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Abstract

The isotopic depletion capabilities of the new Standardized Computer Analyses for Licensing Evaluation control module TRITON, coupled with ORIGEN-S, were evaluated using spent fuel assays from several commercial light water reactors with both standard and mixed-oxide fuel assemblies. Calculations were performed using the functional modules NEWT and KENO-VI. NEWT is a two-dimensional, arbitrary-geometry, discrete-ordinates transport code, and KENO-VI is a three-dimensional Monte Carlo transport code capable of handling complex three-dimensional geometries. To validate the codes and data used in depletion calculations, numerical predictions were compared with experimental measurements for a total of 29 samples taken from the Calvert Cliffs, Obrigheim, and San Onofre pressurized water reactors and the Gundremmingen boiling water reactor. Similar comparisons have previously been performed at the Oak Ridge National Laboratory for the one-dimensional SAS2H control module. The SAS2H, TRITON/KENO-VI, and TRITON/NEWT results were compared for corresponding samples. All analyses showed that TRITON/KENO-VI and TRITON/NEWT produced typically similar or better results than SAS2H. The calculations performed in this validation study demonstrate that the depletion capabilities of TRITON accurately model spent fuel depletion and decay.

KEYWORDS: lattice physics, validation, depletion, isotopics, SCALE, TRITON, KENO, NEWT, Monte Carlo

1. Introduction

The ability to accurately predict the nuclide composition of depleted reactor fuel is important in a wide variety of applications. These applications include, but are not limited to, the design, licensing, and operation of commercial/research reactors and spent fuel transport/storage systems. New complex design projects such as space reactors and Generation IV power reactors also require calculational methods that provide accurate prediction of the isotopic inventory.

The calculation of isotopic compositions of spent fuel has long been a capability of the Standardized Computer Analyses for Licensing Evaluation (SCALE) code system. [1] The release of SCALE 5.1 in 2006 includes expanded depletion capabilities through the significantly upgraded

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TRITON control module. In SCALE 5.1, TRITON is able to perform depletion calculations using NEWT, KENO V.a, or KENO-VI. NEWT is a two-dimensional (2-D) flexible-mesh, discrete-ordinates transport code initially released in SCALE 5, while both KENO V.a and KENO-VI are three-dimensional (3-D) Monte Carlo transport codes that have been in use worldwide for many years. TRITON couples these neutron transport codes with the well-known SCALE point depletion and decay module ORIGEN-S, which tracks more than 1500 nuclides.

NEWT in SCALE 5.1 uses a 2-D version of the SCALE Generalized Geometry Package (SGGP). The SGGP was originally developed for KENO-VI and provides SCALE users with consistent geometry model input that makes it easy to convert input models between NEWT and KENO-VI. SGGP includes many geometric shapes, such as cylinders, boxes, spheres, hexprisms, wedges, cones, and rectangular and hexagonal arrays, and is capable of handling extremely complex geometry models. This system provides NEWT with a much more versatile and robust geometry package than that originally released in SCALE 5.

2. Model Descriptions

To validate the SCALE/TRITON modules and data used in reactor physics depletion calculations, numerical predictions using TRITON/NEWT (the t-depl sequence) and TRITON/KENO-VI (the t6-depl sequence) were compared with experimental measurements for a total of 29 samples taken from the Calvert Cliffs, Obrigheim, and San Onofre pressurized water reactors (PWRs) and the Gundremmingen boiling water reactor (BWR). Similar comparisons have previously been performed at the Oak Ridge National Laboratory using the one-dimensional (1-D) SAS2H control module in SCALE. SAS2H, t6-depl, and t-depl results were compared for corresponding samples.

All TRITON models used the 44-group ENDF/B-V cross-section library and the CENTRM/PMC modules for resonance self-shielding of the cross sections. CENTRM is a 1-D discrete-ordinates code that computes space-dependent, continuous-energy (CE) neutron spectra. PMC uses the CE spectra to collapse the CE cross-section data to multigroup data (in these cases, 44-group data) for use by NEWT or KENO-VI. CENTRM/PMC used 1-D unit cell models that described the square lattice of each assembly being modeled. The fuel diameter used in the unit cells, as well as in the NEWT and KENO-VI geometry models, was that of the cladding inner diameter (ID). This was done by homogenizing the gas gap between the pellet outer diameter and the clad ID with the fuel. Also, although the KENO-VI models were 3-D, end-fitting hardware on the assemblies was not modeled, and reflective boundary conditions were applied on all boundaries. Thus, in terms of neutronics, the KENO-VI models were basically identical to the NEWT models.

The t-depl models all used an order 6 S_N quadrature with inner and outer iteration convergence criteria of 1.0×10^{-4} and an eigenvalue convergence criterion of 1.0×10^{-5}. Coarse-mesh-finite-difference acceleration was also used with the NEWT models. The KENO-VI models all used 2100 neutron generations, skipping the first 100 generations. There were 2000 neutrons in each generation, resulting in a total of 4 million neutron histories. The SAS2H models used the 1-D discrete-ordinates code XSDRNPM coupled with ORIGEN-S for depletion and decay.

3. Comparison of Calculated Results and Measured Data

Provided in this section are comparisons of spent fuel isotopic compositions predicted by the TRITON module using both NEWT and KENO-VI with experimental measurements. For each sample, percent differences between the computed and measured values were calculated for numerous nuclides.

The Calvert Cliffs Unit 1 PWR, currently operated by Constellation Energy, uses ABB-Combustion Engineering-designed fuel assemblies with a 14 × 14 pin square lattice. Each assembly contains 176 fuel pins and five guide tubes. Spent fuel samples were taken from three axial positions in the assemblies D047, D101, and BT03. These pellets then underwent radiochemical measurements at the Materials Characterization Center of Pacific Northwest Laboratory. [2] The measured data to which the TRITON results have been compared come from a previous study regarding the application of isotopic uncertainties in light water reactor depletion calculations. [3] Table 1, which provides a statistical summary by nuclide over all Calvert Cliff samples, shows that the t-depl results are generally comparable and often superior to the SAS2H results. (The t6-depl results were statistically equivalent to the t-depl results.) It can be seen that for both the actinides and fission products, TRITON outperforms SAS2H in most cases.

The San Onofre mixed-oxide fuel samples were prepared by the Battelle Memorial hot-cell facility in Columbus, Ohio. The samples were then sent to the Westinghouse Waltz Mill Analytical Laboratory for comprehensive spectrometric analyses of isotopic concentrations. All of the isotopes measured were actinides, with the exception of the fission product ^{148}Nd. Table 2 shows similar results for San Onofre when comparing both TRITON depletion cases with the previous SAS2H depletion case. [4] TRITON clearly provides better results for ^{236}U, ^{241}Pu, and ^{242}Pu while performing more poorly for the nuclide ^{237}Np. For all other nuclides, the results between cases are consistent.

Obrigheim is a German PWR that uses 14 × 14 fuel assemblies. The radiochemical analyses were performed independently by the laboratories of the European Institute for Transuranic Elements, the Institute for Radiochemistry, the Karlsruhe Reprocessing Plant, and the International Atomic Energy Agency. Each fuel assembly was split lengthwise before dissolution so that two batches per assembly were available for analysis. The measured results used here were from one batch of each fuel assembly. [2] Table 3 shows that the TRITON results for Obrigheim are generally better than or comparable to the SAS2H results, with the exception of ^{240}Pu and ^{242}Pu. For nuclides such as ^{238}Pu and ^{241}Pu, the TRITON results are far superior to the SAS2H results.

Radiochemical isotopic analyses of Gundremmingen BWR spent fuel were conducted by the Ispra and Karlsruhe facilities of the European Joint Research Center. The spent fuel specimens taken from two samples were analyzed at Ispra only; all other sample analyses were performed at both establishments. For twice-measured samples, the average of the two measurements was reported. Isotopic composition measurements from six different pins (from two fuel assemblies) were reported. [5] Table 4 shows a summary of the results for the Gundremmingen BWR. The TRITON results are generally comparable to the SAS2H results.

Table 1: Average percent difference[a] between measured and computed nuclide compositions for TRITON and SAS2H (Calvert Cliffs Unit 1 PWR)

	Average percent difference		Standard deviation	
	t-depl	SAS2H	t-depl	SAS2H
^{234}U	–1.10	0.79	14.60	15.20
^{235}U	0.26	–4.26	3.98	3.51
^{236}U	–0.52	1.12	2.03	1.59
^{238}U	–0.88	–0.74	0.51	0.50
^{238}Pu	–7.23	–9.09	4.84	6.11
^{239}Pu	7.19	–1.19	4.41	2.00
^{240}Pu	2.62	–2.71	0.72	1.03
^{241}Pu	0.98	–4.07	4.31	1.94
^{242}Pu	–1.43	0.22	3.31	3.38
^{237}Np	9.07	9.29	7.62	9.99
^{133}Cs	2.32	2.47	0.89	0.90
^{143}Nd	1.12	–1.10	1.32	1.11
^{145}Nd	0.03	–0.58	0.65	0.70
^{147}Sm	2.78	0.88	4.78	5.91
^{149}Sm	–13.45	–9.98	29.83	31.56
^{150}Sm	12.52	7.35	2.87	2.77
^{151}Sm	20.71	24.98	10.93	6.92
^{151}Eu	–20.85	8.00	36.29	53.20
^{152}Sm	12.47	38.20	20.96	21.49
^{153}Eu	3.81	3.55	6.24	4.84
^{155}Gd	–25.64	–22.30	14.48	12.38
^{241}Am	–2.70	–11.80	17.77	10.94
^{99}Tc	20.98	18.51	20.00	19.36

[a](Calculated/measured –1) × 100%.

Table 2: Average percent difference between measured and computed nuclide compositions for TRITON and SAS2H (San Onofre Unit 1 PWR)

	Average percent difference			Standard deviation		
	t6-depl	t-depl	SAS2H	t6-depl	t-depl	SAS2H
^{234}U	–8.70	–8.84	–8.5	6.37	6.40	6.41
^{235}U	0.96	0.85	–0.9	1.74	1.70	1.04
^{236}U	0.59	1.06	4.3	5.79	5.86	5.73
^{238}U	–0.02	0.00	0.0	0.01	0.01	0.00
^{238}Pu	–43.32	–43.22	–44.4	12.40	12.39	12.21
^{239}Pu	4.55	4.72	5.2	3.05	3.08	3.89
^{240}Pu	1.58	1.67	–1.7	0.58	0.56	2.57
^{241}Pu	0.90	0.80	3.0	6.81	6.83	4.17
^{242}Pu	5.34	5.31	9.6	11.10	11.16	6.50
^{237}Np	–10.70	–10.94	–7.4	4.04	3.87	3.52
^{241}Am	–24.41	–24.54	–23.9	62.45	62.39	62.86
^{243}Am	4.33	5.47	6.4	53.31	55.48	55.02
^{148}Nd	0.26	0.25	–0.3	0.31	0.30	0.35

Table 3: Average percent difference between measured and computed nuclide compositions for TRITON and SAS2H (Obrigheim PWR)

	Average percent difference			Standard deviation		
	t6-depl	t-depl	SAS2H	t6-depl	t-depl	SAS2H
^{235}U	–0.55	–1.24	–2.7	0.80	0.80	0.80
^{236}U	0.41	0.73	1.4	0.40	0.42	0.39
^{238}U	0.02	0.01	0.1	0.00	0.02	0.04
^{238}Pu	–4.12	–2.49	13.7	3.27	3.35	3.85
^{239}Pu	2.45	2.79	2.0	1.62	1.60	1.66
^{240}Pu	4.10	4.63	–0.7	1.38	1.36	1.50
^{241}Pu	–2.08	–1.03	–10.7	1.47	1.42	1.35
^{242}Pu	–9.33	–7.77	–4.4	2.12	2.20	2.19

Table 4: Average percent difference between measured and computed nuclide compositions for TRITON and SAS2H (Gundremmingen BWR)

	Average percent difference			Standard deviation		
	t6-depl	t-depl	SAS2H	t6-depl	t-depl	SAS2H
^{235}U	–4.90	–5.15	–3.0	9.35	9.22	3.79
^{236}U	–4.62	–4.53	–4.3	3.03	3.01	2.35
^{238}U	0.11	0.12	0.1	0.14	0.12	0.09
^{238}Pu	–2.61	–3.31	1.7	12.60	12.40	16.69
^{239}Pu	–3.78	–3.95	–5.0	10.99	10.63	7.36
^{240}Pu	1.54	1.69	–0.9	4.41	4.44	5.62
^{241}Pu	–7.72	–7.86	–7.8	12.28	11.68	7.31
^{242}Pu	–4.03	–4.08	–2.1	8.69	8.41	9.16
^{244}Cm	–11.28	–11.57	–15.8	20.44	19.59	19.31

Figs. 1 and 2 graphically show the average percent differences and the standard deviations from all data presented in Tables 1 through 4. Fig. 1 shows the results for actinides, while Fig. 2 shows results for those nuclides that are fission products. The figures confirm that the TRITON results are generally similar to or better than the SAS2H results.

Figure 1: TRITON/SAS2H results for actinides.

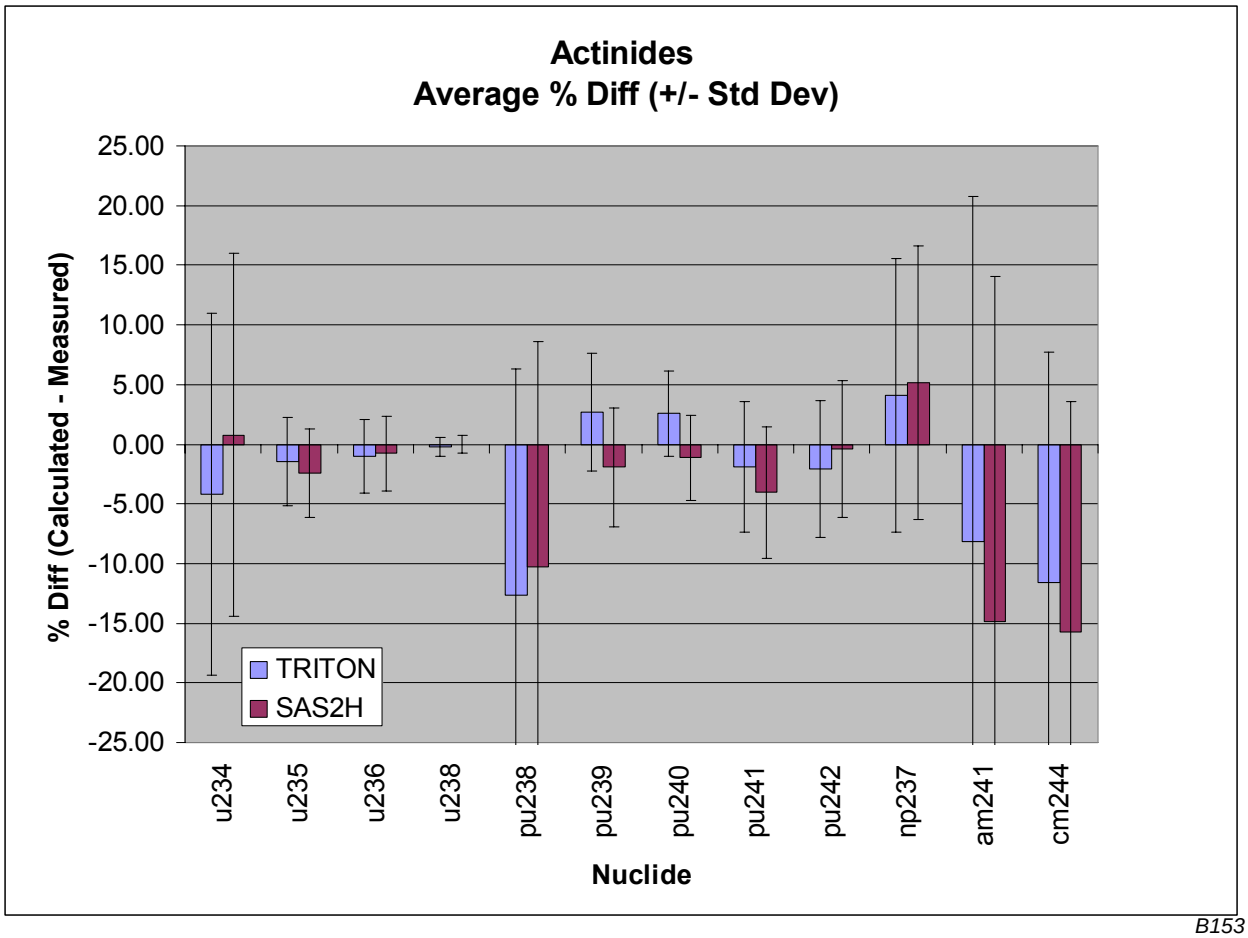
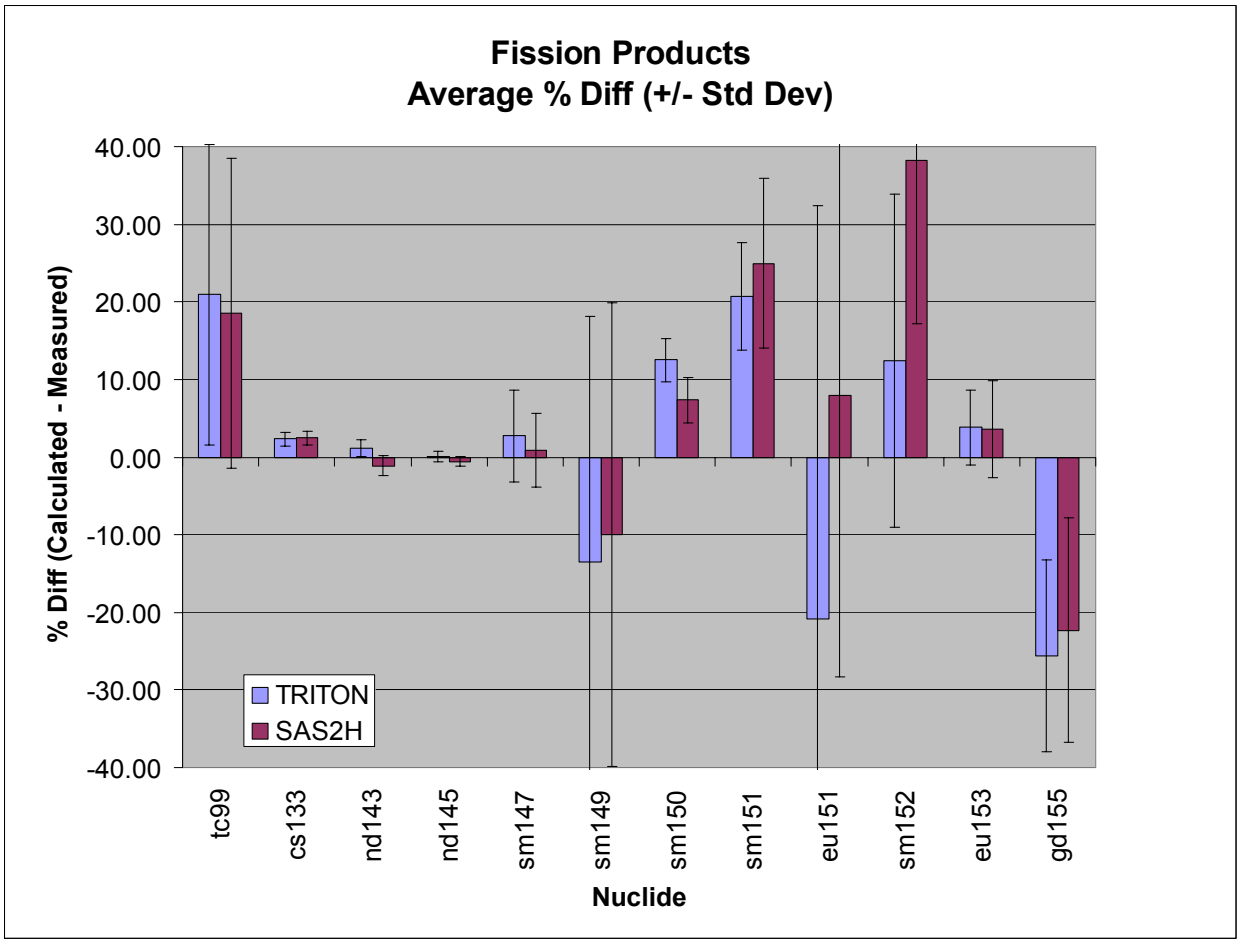


Figure 2: TRITON/SAS2H results for fission products.



4. Conclusions

This study shows that the TRITON control module generally performs comparably to the SAS2H control module and that NEWT and KENO-VI produce nearly identical transport/depletion results when part of the TRITON depletion sequence. TRITON greatly improves the isotopic depletion capabilities of the SCALE code system by handling complex 2-D and 3-D models with rigorous transport codes (NEWT and KENO) coupled with the point depletion and decay module ORIGEN-S, which tracks more than 1500 nuclides.

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