

A recent progress of new BESNA update for burnup and source term analysis

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1. Introduction

A huge amount of spent nuclear fuels from PWR and CANDU reactors have been accumulated in our country. In particular, the interim dry storage of PWR spent nuclear fuel currently stored in spent fuel storage pools is a big issue due to the limitation of the capacity of the spent fuel storage pools. Finally, they are needed to be disposed in a geological repository of which the construction is a long term issue. And so the computationally efficient estimation of the source terms characterizing the spent nuclear fuels is required for safety and performance analyses of the facilities related to the storage of spent nuclear fuels. Recently, we have developed a source term estimation code BESNA for this purpose [1]. The objective of this work is to report the recent improvements in the BESNA code development and to report detailed validation efforts against experimental benchmarks of PWR fuel assemblies and CANDU fuel bundles.

2. BESNA code structures

BESNA is programmed in C++, with supplementary Python scripts semi-automating OpenMC workflows for generating burnup-dependent cross section libraries. As Fig. 1 shows, BESNA is comprised of pre-generated nuclear data and three hierarchies for solver, physics, and control. In the solver level, the CRAM (Chebyshev Rational Approximation Method) solver was developed based on the Eigen library for solving linear algebra with parallel computing capability. The physics level contains decay, irradiation, and burnup calculation modes, for all of which source term evaluations are supported. Notably, setting neutron flux or power density to zero in irradiation or burnup modes activates decay calculation equivalence, enabling seamless simulation of practical scenarios. The control level manages input simulation parameters and nuclear data, assigning them into multiple depletion zones for burnup and source term calculations.

The stand-alone depletion capabilities of BESNA depend on the pre-generated burnup libraries, consisting of burnup-dependent neutron-induced cross sections, and burnup-average fission product yields. We provide an auxiliary program to execute OpenMC transport-coupled depletion on user-defined models, and the simulation results are then tabulated into BESNA

burnup libraries. BESNA contains burnup libraries for two CANDU bundles with 28 or 37 fuel elements, three PWR fuel assemblies with the Westinghouse 14x14 (WH14) or 17x17 (WH17) rod layouts, or the Combustion Engineering 16x16 (CE16) rod layout. For PWR fuel assembly depletion, BESNA supports simulations with initial U-235 enrichment from 1.0 wt% to 6.0 wt% and discharge burnup up to 72 GWd/kgU. CANDU utilizes natural uranium, thus the initial U-235 enrichment is fixed while BESNA can simulate CANDU fuel bundle depletion with discharge burnup up to 15 MWd/kgU. To calculate ring-wise nuclide inventories for validation against CANDU experimental data, the power density ratios of rings to whole bundle are tabulated with ring-wise neutron-induced cross sections, enabling cross section interpolations for each ring during multi-point depletion simulations.

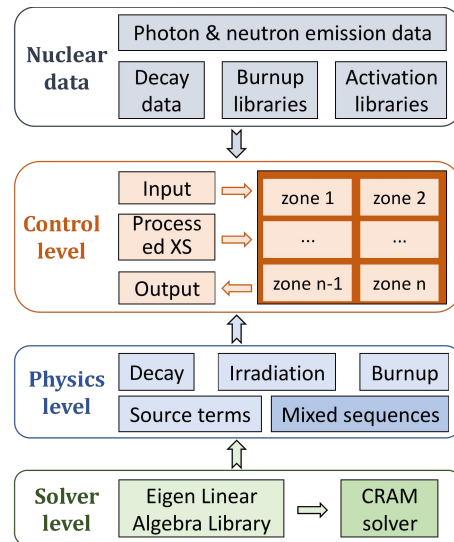


Fig. 1. BESNA code structure.

3. Validation of BESNA

3.1. Takahama-3 reactor SNF inventories

The two measured fuel rods in the Takahama-3 reactor, rod SF95 in the assembly NT3G23 and rod SF97 in the assembly NT3G24, are presented in Fig. 2. The SF95 and SF97 rods are not neighboring to guide tubes or poison rods, thus presenting similar neutron

spectrum to a single fuel rod with reflective boundaries. The STREAM code [2] obtained very close nuclide concentrations through simulating a pin model and an assembly model. Therefore, BESNA can directly use the pre-generated libraries based on the WH17 assembly for SF95 and SF97 rod depletion simulations.

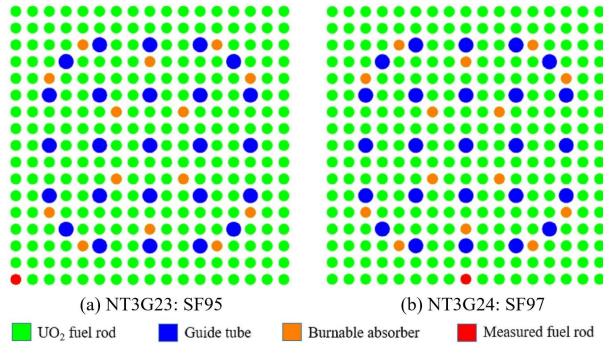


Fig. 2. Radial layout of NT3G23 (a) and NT3G24 (b) fuel assemblies in the Takahama-3 reactor.

There are five fuel segment samples for the SF95 rod and six fuel segment samples for the SF97 rod. All of them have initial U-235 enrichment of 4.11 wt% and are obtained in different axial rod positions. Sample 1 of the SF97 rod is cut from the top position, for which neutron leakages have great impacts on its spectrum. Only the left five samples from the SF97 rod are simulated, while all the five SF95 samples are considered. The isotopic assay data for fuel rods SF95 and SF97 are used for BESNA validation, including the ten samples with discharge burnup ranging from 14.3 to 47.3 MWd/kgU. In BESNA, the power histories for all samples from SFCOMPO-2.0 database are used. Note that samarium isotopes were measured after cooling for 3.96 years while all other isotopes were measured without cooling.

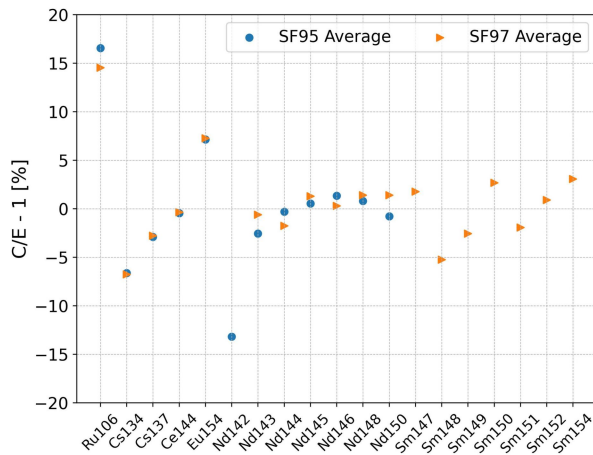


Fig. 3. Average C/E-1 values for fission products in the SF95 and SF97 fuel rod samples.

Figs. 3 and 4 present C/E-1 values individually averaged from five fuel samples of the rods SF95 and

SF97. All these results are simulated by BESNA and then compared with measured data. Note that samarium isotopes, Np-237, and Cm-247 were not measured in all samples of the SF95 rod, while there is no measured Nd-142 data for the SF97 rod. BESNA presents similar prediction errors for all nuclides measured in both SF95 and SF97 rod samples. Except for Ru-106 and Nd-142, all fission products have average estimation errors less than 10%, where most of these errors are less than 5%.

As shown in Fig. 4, most uranium and plutonium isotopes have prediction errors below 5% while U-234 shows an approximately 10% error. BESNA has a large estimation error for Am-242, which exceeds 30% and is not presented in Fig. 4. Since reasonable results for Am-241 and Am-243 are obtained, the large Am-242m error may be attributed to energy-independent capture branching ratio data. BESNA shows opposite errors in the SF95 and SF97 rod samples for Cm-242, which has large measurement uncertainties. For other curium isotopes, their prediction errors are within 10% while the Cm-247 error is around 15% for the rod SF97.

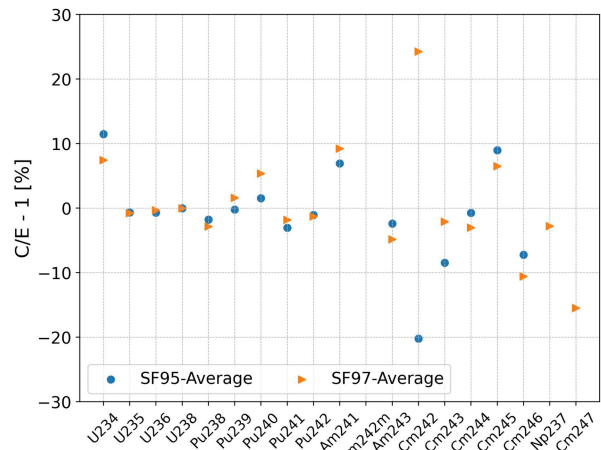


Fig. 4. Average C/E-1 values for actinides in the SF95 and SF97 fuel rod samples.

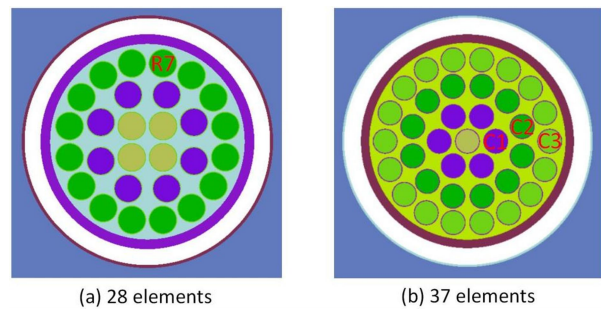


Fig. 5. The CANDU 28-element bundle in the Pickering A-1 reactor (a) and the CANDU 37-element bundle in the Bruce-1 reactor (b).

3.2. CANDU SNF inventories

The Pickering A-1 CANDU 28-element and the Bruce-1 37-element fuel bundles in SFCOMPO-2.0 are

selected for BESNA validation. Their OpenMC constructed geometry models are shown in Fig. 5, one and three fuel rod samples were individually measured for the CANDU 28-element and 37-element bundles.

The CANDU 28-element fuel bundle consists of inner, middle, and outer fuel element rings, while nuclide inventory measurements for the outer fuel ring are provided in SFCOMPO-2.0. The CANDU 37-element fuel bundle is composed of one central element and inner, middle and outer fuel element rings, whereas atomic ratios for uranium and plutonium isotopes are provided in SFCOMPO-2.0. Note that the CANDU 28-element and 37-element bundles have been cooled for 5590 days and 1162 days before measurements, respectively. Both ring-wise and bundle-wise burnup libraries are provided in BESNA, while the former are used in validations since only the experimental data for a few fuel elements are accessible in SFCOMPO-2.0.

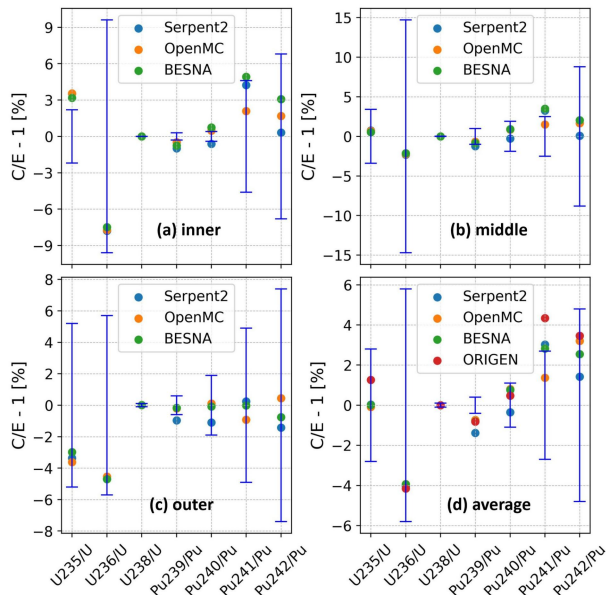


Fig. 6. C/E-1 for uranium and plutonium atomic ratios in the CANDU 37-element fuel rings and whole bundle.

Except for BESNA, the simulation results from transport-coupled depletion code OpenMC and Serpent, and the stand-alone depletion code ORIGEN are also presented for comparisons. The three codes employed the ENDF/BVII.1 library while ORIGEN with the ENDF/B-VII.0 library provided bundle-average results [3]. The C/E-1 values for uranium and plutonium atomic ratios are given in Fig. 6, demonstrating the three codes overestimate the inner ring burnup and underestimate the outer ring burnup according to U-235 atomic ratios. All C/E-1 values for the outer fuel ring are within measurement uncertainties for OpenMC and BESNA. For the bundle-average uranium and plutonium isotopes, Pu-239 and Pu-241 are out of measurement bounds but all C/E-1 values for the four codes are below 5%, demonstrating their excellent prediction accuracy.

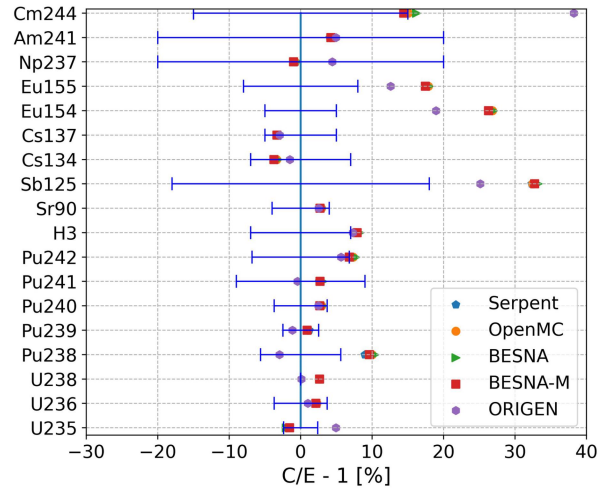


Fig. 7. C/E-1 for actinides and fission products in the CANDU 28-element outer fuel ring.

Fig. 7 present the C/E-1 values for actinides and fission products in the CANDU 28-element outer fuel ring. Serpent, OpenMC, and BESNA calculate depletion in the outer ring based on the bundle-average power history, whereas BESNA-M and ORIGEN use the outer ring power history directly. Serpent, OpenMC, and BESNA yield closely aligned actinide and fission product predictions, since all of them employ the ENDF/B-VII.1 nuclear data. The direct use of the outer element power history in BESNA leads to slight improvements in nuclide predictions, indicating consistency between the power distributions obtained from WIMS-AECL [3] and OpenMC.

As shown in Fig. 7, ORIGEN underestimates fuel burnup whereas the other codes overestimate it, primarily through U-235 depletion. Consequently, Serpent, OpenMC, and BESNA overestimate all plutonium isotopes. ORIGEN predictions for all plutonium isotopes fall within measurement uncertainties, while the other codes exhibit errors of approximately 10% for Pu-238.

Fission yields for H-3 are absent in the ENDF/BVII.1 library used for the OpenMC and Serpent simulations. To address this limitation, we processed and incorporated the JEFF/A-3.1 H-3 fission yields into BESNA burnup libraries, enabling good estimation of H-3 specific radioactivity.

All codes predict the radioactivity for Sr-90, Cs-134, Cs-137, Np-237, and Am-241 within experimental uncertainties. However, predictions for Sb-125, Eu-154, and Eu-155 are overestimated. Notably, ORIGEN exhibits more accurate prediction for Sb-125, and europium isotopes compared to the other codes. While ORIGEN substantially overestimates Cm-244 radioactivity, the other codes yield results within approximately the measurement uncertainty bounds. Overall, BESNA using the OpenMC pre-generated

burnup libraries achieves simulation accuracy comparable to that of Serpent, OpenMC, and ORIGEN.

3.3. Ringhals-3 reactor SNF decay heats

Svensk Kärnbränslehantering AB (SKB) conducted decay heat and gamma radiation measurements on spent fuel assemblies at Swedish central interim storage facility CLAB [4], including 50 BWR and 34 PWR SNF assemblies. These assemblies possessed wide variations in initial U-235 enrichment, burnup, and cooling time, and contain no inserts (e.g., boron glass rods, neutron sources). There are two PWR fuel types in SKB facility, 15x15 and 17x17 rod layouts, for the latter BESNA provides corresponding pre-generated burnup libraries. Detailed data, including initial uranium loading, discharge burnup, cooling times between discharge and measurement, measured decay heats, and associated uncertainties are provided for 16 fuel assemblies. These fuel assemblies cover three types of U-235 enrichment with burnup ranging from 20 to 47 MWd/kgU. We employ BESNA to predict decay heats for the Ringhals-3 PWR assemblies and compares BESNA results with experimental data concluded in the report [4].

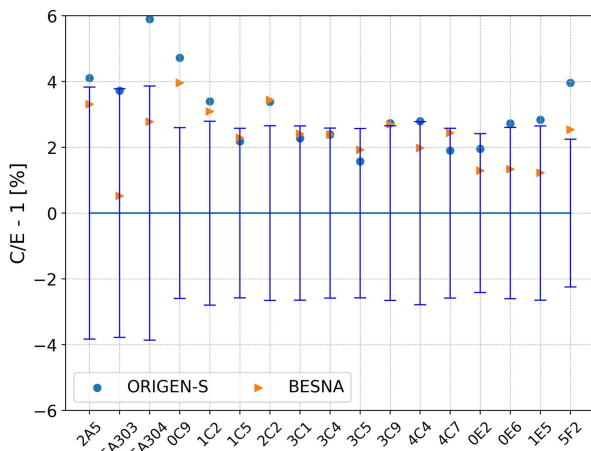


Fig. 8. C/E-1 of decay heat for 17x17 fuel assemblies in the Ringhals-3 reactor.

Fig. 8 compares C/E-1 values for decay heat predictions between ORIGEN-S [4] and BESNA. Approximately 25% of fuel assemblies exhibit BESNA prediction errors exceeding measurement uncertainties, while the remainder fall within statistical bounds. Both codes show positive simulation errors, while BESNA demonstrates better agreement with experimental data than ORIGEN-S. BESNA maintains good overall accuracy with an average C/E-1 of 2.3% for decay heat predictions. The observed discrepancies arise because the BESNA built-in burnup libraries cannot fully capture assembly-specific variations in moderator density and boron concentration histories across the 16

fuel assemblies. These results prove that BESNA is reliable for SNF decay heat estimations.

4. Conclusions

The stand-alone depletion capabilities of BESNA was validated against experimental data from CANDU spent fuel bundles and PWR spent fuel assemblies. Most concentration prediction errors are within 10% for uranium and plutonium isotopes while below 20% for curium isotopes and fission products. Additionally, BESNA always gives accurate estimations for PWR fuel assembly burnup, with excellent predictions for most neodymium isotopes. BESNA maintains good overall accuracy with an average calculation error of 2.3% for decay heat predictions of the Ringhals-3 reactor fuel assemblies. For nuclide inventories and decay heat, BESNA shows comparable predictions with OpenMC, Serpent, and ORIGEN. Overall, the presented results demonstrate that BESNA has capabilities in source term analysis for CANDU and PWR spent nuclear fuels.

5. Acknowledgments

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