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VERIFICATION OF SCALE MODULES AGAINST CMS5/SNF SEQUENCE FOR DEPLETION AND DECAY CALCULATIONS OF BWR FUEL ASSEMBLIES

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ABSTRACT

This study presents code-to-code comparisons between the TRITON and Polaris modules of the SCALE code system and the coupled CASMO/SIMULATE/SNF (CMS5/SNF) code sequence for evaluating the isotopic composition of spent nuclear fuel on a long-term basis. The models are based on spent fuel assemblies from a Swiss boiling water reactor. The parameters for the comparisons are: nuclide vectors, total activity, neutron source, and decay heat starting from 2019 and up to 100,000 years of decay. Where notable, the deviations in fission products and actinides are discussed with respect to differences between the codes and models. Overall, the results proved to be in good agreement for the prediction of spent fuel nuclide vectors. Good consistency was observed for the total activity and decay heat power. Most fission products and actinides considered in this work are in good agreement, with few exceptions which show systematic deviations, e.g. Mo-93, Sn-121m, Am-242, Am-242m and Cm-242.

INTRODUCTION

The disposal of spent nuclear fuel in deep geological repositories (DGR) is the preferred solution for nuclear waste management in Switzerland [1]. NAGRA has the mandate to prepare and implement such solutions [2], which requires a demonstration that the disposal facilities comply with operational and long-term safety requirements. Estimation of the long-term maximum surface dose rates, decay heat, and criticality safety are key components of the safety assessment of the repository. These safety parameters depend on the time-dependent isotopic inventory of the spent fuel, which is evaluated by means of detailed simulations of the fuel irradiation and decay.

In NAGRA, such calculations are performed using the SCALE package [3], and inputs such as integrated fuel irradiation data, as provided from the utilities, and lattice-specific ORIGEN microscopic cross-section libraries to deplete and decay the fuel types. The foreseen update of the radioactive waste database in NAGRA [4], includes modeling of the individual assemblies along with an evaluation of the computational biases of the models.

In this study, sequences that are candidates for evaluating the long-term spent fuel isotopic compositions are investigated. The tools are TRITON, Polaris and ORIGEN-ARP of the SCALE code system [3], and the CMS5/SNF sequence [5]. The SCALE modules are referenced to the CMS5/SNF. The study aims to provide an insight into the methodological specifics and their applicability for spent fuel analyses for the DGR. The methods are applied to two BWR assemblies, for a timespan relevant for the DGR operational phase [2]. The analyses focus on fission products and actinides relevant for the safety of the repository; these were defined by NAGRA based on their contributions to the maximum long-term surface dose rates [6].

The study is limited to two fuel assemblies; and, further analysis is foreseen to investigate conditions that impact the code-to-code results of the spent fuel analysis on a long-term basis. The parameters include the fuel and structural material impurities, cladding activation, assembly designs, discharge burnup, control blade patterns and the effects from the neighboring assemblies.

MODELS, CODES AND LIBRARIES

Two fuel assemblies, designated hereafter as GE8 and GE11, irradiated in a Swiss BWR, were selected for the purpose of this study. The assemblies differ in terms of design, enrichment, gadolinium loads and operating histories, including depletion times in the vicinity of control blade. GE8 is the main focus of the analysis, which is an 8x8 assembly and GE11 is a 9x9. GE8 was irradiated without an inserted control blade, where GE11 was irradiated with a control blade inserted for intervals of its exposure, which adds up to ~0.043 of the discharge burnup. The assemblies were irradiated for five and six cycles and reached burnup of ~40 and 56 GWd/tHM, respectively. Because the assemblies had different discharge dates, and hence different decay times, the decay was referenced to 2019 with 10, 100, 1000 and 100,000 year decay increments.

The codes and methodologies chosen for this study are well known and established as standards in the nuclear industry: the SCALE code system [3] and the CMS5/SNF sequence [5]. The main difference between the utilized modules and sequence is the way of implementing the irradiation history. The CMS5/SNF inherently applies a 3D core model to any assembly irradiated in the core, accounting for the exact irradiation conditions. The SCALE models in this study are 2D lattice models assuming an infinite mesh with no account taken of the neighboring assemblies.

The CMS5/SNF methodology is outlined in Figure 1. The isotopic library, generated by the lattice physics code CASMO5 [7], provides isotopic concentrations, cross-sections and fluxes, tabulated via exposure, moderator density, control blade and fuel temperature histories. The nodewise exposure and accumulated history parameters, obtained from qualified operational reactor data and core simulation using the nodal reactor code SIMULATE [8], are used as entry points in the interpolation routines and, together with the power history model in SNF [5,9], are used to compute the time-dependent isotopic concentrations. CMS5/SNF computes the isotopic concentrations and all relevant spent fuel parameters such as decay heat power, activity, neutron and photon sources on a nodal basis following the axial nodalization of the reactor core model.

SIMULATE and SNF share the same cross-section library, generated by CASMO5 and based on ENDF/B-VII.R1. The basic decay data in SNF are also based on ENDF/B-VII.R1 [10], which includes nuclide transmutation chains; decay heat production; radiation emission spectra for photons; electrons and alpha particles from radioactive decay; neutrons from radioactive decay, spontaneous fission, and others. These data are compiled from fundamental (ENDF/B-VII.R1 [10], ENSDF [11], TENDL-2012 [12]) and processed (ESTAR and ASTAR [13]) sources for 890 isotopes. The evaluation and validation of the decay data in SNF is reported in [14].

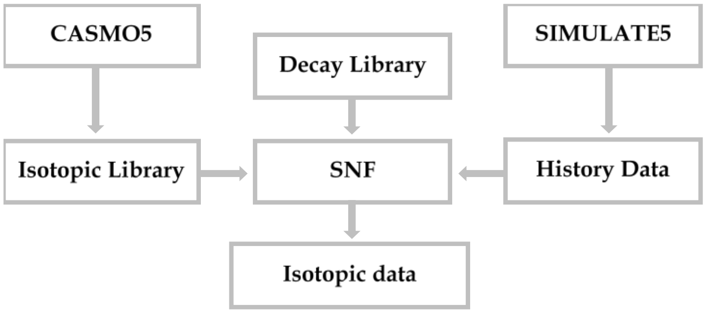

Figure 1. Studsvik's system for spent fuel analyses.

The SCALE code system [3] is widely used for nuclear system design and safety analyses. Polaris, TRITON and ORIGEN-ARP modules of the SCALE 6.2.3 are used in this study along with the SCALE 252g and 56g multigroup (MG) libraries [3]. The MG libraries are based primarily on the ENDF/B-VII.R1 nuclear data library along with supplemental nuclear data from JEFF-3.0/A.

Polaris and TRITON are 2D lattice physics modules that are used for the analysis of LWR fuel assemblies [3]. Both are coupled to ORIGEN to perform the depletion and decay calculations. TRITON is also used to generate cross sections for ORIGEN-ARP module for the transmutation and decay calculations. All parameters are direct output of the modules, except for the neutron sources, which are evaluated in ORIGEN.

Five modeling approaches have been considered in reference to the CMS5/SNF full core models:

1) TRITON – individual nodes with cycle-average irradiation conditions;
2) TRITON – four lattices with cycle/axial burnup weighted-average irradiation conditions;
3) Polaris – individual nodes with exact nodal irradiation conditions as implemented in CMS5;
4) Polaris – four lattices with cycle and axial burnup weighted-average irradiation conditions;
5) ORIGEN-ARP – four lattices with cycle/axial burnup weighted-average irradiation conditions;

The all-nodes models follow the axial nodalization of the SIMULATE core model. In this way, the operational parameters such as power density, void and temperatures, exported from the core-follow calculations, were implemented in the SCALE models on a node by node basis. The number of exposure intervals is 292 for the GE8 as shown in Figure 2. The core-follow simulation was reproduced for each node by the same number of exposure steps as in the core simulation. Similarly, all axial nodes are modeled in TRITON. However, due to the significant computational requirements, the irradiation history was applied as burnup-weighted, cycle-average parameters.

The assembly axial profile is shown in Figure 2. Axially, the assembly is profiled by 5 lattices, top and bottom natural uranium blankets and four lattices with different fuel pin layouts, enrichments and burnable absorber contents. Each axial node (25 in total) is "filled out" entirely by only one lattice, hence the modeling in Polaris, TRITON and CMS5/SNF is nodewise fully consistent.

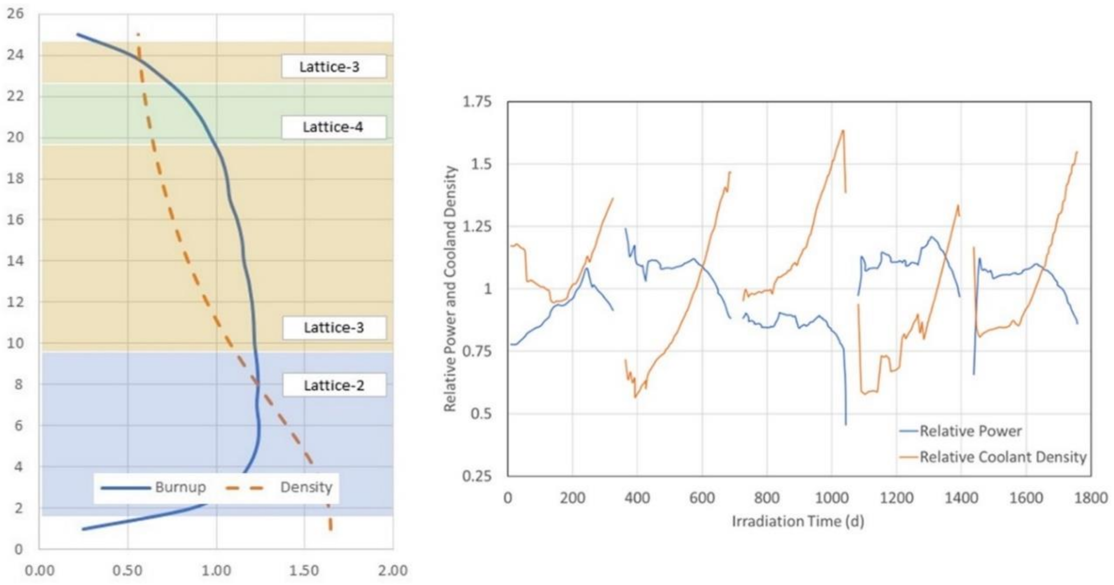

Figure 2. Relative power and coolant density (right) in node 13 of the GE8 distributed over 292 exposure steps, and axially normalized burnup of 25 axial nodes and moderator density (left).

RESULTS

The results are relative deviations between the SCALE modules and the CMS5/SNF sequence (the latter results are the reference) for the concentrations, decay heat, neutron source and total activity. The relative deviations are calculated as $\Delta = {}^{SCALE}/_{CMS5} - 1$. The results include dose rate-relevant nuclides as defined by NAGRA implementing a 0.1 ppm cut-off (i.e. 0.1 g/tU), except for Mo-93 and Ho-166m. Stable nuclides, e.g. Nd-145, Nd-148 and Gd-155, were included in the comparisons due to their importance in burnup credit criticality calculations.

Table 1 shows relative deviations of average concentrations of isotopes and parameters in 9 nodes distributed axially in the GE8 and GE11. The SCALE results were evaluated using Polaris and the 252g MG library following the exact irradiation histories, and up to 100k years of decay.

Table 2 shows relative deviations between SCALE modules and the CMS5/SNF sequence in the GE8 at year 2119 and in 3 nodes (5, 13 and 21) located in three lattices. The SCALE modules used are Polaris and TRITON, using both the 56g and 252g MG libraries.

Table 3 shows relative deviations between the Polaris and the CMS5/SNF sequence in nodes of the GE8 at year 2119. The results of the even nodes are listed along with lattice averages. The 5 lattices are computationally divided into 25 nodes as: 1, 8, 12, 3, and 1 node, respectively. In these models, Polaris uses the 252g MG library and exact operational history (292 exposure intervals).

Table 4 shows relative deviations between the SCALE modules and the CMS5/SNF sequence for the average concentrations in each lattice. The SCALE modules use the 252g MG library and the cycle-average histories. Lattice-specific models implementing burnup-weighted histories were modeled in SCALE and compared to the average concentration over the whole lattice in SNF. In addition, a model that implements the entire assembly-weighted histories is presented, which is a typical approach of modeling a spent fuel assembly using a single, representative-node model.

Table 1. Deviations in average concentrations of 9 nodes in GE8 and GE11 during long-term decay.

Assembly	GE8				GE11			
Year/Iso	2029	2119	3019	100K	2029	2119	3019	100K
Se-79	3%	3%	3%	3%	4%	4%	4%	4%
Sr-90	0%	0%	0%	-	0%	-1%	-1%	-
Zr-93	1%	1%	1%	1%	0%	0%	0%	0%
Nb-93m	2%	1%	1%	1%	2%	0%	0%	0%
Nb-94	3%	3%	3%	3%	8%	7%	7%	7%
Mo-93	-85%	-85%	-85%	-	-82%	-82%	-82%	-
Mo-95	0%	0%	0%	0%	0%	0%	0%	0%
Tc-99	1%	1%	1%	1%	1%	1%	1%	1%
Ru-101	1%	1%	1%	1%	1%	1%	1%	1%
Rh-103	2%	2%	2%	2%	4%	4%	4%	4%
Pd-107	2%	2%	2%	2%	2%	2%	2%	2%
Cd-113	5%	5%	5%	5%	3%	2%	2%	2%
Sn-121m	52%	52%	52%	-	54%	53%	53%	-
Sn-126	10%	10%	10%	10%	10%	10%	10%	10%
I-129	7%	7%	7%	7%	8%	8%	8%	8%
Cs-135	1%	3%	3%	3%	6%	5%	5%	5%
Cs-137	-3%	-3%	-3%	-	-3%	-3%	-3%	-
Nd-145	1%	1%	1%	1%	1%	1%	1%	1%
Nd-148	1%	1%	1%	1%	1%	1%	1%	1%
Sm-151	-5%	-5%	-5%	-	-6%	-7%	-7%	-
Eu-153	-3%	-1%	-1%	-1%	-2%	-1%	-1%	-1%
Gd-155	-11%	3%	3%	3%	-5%	3%	3%	3%
Ho-166m	-2%	-2%	-2%	-	-9%	-9%	-9%	-
Ra-226	-5%	-3%	0%	2%	-5%	0%	4%	6%
Pa-231	-1%	-1%	-1%	-2%	-15%	-10%	1%	1%
U-234	-4%	-1%	0%	0%	0%	3%	5%	4%
U-235	-1%	-1%	-1%	-2%	5%	6%	6%	1%
U-236	3%	3%	3%	3%	3%	3%	3%	3%
U-238	0%	0%	0%	0%	0%	0%	0%	0%
Np-237	5%	4%	1%	1%	6%	5%	3%	3%
Pu-238	5%	5%	3%	-	10%	8%	6%	-
Pu-239	-2%	-2%	-2%	-2%	-3%	-4%	-4%	-3%
Pu-240	2%	2%	2%	3%	4%	3%	3%	3%
Pu-241	0%	-1%	-2%	-1%	2%	0%	-6%	-5%
Pu-242	2%	2%	2%	2%	3%	3%	3%	3%
Am-241	0%	0%	0%	-6%	2%	1%	1%	-10%
Am242	-26%	-26%	-26%	-	-22%	-23%	-23%	-
Am-242m	-26%	-26%	-26%	-	-22%	-23%	-23%	-
Am-243	4%	4%	4%	4%	4%	4%	4%	5%
Cm-242	-26%	-26%	-26%	-	-22%	-24%	-24%	-
Cm-243	2%	1%	-	-	12%	6%	-	-
Cm-244	3%	3%	-	-	2%	1%	-	-
Cm-245	-2%	-2%	-2%	-1%	-4%	-6%	-6%	-5%
Cm-246	7%	7%	7%	8%	6%	6%	6%	7%
DH (W)	0%	1%	0%	0%	-1%	2%	1%	2%
A (Bq)	-2%	-2%	-13%	-23%	-2%	-2%	-11%	-18%

Table 2. Deviations in concentrations in GE8 at year 2119 – “x” denotes out of range.

Module History	Polaris - 56g Cycle Average			Polaris - 252g Cycle Average			Polaris - 252g 292 Exposure Step			TRITON - 56g Cycle Average			TRITON - 252g Cycle Average		
Node No.	5	13	21	5	13	21	5	13	21	5	13	21	5	13	21
Se-79	4%	4%	5%	3%	4%	4%	3%	3%	4%	3%	4%	4%	2%	3%	3%
Sr-90	1%	0%	0%	1%	1%	0%	0%	0%	0%	1%	1%	1%	0%	0%	0%
Zr-93	1%	1%	1%	1%	1%	1%	0%	0%	1%	0%	0%	1%	0%	0%	1%
Nb-93m	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%
Nb-94	X	X	X	9%	7%	-2%	7%	6%	-3%	X	X	X	5%	4%	-5%
Mo-93	X	X	X	-85%	-84%	-86%	-85%	-84%	-87%	X	X	X	-86%	-85%	-88%
Mo-95	1%	1%	1%	1%	1%	1%	0%	0%	0%	0%	0%	1%	0%	0%	1%
Tc-99	1%	1%	1%	2%	2%	2%	1%	1%	1%	4%	4%	4%	4%	4%	4%
Ru-101	1%	1%	1%	2%	2%	2%	1%	1%	1%	0%	0%	1%	0%	1%	1%
Rh-103	1%	1%	2%	2%	3%	3%	2%	3%	3%	2%	3%	4%	0%	1%	2%
Pd-107	3%	3%	4%	3%	3%	4%	1%	2%	2%	0%	1%	1%	1%	1%	1%
Cd-113	15%	16%	17%	10%	10%	10%	5%	3%	6%	6%	8%	8%	3%	5%	5%
Sn-121m	59%	62%	64%	52%	54%	55%	49%	52%	53%	55%	58%	60%	48%	51%	51%
Sn-126	13%	14%	16%	10%	11%	12%	9%	10%	11%	10%	12%	13%	8%	9%	10%
I-129	3%	3%	4%	3%	3%	3%	6%	7%	7%	1%	2%	2%	1%	1%	2%
Cs-135	2%	1%	1%	2%	0%	0%	3%	4%	2%	-2%	-3%	-3%	-1%	-1%	-2%
Cs-137	-2%	-2%	-2%	-2%	-2%	-2%	-3%	-3%	-3%	-3%	-3%	-3%	-3%	-3%	-3%
Nd-145	1%	1%	1%	1%	1%	1%	0%	0%	1%	0%	0%	0%	0%	0%	1%
Nd-148	2%	1%	1%	2%	1%	1%	1%	1%	1%	1%	1%	0%	1%	1%	0%
Sm-151	4%	3%	0%	2%	1%	-2%	-4%	-5%	-5%	-4%	-4%	-7%	-5%	-4%	-7%
Eu-153	1%	2%	0%	0%	0%	-3%	-1%	-1%	-1%	-3%	-3%	-5%	-1%	-1%	0%
Gd-155	-4%	-2%	-13%	-9%	-8%	-20%	2%	4%	3%	-11%	-10%	-22%	0%	0%	0%
Ho-166m	-4%	-3%	-6%	0%	2%	-2%	3%	-5%	-3%	-13%	-12%	-13%	-13%	-13%	-14%
Ra-226	-1%	0%	0%	-3%	-2%	-3%	-4%	-3%	-3%	-6%	-5%	-6%	-6%	-5%	-5%
Pa-231	-9%	-5%	8%	-11%	-7%	6%	-13%	-7%	6%	-16%	-11%	2%	-15%	-10%	3%
U-234	3%	4%	2%	1%	1%	0%	-1%	0%	-1%	-3%	-2%	-4%	-3%	-2%	-4%
U-235	1%	2%	1%	-1%	0%	0%	-4%	0%	-1%	-11%	-6%	-5%	-10%	-5%	-4%
U-236	3%	2%	3%	3%	2%	3%	3%	2%	3%	3%	3%	3%	3%	2%	3%
U-238	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Np-237	4%	5%	6%	4%	5%	6%	2%	4%	5%	0%	2%	3%	0%	2%	2%
Pu-238	10%	11%	13%	8%	8%	10%	4%	5%	6%	2%	4%	4%	2%	4%	4%
Pu-239	0%	0%	0%	-1%	-1%	-2%	-3%	-2%	-2%	-5%	-4%	-6%	-4%	-3%	-5%
Pu-240	-2%	-3%	-4%	1%	1%	0%	2%	3%	1%	0%	0%	-1%	1%	1%	-1%
Pu-241	3%	5%	6%	2%	3%	3%	-3%	-1%	0%	-3%	-1%	-1%	-4%	-2%	-2%
Pu-242	6%	7%	10%	4%	4%	6%	2%	2%	3%	2%	3%	4%	2%	2%	3%
Am-241	3%	5%	6%	1%	3%	3%	-2%	0%	0%	-3%	-1%	-1%	-3%	-1%	-1%
Am242	-21%	-17%	-18%	-24%	-21%	-21%	-28%	-26%	-25%	-31%	-26%	-26%	-31%	-26%	-26%
Am-242m	-21%	-17%	-18%	-24%	-21%	-21%	-28%	-26%	-25%	-31%	-26%	-26%	-31%	-26%	-26%
Am-243	3%	4%	6%	8%	9%	11%	2%	4%	6%	3%	5%	6%	2%	4%	5%
Cm-242	-22%	-18%	-19%	-24%	-21%	-21%	-28%	-26%	-26%	-31%	-26%	-27%	-31%	-26%	-26%
Cm-243	8%	10%	11%	5%	6%	8%	1%	1%	1%	2%	6%	6%	-1%	3%	3%
Cm-244	6%	7%	7%	9%	11%	11%	1%	3%	3%	-3%	-1%	-4%	-1%	3%	1%
Cm-245	10%	14%	12%	7%	10%	8%	-4%	-1%	-1%	-5%	0%	-5%	-2%	5%	1%
Cm-246	16%	18%	20%	14%	16%	17%	4%	10%	7%	0%	3%	-4%	4%	10%	5%
DH (W)	3%	4%	5%	2%	3%	3%	0%	1%	1%	-1%	0%	0%	-1%	0%	0%
A (Bq)	-1%	-1%	-1%	-1%	-1%	-2%	-2%	-2%	-2%	-2%	-2%	-3%	-3%	-3%	-3%
N (1/s)	10%	11%	7%	10%	11%	7%	4%	7%	2%	0%	2%	-3%	5%	9%	2%

Table 3. Deviations at year 2119 in nodes of GE8 (even numbers) using Polaris and the 252g library vs. CMS5/SNF, and the average of 8, 12, and 3 models in lattice 2, 3 and 4, respectively.

Node	2	4	6	8	10	12	14	16	18	20	22	24	Avg L2 #8	Avg L3 #12	Avg L4 #3
Lattice	2				3a					4		3b			
Se-79	3%	3%	3%	3%	3%	3%	4%	4%	4%	4%	4%	4%	3%	4%	4%
Sr-90	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%
Zr-93	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%
Nb-93m	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%
Nb-94	-3%	7%	8%	8%	8%	7%	6%	4%	2%	-1%	-6%	-19%	6%	1%	-3%
Mo-93	-90%	-85%	-84%	-84%	-84%	-84%	-84%	-84%	-85%	-86%	-88%	-92%	-86%	-85%	-87%
Mo-95	1%	0%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	0%	1%	1%
Tc-99	2%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	2%	1%	1%	1%
Ru-101	2%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	2%	1%	1%	1%
Rh-103	2%	2%	2%	2%	3%	3%	3%	3%	3%	3%	3%	3%	2%	3%	3%
Pd-107	2%	2%	2%	2%	2%	2%	2%	2%	2%	2%	2%	2%	2%	2%	2%
Cd-113	10%	6%	3%	2%	4%	4%	3%	3%	4%	5%	7%	10%	5%	5%	6%
Sn-121m	49%	50%	51%	52%	52%	53%	53%	54%	54%	54%	54%	55%	50%	53%	54%
Sn-126	10%	9%	9%	10%	10%	10%	11%	11%	11%	11%	12%	13%	9%	11%	11%
I-129	8%	7%	7%	7%	7%	7%	7%	7%	7%	8%	8%	9%	7%	7%	8%
Cs-135	3%	2%	2%	2%	3%	3%	2%	2%	1%	1%	0%	0%	2%	2%	0%
Cs-137	-2%	-2%	-2%	-2%	-2%	-2%	-2%	-2%	-2%	-2%	-2%	-2%	-2%	-2%	-2%
Nd-145	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%
Nd-148	1%	2%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%	1%
Sm-151	-1%	-3%	-5%	-5%	-4%	-4%	-6%	-6%	-5%	-5%	-4%	-3%	-4%	-5%	-5%
Eu-153	-4%	-2%	-2%	-2%	-2%	-2%	-2%	-2%	-2%	-3%	-5%	-6%	-3%	-3%	-4%
Gd-155	-18%	-10%	-9%	-8%	-5%	-5%	-7%	-8%	-10%	-17%	-22%	-34%	-11%	-11%	-19%
Ho-166m	14%	8%	2%	-1%	-1%	-2%	-5%	-5%	-4%	-3%	0%	8%	4%	-2%	-2%
Ra-226	-4%	-4%	-4%	-3%	-3%	-3%	-3%	-3%	-3%	-3%	-3%	-3%	-4%	-3%	-3%
Pa-231	6%	-11%	-14%	-12%	-10%	-9%	-6%	-5%	-2%	3%	9%	14%	-9%	-2%	6%
U-234	-3%	-1%	-1%	0%	0%	1%	0%	0%	0%	-1%	-2%	-6%	-1%	-1%	-2%
U-235	-4%	-6%	-5%	-3%	-2%	-1%	-2%	-2%	-2%	-2%	-1%	-1%	-4%	-1%	-1%
U-236	4%	3%	3%	3%	3%	3%	2%	2%	2%	3%	3%	5%	3%	3%	3%
U-238	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Np-237	4%	3%	2%	3%	3%	4%	4%	4%	4%	5%	5%	6%	3%	4%	5%
Pu-238	8%	5%	5%	5%	6%	6%	6%	6%	6%	7%	8%	10%	5%	6%	7%
Pu-239	1%	-2%	-4%	-4%	-2%	-1%	-3%	-3%	-3%	-2%	-2%	-1%	-2%	-2%	-2%
Pu-240	3%	3%	3%	3%	4%	4%	3%	2%	2%	1%	1%	2%	3%	3%	1%
Pu-241	0%	-1%	-2%	-2%	0%	0%	0%	0%	0%	1%	1%	0%	-1%	0%	0%
Pu-242	2%	2%	3%	2%	2%	2%	2%	3%	3%	3%	4%	4%	2%	3%	3%
Am-241	0%	-1%	-2%	-2%	0%	1%	0%	0%	0%	1%	1%	0%	-1%	0%	1%
Am242	-25%	-27%	-28%	-28%	-25%	-25%	-26%	-27%	-26%	-26%	-25%	-25%	-27%	-26%	-25%
Am-242m	-25%	-27%	-28%	-28%	-25%	-25%	-26%	-27%	-26%	-26%	-25%	-25%	-27%	-26%	-25%
Am-243	4%	4%	3%	3%	4%	4%	5%	6%	6%	6%	7%	5%	3%	5%	6%
Cm-242	-25%	-27%	-29%	-28%	-26%	-25%	-27%	-27%	-27%	-26%	-25%	-25%	-27%	-26%	-26%
Cm-243	5%	3%	1%	1%	3%	3%	2%	2%	2%	2%	3%	2%	2%	2%	2%
Cm-244	5%	4%	4%	4%	5%	5%	5%	6%	6%	5%	5%	2%	3%	5%	5%
Cm-245	5%	0%	-3%	-3%	0%	1%	0%	0%	1%	0%	1%	-3%	-2%	0%	0%
Cm-246	8%	8%	8%	9%	11%	12%	11%	11%	11%	10%	10%	2%	7%	9%	9%
DH (W)	1%	0%	0%	0%	1%	1%	1%	1%	1%	1%	1%	1%	0%	1%	1%
A (Bq)	-2%	-2%	-2%	-2%	-2%	-2%	-2%	-2%	-2%	-2%	-2%	-3%	-2%	-2%	-2%
N (1/s)	2%	5%	6%	7%	8%	8%	7%	7%	6%	4%	2%	-1%	5%	5%	3%

Table 4. Deviations at year 2119 in lattices of GE8 – concentrations in lattice representative model vs nodal averages.

Ref.	Polaris Avg. nodal conc.				CMS5/SNF Avg. nodal conc.											
Module	Polaris				Polaris				TRITON				ORIGEN-ARP			
Lattices	L2	L3	L4	All	L2	L3	L4	All	L2	L3	L4	All	L2	L3	L4	All
Se-79	0%	1%	0%	3%	4%	5%	5%	7%	3%	5%	4%	6%	3%	4%	4%	6%
Sr-90	0%	1%	0%	4%	1%	2%	0%	4%	1%	2%	1%	4%	0%	1%	0%	3%
Zr-93	0%	1%	0%	3%	1%	1%	1%	3%	1%	1%	1%	3%	0%	1%	0%	2%
Nb-93m	0%	1%	0%	3%	1%	2%	1%	3%	1%	1%	1%	3%	0%	1%	0%	2%
Nb-94	-1%	-3%	0%	-8%	X	X	X	X	X	X	X	X	X	X	X	X
Mo-93	-2%	-5%	-1%	-10%	X	X	X	X	X	X	X	X	X	X	X	X
Mo-95	0%	1%	0%	3%	1%	2%	1%	3%	0%	1%	1%	3%	-1%	1%	0%	2%
Tc-99	0%	1%	0%	2%	2%	2%	1%	4%	4%	5%	4%	6%	-1%	1%	1%	3%
Ru-101	0%	0%	0%	1%	2%	2%	1%	2%	0%	1%	1%	1%	0%	0%	0%	1%
Rh-103	0%	2%	0%	3%	2%	3%	2%	4%	2%	5%	4%	6%	-1%	3%	3%	5%
Pd-107	0%	-2%	0%	-5%	3%	1%	4%	-2%	0%	-1%	0%	-4%	1%	-1%	1%	-3%
Cd-113	-1%	-1%	0%	-1%	15%	15%	17%	14%	6%	7%	8%	7%	32%	22%	24%	30%
Sn-121m	0%	-1%	0%	-2%	59%	61%	64%	58%	55%	58%	60%	55%	54%	57%	59%	56%
Sn-126	0%	-1%	0%	-2%	13%	14%	16%	11%	10%	12%	13%	10%	9%	11%	13%	10%
I-129	0%	0%	0%	-1%	3%	3%	4%	3%	1%	2%	2%	1%	2%	2%	3%	3%
Cs-135	0%	1%	0%	3%	2%	1%	1%	5%	-2%	-2%	-3%	1%	3%	-1%	0%	6%
Cs-137	0%	0%	0%	1%	-2%	-2%	-2%	-1%	-3%	-3%	-3%	-2%	-3%	-3%	-3%	-2%
Nd-145	0%	1%	0%	3%	2%	2%	1%	4%	0%	1%	1%	3%	0%	1%	0%	3%
Nd-148	0%	0%	0%	1%	2%	1%	1%	2%	1%	1%	0%	1%	0%	0%	0%	1%
Sm-151	0%	-1%	0%	0%	3%	1%	0%	2%	-4%	-6%	-7%	-5%	21%	5%	6%	14%
Eu-153	0%	1%	0%	1%	2%	2%	0%	2%	-3%	-2%	-5%	-2%	4%	0%	-3%	1%
Gd-155	0%	0%	0%	-2%	-5%	-5%	-13%	-8%	-12%	-13%	-22%	-15%	-5%	-14%	-23%	-15%
Ho-166m	-9%	-16%	-3%	-39%	-13%	-19%	-9%	-41%	-21%	-26%	-16%	-46%	22%	4%	17%	-26%
Ra-226	-1%	-1%	0%	6%	-1%	-1%	0%	6%	-6%	-6%	-6%	1%	-1%	-5%	-4%	3%
Pa-231	-1%	-3%	0%	8%	-6%	-3%	8%	9%	-12%	-8%	2%	4%	-2%	-3%	7%	13%
U-234	-1%	-1%	0%	2%	2%	2%	2%	5%	-4%	-4%	-4%	-1%	7%	-2%	-1%	4%
U-235	-5%	-8%	0%	7%	-4%	-8%	1%	8%	-14%	-13%	-5%	2%	2%	-9%	0%	13%
U-236	1%	2%	0%	7%	3%	5%	3%	10%	4%	5%	3%	10%	0%	4%	2%	9%
U-238	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Np-237	0%	2%	0%	2%	5%	7%	7%	7%	1%	4%	3%	4%	21%	12%	13%	16%
Pu-238	-1%	-2%	0%	-7%	10%	9%	13%	4%	2%	2%	4%	-3%	22%	7%	10%	7%
Pu-239	0%	0%	0%	0%	0%	0%	0%	0%	-5%	-4%	-6%	-5%	1%	-2%	-4%	3%
Pu-240	0%	2%	0%	0%	-2%	-2%	-4%	-3%	1%	2%	-1%	0%	-36%	-15%	-17%	-14%
Pu-241	0%	3%	0%	2%	4%	8%	6%	7%	-2%	2%	-1%	1%	19%	18%	20%	24%
Pu-242	0%	-3%	0%	-7%	6%	4%	9%	-1%	2%	-1%	3%	-5%	11%	3%	9%	-1%
Am-241	1%	3%	0%	2%	4%	8%	6%	7%	-2%	2%	-1%	1%	18%	18%	20%	24%
Am242	1%	6%	1%	5%	-19%	-14%	-18%	-15%	-29%	-22%	-26%	-23%	-1%	-8%	-9%	1%
Am-242m	1%	6%	1%	5%	-19%	-14%	-18%	-15%	-29%	-22%	-26%	-23%	-1%	-8%	-9%	1%
Am-243	-2%	-7%	-1%	-15%	1%	-3%	5%	-11%	0%	-2%	5%	-11%	35%	10%	20%	4%
Cm-242	1%	6%	1%	5%	-20%	-14%	-18%	-15%	-29%	-22%	-26%	-23%	-1%	-8%	-10%	1%
Cm-243	-1%	-3%	-1%	-9%	8%	7%	10%	0%	2%	3%	6%	-4%	25%	11%	16%	10%
Cm-244	-7%	-16%	-3%	-29%	-1%	-10%	5%	-24%	-10%	-17%	-6%	-30%	31%	-9%	4%	-17%
Cm-245	-11%	-18%	-4%	-34%	-1%	-8%	8%	-26%	-15%	-19%	-8%	-35%	39%	-11%	0%	-18%
Cm-246	-16%	-29%	-7%	-47%	-2%	-17%	12%	-38%	-16%	-28%	-10%	-47%	16%	-31%	-15%	-44%
DH (W)	0%	1%	0%	0%	3%	5%	5%	3%	-1%	1%	0%	-1%	9%	8%	9%	10%
A (Bq)	0%	1%	0%	1%	-1%	0%	-1%	0%	-2%	-2%	-3%	-2%	0%	0%	0%	1%

DISCUSSION

The relative deviations between the used SCALE modules and the CMS5/SNF sequence resulting from this work are compared to the standard deviations of the results of a reference benchmark as shown in Table 5. The reference benchmark was conducted by the Expert Group on Used Nuclear Fuel Criticality (EGUNF) of the OCED/NEA and addressed calculations of isotopic compositions of a BWR fuel assembly using various codes, including Polaris and TRITON [15].

The methodology in this work does not strictly follow the code-to-code benchmark requirements. Nevertheless, the assembly average deviations between the sequences of the present work are close to the 95% confidence interval (2σ) of the results of the reference EGUNF benchmark for most of the isotopes. In particular, the deviations of the Polaris results using the 252g MG library are all within the 2σ interval, except for U-236 which deviates by 2.6σ. The comparison with the reference benchmark provides confidence in the presented methodologies and computational methods.

Table 5. Standard deviations of the results in a reference benchmark [15], and assembly deviations between Polaris/TRITON and CMS5/SNF.

Benchmark	EGUNF*	Polaris 56g	Polaris 252g	TRITON
Parameter	2σ	Δ	Δ	Δ
Void%	0%, 40%, 70%	All nodes	All nodes	All nodes
Years of decay	5	2119	2119	2119
Tc-99	2–3%	1%	1%	4%
Rh-103	2%	2%	2%	3%
Nd-148	1%	1%	1%	0%
Sm-151	13–15%	2%	-4%	-4%
Gd-155	11–15%	-6%	-12%	-14%
U-234	1–2%	3%	-1%	-9%
U-235	1–2%	1%	-2%	-6%
U-236	2%	3%	3%	3%
Np-237	5%	5%	4%	2%
Pu-238	11–13%	12%	6%	5%
Pu-239	5–7%	0%	-2%	-4%
Pu-240	4%	-3%	3%	0%
Pu-241	4–9%	5%	0%	-1%
Pu-242	8–10%	7%	3%	3%
Am-241	5–9%	5%	0%	-1%

* Reference results of the EGUNF benchmark [15].

The deviations in average concentrations of the GE8 are relatively lower than those of GE11 as shown in Table 1, particularly for the plutonium isotopes, U-235, Cm-245 and most of the fission products. The latter assembly is controlled during intermittent exposure intervals, while GE8 is irradiated without a control blade inserted in the vicinity. While the deviations are still within the expected range, the effect of the control blades requires further investigations on a larger number of assemblies exposed to different levels of control blade usage and control blade types.

As shown in Table 1 for the GE8, most of the major and minor actinides are in good agreement. Exceptions for americium and curium isotopes are noted; Am-241 shows slight deviations, while Am-242, Am-242m and Cm-242 are all underpredicted, on average by about 22%. This pattern is also shown when using TRITON, the different SCALE MG libraries, and the nodewise results.

The underprediction could be attributed to the difference in the capture branching fraction in Am-241 to Am-242/Am-242m. In CMS5/SNF, the branching ratio to Am-242m is 13%, while in the SCALE modules it is 10%. With the long decay time, the short-lived Am-242 and Cm-242 reach quasi-equilibrium with the long-lived Am-242m.

The fission products are in good agreement with two exceptions observed for Mo-93 and Sn-121m – which are present with very small concentrations below the cut-off of 0.1 ppm. The reason might be sought in using different nuclear data. In SCALE, the nuclear data for Mo-93 and Sn-121m are from JEFF-3.0, while CMS5/SNF utilizes TENDL-2012-based nuclear data, which highlights the important role of the nuclear data regarding the calculation of this repository-relevant nuclide.

For integral parameters such as the total activity, the short-term results agree between models. However, underprediction that increases with the decay time is observable. The main reason is identified in the decay of Pu-239, which, in SCALE/ORIGEN data, decays directly to the ground state U-235, while the CMS5/SNF accounts for the intermediate short-lived metastable U-235m. Such a discrepancy is not prominent considering that the decay energy is conserved.

As shown in Table 3. for the nodal results, the 1-2% overpredictions of the decay heat in Polaris can be attributed to the major contributors to the decay heat (Am-241 and Pu-238). The models in which these isotopes show larger deviations between the sequences are those using an average exposure history and the 56g MG library in Polaris (as shown in Table 2), resulting in deviations in the decay heat of about 2-5%.

The neutron source shows a trend of overprediction in the middle of the assembly (along with burnup), which goes up to 8% (see Table 3 for nodal values). The trend of overprediction of the neutron source can be directly attributed to the major (α,n) contributors (Am-241 and Pu-238) as well as to the spontaneous fission term contributors (Cm-244 and Cm-246).

As shown in Table 2, using Polaris and the 252g MG library and implementing a detailed exposure history yields comparatively better agreement, particularly for the actinides. The Polaris models that implement cycle-averaged histories deviate in evaluating the minor actinides, while the TRITON models deviate largely in evaluating U-235 (4-11% on average). The results for the fission products also follow the better agreement in the same Polaris models. The use of the coarse 56g MG library misevaluated the Nb-94 and Mo-93 in both Polaris and TRITON compared to the finer 252g library, but with a considerable reduction in computational requirements.

The results of the 23 node-wise models of Polaris show weak trends, except for a peaking neutron source with the burnup. The nodes are distributed over three different lattices and axially varying void fraction. The weak trends in the node-wise deviations agree with the thermal spectral ratios shown in Table 6. The fluxes are integrated over the assembly life in the core and computed for three different axial nodes, as an illustration of the code consistency at different H/U ratios.

Table 6. EOL average flux ratio in nodes of GE8 (0.625 eV group boundary).

Node Number	Flux	Flux Ratio Polaris 252g	 TRITON 252g	 SIMULATE 2g
5	Thermal	0.25	0.21	0.23
13	Thermal	0.19	0.16	0.17
21	Thermal	0.15	0.14	0.14

As shown in Table 5, comparing the results of Polaris using the lattice average properties and irradiation histories to the Polaris-evaluated average concentrations on nodal basis shows inherent deviations related to the former models. The fission products are reproduced within 2% in the lattice-wise models, with the actinides showing relatively larger deviations. The lattice with the largest deviations (particularly for the minor actinides) is lattice 3, which is composed of 12 nodes that are distributed axially over regions of largely varying coolant density. However, the lattices that consist of a smaller number of nodes, particularly lattice 4, show smaller deviations, which suggests that implementing such an approach should be done over fewer nodes avoiding large gradients in the moderator density and largely different burnups. These deviations contribute to the deviations between SCALE modules and CMS5/SNF when comparing the Polaris/TRITON evaluations using single lattice and assembly models. However, the deviations are still comparable to the node-by-node deviations, particularly for the fission products, activity and decay heat.

The results using ORIGEN-ARP show large deviations, particularly for the major and minor actinides. The ORIGEN-ARP models in this study interpolate between lattice-combined transition matrices that are generated using the current TRITON models into the actual average operating conditions of the lattice. The deviations in actinides are attributed to the use of lattice-combined cross-sections instead of the material-specific cross-sections. ORIGAMI (a SCALE module) could utilize the material-specific cross-sections, which would improve the evaluations of the actinides, but the use of ORIGAMI is outside the scope of the present work.

CONCLUSIONS

This work presents comparisons between the SCALE modules Polaris, TRITON and ORIGEN-ARP versus the CMS5/SNF sequence in the evaluation of isotopes relevant for the long-term safety of spent fuel disposal in DGR for decay times up to 100,000 years. Safety-relevant parameters such as decay heat, total activity and neutron source terms are also presented. The sequences are applied to two assemblies irradiated in a Swiss BWR.

The deviations of selected key nuclides with reference to CMS5/SNF compared against the deviations in the reference benchmark of EGUNF in terms of 2 standard deviations show very good consistency for Polaris as well as TRITON.

Overall, the codes and methodologies presented in this paper are in good agreement for most of the safety-relevant isotopes (fission products and actinides) and the integral parameters such as decay heat, activity and neutron source. The spread of the deviations is within the expected range for evaluation of isotopic composition of spent fuel assemblies and the other parameters. Some isotopes have shown near-systematic deviations, namely Mo-93, Sn-121m, Am-242, Am-242m and Cm-242. The SCALE modules underestimate these isotopes relative to the CMS5/SNF sequence, except for Sn-121m which is overestimated. The observed deviations are sought to be attributed to differences in the utilized nuclear data.

TRITON is at a disadvantage in terms of computational requirements and complexity of the inputs, which reduces its suitability for large numbers of spent fuel assemblies, even with the gain in the consistency of the results. ORIGEN-ARP is faster but at a disadvantage in terms of reproducing the actinides. The integrated CMS5/SNF and Polaris are promising in terms of computational requirements and consistency of the results. Further improvements in the computational requirements of Polaris would be helpful, particularly in terms of generating material-specific cross-sections to be utilized in ORIGAMI, which is planned as part of future work and evaluations.

Additionally, the use of different nuclear data highlights the need for further investigation of the individual roles of the material nuclear data in the evaluation of the spent fuel isotopic composition. The validity of using lattice- or assembly-specific models to evaluate the whole assembly isotopic composition as compared to node-wise explicit modeling should be verified with a wider range of assembly designs. Additionally, the effect of the control blades on such evaluations should be investigated and applied to a wide range of assembly and control blade designs.

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