembly-wise power distribution without considering axial power distribution is considered to determine the fixed source densities over the fuel assemblies. The initial source spectrum was calculated by integrating the prompt neutron spectrum for 47group structure.

The fuel assembly-wise power distribution is come from Ref. 7.

For MCNP6 calculation, an octant core as illustrated in Fig. 1 was used. Reflective boundary conditions were applied within the active core, while vacuum conditions were implemented outside the reactor. The ENDF/B-VIII.0 library was used in neutron transport calculation. The geometry splitting was employed to reduce variance. The multi-group fluxes were tallied using the F4 tally within each reactor pressure zone.

For Monaco/MAVRIC module, the whole core model was considered by applying vacuum condition outside the reactor. The transport calculation was conducted using the 200n47g multi-group library based on ENDF/B-VII.0 in SCALE 6.2. For variance reduction, an importance map generated by MAVRIC module using the FW-CADIS method was used in the Monaco multi-group Monte Carlo calculations. Multi-group fluxes were estimated through the volume tally for each reactor pressure vessel zone.

For STRAUM, an octant core was modeled by GMSH [8] and 2,228,762 tetrahedral meshes were generated, as shown in Fig. 2. A 47 multi-group library based on BUGLE-96 neutron structure was generated for STRAUM transport calculation by using the MATXST program [1] and ENDF/B-VIII.0. The Gauss-Chebyshev angular quadrature with 3 azimuthal and 3 polar directions per octant was chosen to solve the transport equation. The BiCGSTAB method was used to accelerate the source iteration.

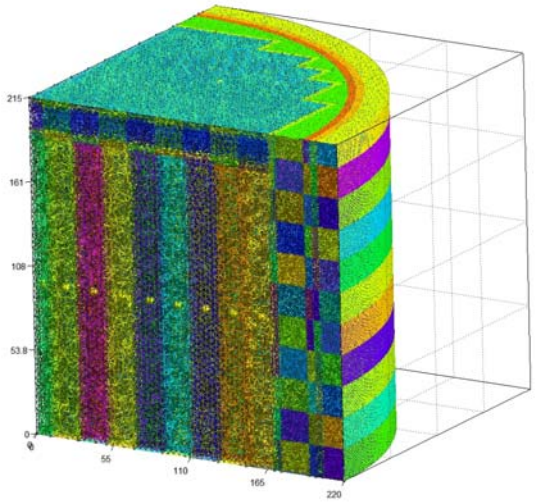


Fig. 2. Geometry modeling for STRAUM

2.3 Activation calculation

Activation calculations were conducted with a simple irradiation scenario which considers 300 days irradiation followed by 100 days cooling. Three codes, FISPAC-II, BESNA, and ORIGEN were used for the activation calculation. In FISPACT-II, the multi-group fluxes obtained MCNP6 and the JEFF-3.3/A library were used. In ORIGEN, the activation calculation was performed using multi-group fluxes from Monaco/MAVRIC and the JEFF-3.0/A library. Meanwhile, BESNA activation calculation was conducted using multi-group neutron fluxes from STRAUM and the activation library based on JEFF-3.1/A library. Specific activities were evaluated over a span of every 50 days during the irradiation times and every 20 days during the cooling times.

3. Results

3.1 Transport code verification

This section provides a comparison of the neutron fluxes calculated by each code. Table 2 gives the total neutron flux from MCNP6, along with the ratios of the total fluxes by Monaco/MAVRIC and STRAUM to the total neutron flux by MCNP6 for the target vessel regions. Additionally, the statistical errors for the tallies are provided for MCNP6 and Monaco/MAVRIC.

Table 2. Comparison of total fluxes over the target vessel zones

zone	MCNP6	MONACO	STRAUM
	Flux (#/cm^2-sec) (statistical uncertainty %)	Ratio of total flux to MCNP6 total flux (%) (Statistical uncertainty %)	Ratio of total flux to MCNP6 total flux (%)
1	1.694E+10 (0.37)	110 (0.495)	100
2	6.337E+10 (0.17)	110 (0.41)	102
3	1.079E+11 (0.13)	110 (0. 33)	102
4	1.188E+11 (0.11)	110 (0. 31)	102
5	1.202E+11 (0.12)	110 (0. 31)	102
6	1.202E+11 (0.12)	110 (0. 31)	102
7	1.200E+11 (0.12)	110 (0. 31)	102
8	1.203E+11 (0.12)	110 (0. 31)	102
9	1.207E+11 (0.12)	110 (0. 31)	102
10	1.204E+11 (0.12)	110 (0. 31)	102
11	1.203E+11 (0.13)	110 (0. 31)	102

As shown in Table 2, the statistical errors of the total flux tallies are quite small (<1%) both for MCNP6 and Monaco/MAVRIC Monte Carlo calculations. The minimum total neutron flux was observed in Zone 1, which is the outer most region of the core. The total neutron fluxes from Monaco/MAVRIC and STRAUM were higher by 10% and 2%, respectively, than the ones by MCNP6. This discrepancy was attributed to difference in the methods employed by the transport codes and in the cross section libraries. STRAUM solve the transport calculation using the S_N method, in contrast to MCNP6 and Monaco/MAVRIC using the Monte Carlo method. Furthermore, the STRAUM calculations used a 47 multi-group library, whereas MCNP6 used a continuous cross section library, and Monaco/MAVRIC used 200n47g fine multi-group cross section library from SCALE 6.2.

3.2 Activation Calculation code verification

Before going to the direction comparison for the benchmark problem, a simple test calculation with the same multi-group neutron fluxes was performed to check the accuracies of the activation calculation codes and their associated libraries in this subsection. The activation calculations with FISPACT-II, ORIGEN, and BESNA were conducted by using the same multi-group fluxes of Zone 1 obtained from STRAUM. Fig. 3 presents the specific activities at each irradiation time and cooling time. We used the CRAM (Chebyshev Rational Approximation Method) option both in BESNA and ORIGEN for solving the Bateman equation.

As depicted in Fig. 3, the specific activities from BESNA are lower by 5 % and 2.5 % than FISPACT-II during irradiation and cooling periods, respectively. On the other hand, the BESNA results have good agreements with ORIGEN, where the discrepancies are less than 1% discrepancies during both irradiation and cooling time periods.

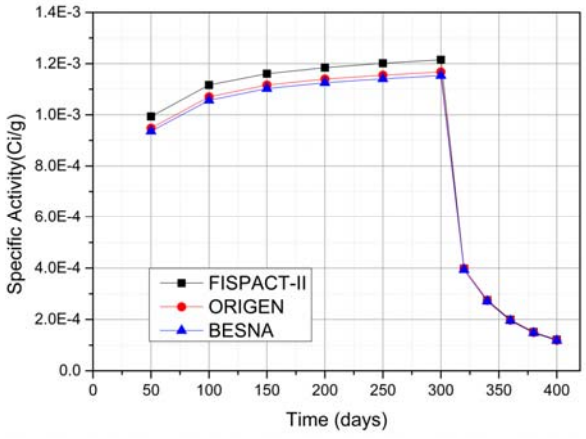
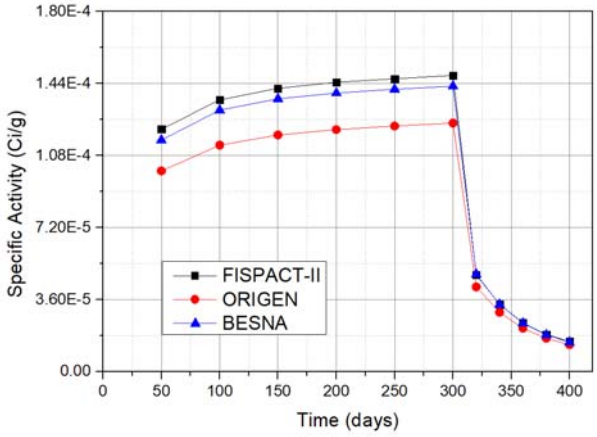


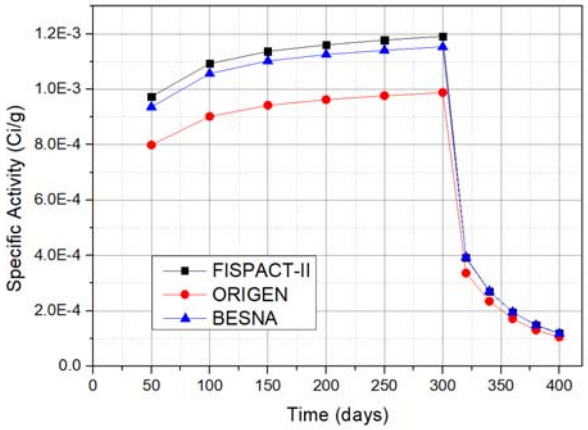
Fig. 3. Activation calculation with FISPACT-II, ORIGEN, and BESNA using same multi-group flux

3.3 Activation results for the benchmark problem

In this section, the activation calculations were conducted using FISPACT-II, ORIGEN, and BESNA with the neutron fluxes from MCNP6, Monaco/MAVRIC, and STRAUM, respectively, for the benchmark problem. Fig. 4 compares the changes of the specific activities estimated with these codes as time in Zones 1 and 11.



a. Zone 1



b. Zone 11

Fig. 4. Comparison of the specific activity changes as time

In Zone 1, the specific activities calculated using Monaco/MAVRIC-ORIGEN are lower by ~16 % during irradiation and by ~11% during cooling time than MCNP6-FISPACT-II. On the other hand, the specific activities by STRAUM-BESNA are lower by ~3% during irradiation time and by ~1% during cooling time than MCNP6-FISPACT-II. In Zone 11, Monaco/MAVRIC-ORIGEN gives lower specific activities by ~17% over the irradiation and ~12% during over the cooling period than MCNP6-FIPSACT-II. However, STRAUM gives lower specific activities by ~3% over the irradiation time and by ~1% over the cooling time. From Table 2, the total fluxes from Monaco/MAVRIC were higher than MCNP6 and STRAUM but the specific activities by Monaco/MAVRIC-ORIGEN were lower than MCNP6-FISPACT-II and STRAUM-BESNA. To understand this fact, we analyzed the energy group-wise contributions to the total specific activities in Zone 11, which is given in Fig. 5.

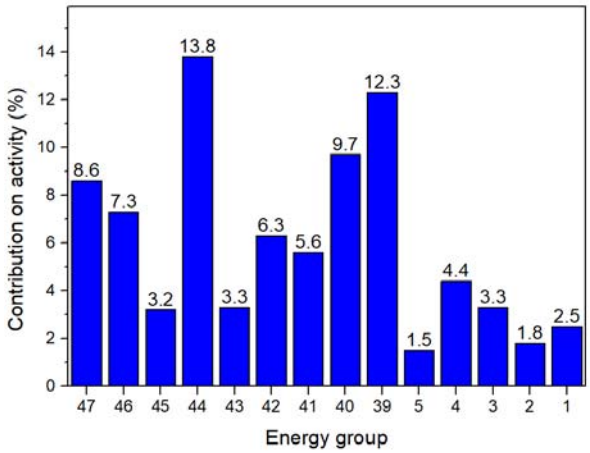
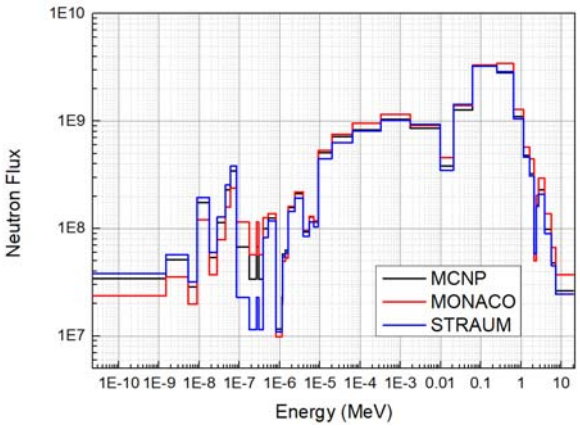
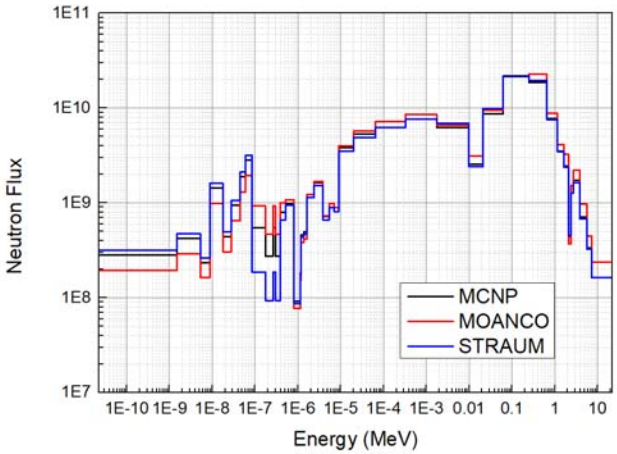


Fig.5. Importance of 49 energy group in activation calculation

Fig. 5 shows the contributions (%) of fourteen energy groups having high contributions to the total specific activity. As shown in Fig.5, the low energy groups show large contribution and so the neutron fluxes in these groups are important in the activity. Fig.6 shows the multi-group neutron spectra calculated among MCNP6, Monaco/MAVRIC, and STRAUM.



a. Zone 1



b. Zone 11

Fig. 6. Comparison of the neutron spectra in vessel regions

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Interestingly, within the low energy groups, the neutron fluxes of MCNP and STRAUM are higher than Monaco/MAVRIC, which explains the higher specific activity by MCNP6-FISPACT-II and STRAUM-BESNA in spite of its lower total flux than Monaco/MAVRIC-ORIGEN.

4. Conclusion

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In this work, a verification of the activation code system of STRAUM-BESNA was conducted for a PWR reactor vessel benchmark problem considering a simple irradiation and cooling scenario. We evaluated the specific activities in the axially eleven region of the

vessel using STRAUM-BESNA, Monaco/MAVRIC-ORIGEN and MCNP6-FISPACT-II. In transport calculation, the total fluxes by STRAUM over the vessel regions were estimated to be higher by ~2% and lower by 8% than MCNP6 and Monaco/MAVRIC, respectively. On the other hand, the comparison of the activation calculations by BESNA, ORIGEN, and FISPACT-II with the same neutron spectrum for a vessel region showed that BESNA results give good agreements within 1% with the ORIGEN ones and agreements within 5% with the FISPACT-II ones.

In the activation calculations using neutron transports codes coupled with their corresponding activation calculation ones, STRAUM-BESNA calculated the specific activities lower over irradiation period by 3% and cooling period 1% for the top vessel zone, the ones for bottom vessel zone were lower by 3% and 1% for irradiation and cooling period, respectively, than MCNP-FISPACT-II. On the other hand, the specific activities calculated using Monaco/MAVRIC-ORIGEN are lower by 16 % during irradiation and by 11% during cooling time than MCNP6-FISPACT-II for the top vessel zone while the ones over the irradiation and cooling time periods were lower by 17% and 12%, respectively than MCNP6-FISPACT-II for the bottom vessel zone.

Acknowledgments

This work was supported by the NRF (National Research Foundation of Korea) through Project No. NRF-2019M2D2A1A02057890.

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