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Recoverable Energy per Fission Discrepancies in NEA FHR Benchmark Depletion Studies

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ABSTRACT

Multiple participants simulated an NEA benchmark problem involving a Fluoride Salt High Temperature Reactor (FHR) assembly. Significant differences between Monte Carlo codes in depletion calculations developed with higher burnup despite past consistencies observed for static cases. In the initial "semi-blind" comparison, the ^{235}U percent difference was observed to be up to 3.5% at 70 GWd/tHM when comparing SCALE6.2.4, OpenMC, and Serpent 2 results - this large difference was found to be due to the recoverable energy per fission used by each code. Benchmark participants were then asked to attempt to modify the recoverable energy per fission to create more consistent results between different codes. Multiple methods of correcting

discrepancies through modification of input power, depletion chain data, or the energy resource in each code was tested. It is observed that for two different benchmark problems, correcting the recoverable energy per fission through modification of the input power produces consistent results up to 30 GWd|tHM. Despite corrections, similarities again diverge midway through the cycle. However, corrections to the energy resource or depletion chain in addition to using a more accurate depletion algorithm in each code was found to result in nearly exact agreement in ^{235}U and very good agreement for other isotopes of interest. Tracking of energy deposition through coupled neutron-gamma simulations was also performed resulting in more a accurate energy deposition and rate of depletion; these results were compared to other codes default energy depletion settings.

KEYWORDS: NEA Benchmark, FHR, Monte Carlo, recoverable energy per fission, depletion

1. INTRODUCTION

The Fluoride salt High Temperature Reactor (FHR) benchmark problem [1] is an OECD-NEA benchmark covering a FLiBe cooled and graphite moderated FHR with a plank type fuel design. Much of the benchmarking work presented so far compared results of static (i.e., no depletion) 2D simulations of this reactor [2] in addition to a variety of sensitivity studies exploring the effect of core parameters [3] on depletion and static results. The presented work covers the time dependent depletion behavior. When performing static cases, there were only minor discrepancies in results between different users using different codes. However, when moving to depletion cases, it was found that the isotopic behavior seemed highly dependent on the code being used with large differences in results, getting larger as the depletion progressed. Further analysis showed strong indications that these differences were attributed to the recoverable energy, E_R, used in each code. Therefore, three separate codes were chosen for further analysis: SCALE6.2.4, OpenMC, and Serpent 2. A brief overview of how each of these codes handles the recoverable energy parameter and other important depletion parameters is now given.

1.1. SCALE6.2.4 Depletion Behavior and Settings

SCALE6.2.4 [4] is a code suite developed and maintained by Oak Ridge National Laboratory (ORNL) and has been historically used for shielding, depletion, criticality safety, and sensitivity analysis. Depletion calculations in SCALE6.2.4 make use of the T6-DEPL sequence which couples the Monte Carlo code KENO-VI with the ORIGEN sequence. The predictor-corrector depletion algorithm in T6-DEPL is dubbed the Ce/CM method and is described in detail by Isotalo [5]. Depletion calculations in the SCALE code system, by default, use values for the recoverable energy that are determined based on the product of the fission and capture cross sections with the fission and capture energy release values, respectively. The energy release values for capture and fission are denoted κ_c and κ_f, respectively. These energy release values are fixed within ORIGEN's source code and are constant hard-wired values that a user has no control of. For commonly depleted isotopes such as ^{235}U, fixed values are applied to $\kappa_{c,i}$ and $\kappa_{f,i}$. However, for more obscure isotopes, default values of 5.0 MeV and 200 MeV are used for the capture and fission energy values, respectively. For benchmarking and inter-code comparisons, modifications must be made to κ_c and κ_f to ensure consistent physics between codes. It is emphasized that the adjustment of the energy resource is by no means an option that an ordinary user of SCALE6.2.4 would have

available. The artificial adjustment is necessary to investigate more meaningful differences in results rather than artificial differences created by a different energy resource.

1.2. OpenMC Depletion Behavior and Settings

OpenMC is an open-source Monte Carlo code originally developed by the Computational Reactor Physics Group at MIT [6]. OpenMC allows the user to choose from a variety of different depletion algorithms with varying accuracy. Depletion calculations in OpenMC use either fixed Q values or variable estimates of the true heating rate. Past work by Romano et al. [7] in the development of OpenMC has shown that disagreement between OpenMC and Serpent 2 depletion results can be mainly attributed to the behavior of probability tables in each code, default recoverable energy values, the use of truncated depletion chains, and the interpolation behavior for determining fission product yields. Different options to address these differences and issues are implemented in OpenMC and no modifications of the source code are necessary to obtain consistent physics between OpenMC and Serpent 2. Depletion results obtained using OpenMC default behavior, modified fission Q values, and coupled neutron-gamma transport are presented for comparison.

1.3. Serpent 2 Depletion Behavior and Settings

Serpent 2 [8] is a Monte Carlo code originally developed at VTT and is widely used for reactor physics analysis. Serpent 2, by default, uses the predictor corrector method dubbed CE/LI by Isotalo and Sahlberg [9]. The default treatment of recoverable energy per fission in Serpent 2 is based on a static value of 202.27 MeV for ^{235}U with other values scaled based on the data library being used and the relative Q values of a given isotope and ^{235}U [10].

1.4. Other considerations for consistent depletion results

Other considerations when performing depletion calculations are related to behavior in each code that a typical user may or may not have the option to modify. Differences between Serpent 2 and OpenMC are discussed extensively by Romano et al. [7] but are now summarized here with the inclusion of SCALE6.2.4 behavior. The first most obvious difference is the depletion chain used and the number of isotopes tracked through depletion and through the transport step of each depletion solver. All codes offer separate options and capabilities. Notably, SCALE6.2.4 uses the “addnux=” option in order to allow a user to increase or decrease the number of nuclides that are tracked throughout each transport simulation while OpenMC offers many different depletion chain options. All results presented use the largest (most complete) depletion chain available. Probability table temperature treatment is another difference that might appear between codes since Serpent 2.1.31 does not offer temperature interpolation treatment in probability tables [7]. Additionally, the interpolation done when determining fission energy yields has an impact on the production of fission products; however, it is noted that all codes are able to create similar behavior by interpolation between fast and thermal fission product yield libraries by using a calculated average energy causing fission. Finally, the capture branching ratios and methods of calculating them used by each code are slightly different. SCALE6.2.4 uses JEFF 3.0 energy dependent branching ratios that are folded into a single energy independent branching ratio. Both OpenMC and Serpent 2 use energy-independent capture branching ratios. OpenMC also offers various different branching ratio options, including options that are identical to the Serpent 2 default branching ratios.

As one would expect, the differences between each codes treatment of E_R and other depletion parameters results in a large difference in produced isotopic results. Therefore, it is necessary to both quantify this difference when ignored and when accounted for through modification of problem power, input, code modification, or postprocessing. The differences can be expected to be minimized by enforcing the use of a similar E_R value in different codes, but one of the objectives of this phase of the benchmark was to first see what differences would result from a standard use of each code with default E_R value and treatment, and then how much that difference can be reduced if as-consistent-as-practical treatment is applied in all codes.

2. RESULTS AND DISCUSSION

2.1. NEA FHR Benchmark, Phase I-B

Phases I-A and I-B of the benchmark consider FHR a single fuel assembly (Figure 1), the former without depletion, and the latter with depletion. Case I-B-1 is the reference full power depletion case, while Case I-B-4 additionally employs burnable absorbers. For more detailed discussion and specification of the benchmark model, see Petrovic et al. [1].

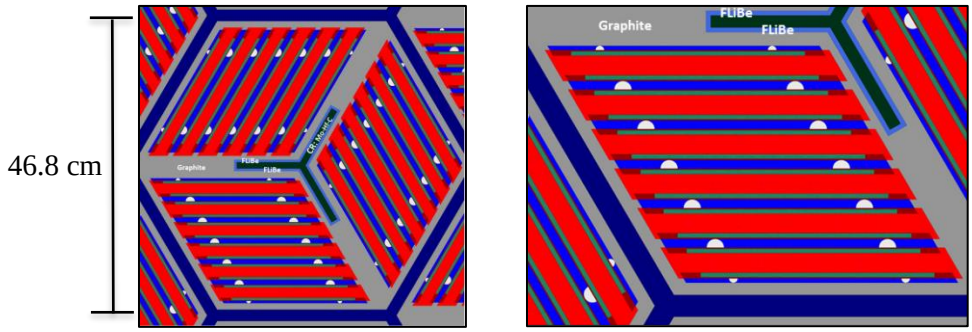

Figure 1. FHR single assembly (left) and assembly "third" (right) with flat-to-flat dimension shown.

2.2. Preliminary Results Before Recoverable Energy per Fission Corrections

Original burnup results as predicted by the three codes are first shown in Figure 2; the results were obtained using a semi-blind analysis. Benchmark specifications were given to participants; then, trivial complications and errors (e.g. simple geometry or material definition mistakes) were corrected in order to accurately preserve methodologies carried out by a typical user in each code. However, no artificial harmonization of results in order to force similar results between codes was performed. Original concentrations of ^{235}U and the relative percent difference of each result to GT-Serpent 2 results are presented for Cases I-B-1 and I-B-4 in Figure 2. The relative difference between OpenMC and Serpent 2 in each model is approximately the same while differences between SCALE6.2.4 and Serpent 2 are slightly different for each model. For this paper, only single-zone depletion is used for both fuel and burnable absorbers. Statistical eigenvalue 1σ

uncertainty for original UIUC results is less than 50 pcm; all other calculations presented in this paper were converged with a maximum eigenvalue uncertainty of 27 pcm.

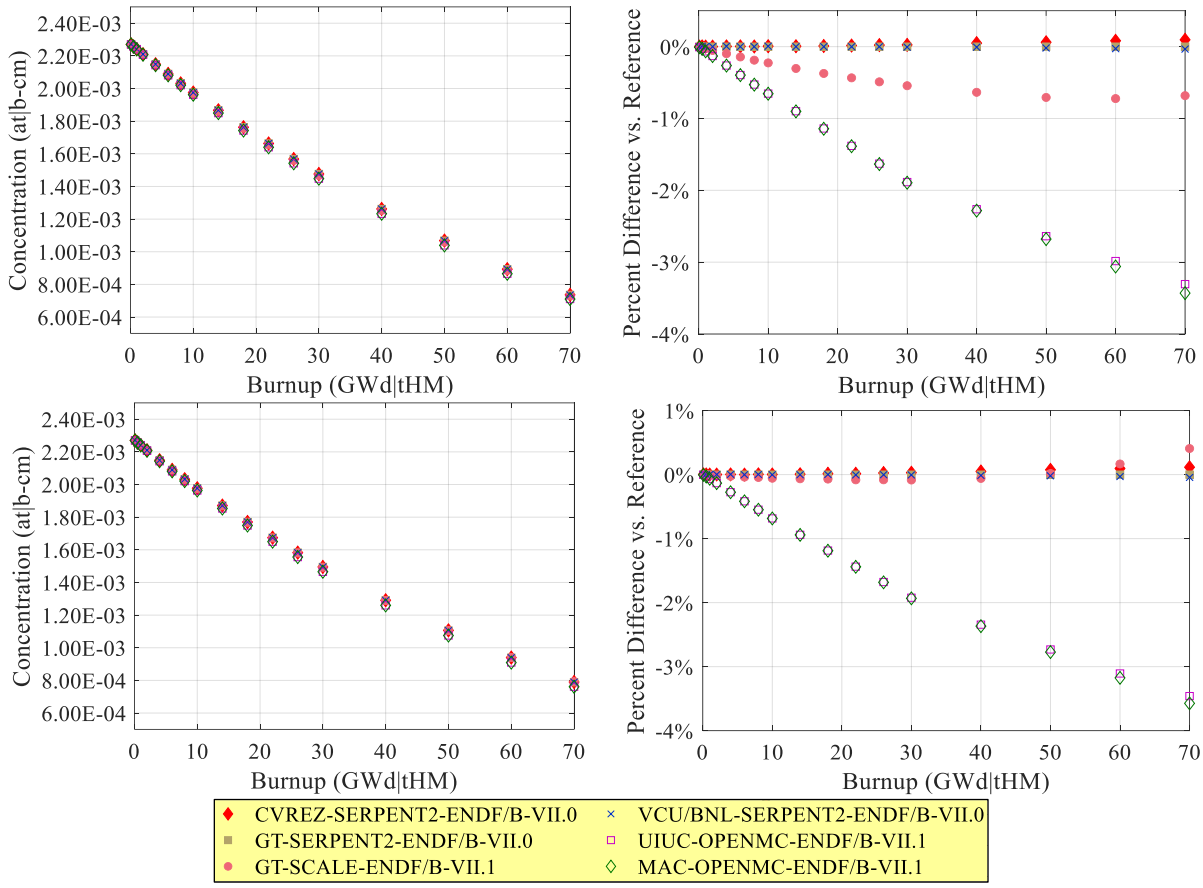

Figure 2. ^{235}U number densities (left column) and percent difference relative to GT-Serpent 2 (right column) before corrections for Case I-B-1 (top) and I-B-4 (bottom).

2.3. Serpent 2 Results after Energy per Fission Correction

Serpent 2 participants were then asked, without prescribing a set methodology, to correct the difference in results that is due to the energy per fission used by each code. VCU/BNL corrected their results by increasing the power density to maintain approximately the same fission rate as OpenMC but with results reported at a scaled burnup in addition to using the newer ENDF/B/VII.1 library. CVREZ corrected their results by modifying the power density from 200 W/g to 190.8 W/g. Then, the values of burnup on the CVREZ x-axis are modified to correct the values to the same burnups as that of OpenMC during postprocessing. Since the results are now offset and being reported at different effective burnup values, the CVREZ, UIUC, and MAC results were then fitted to a 4th order polynomial to make relative comparisons for the full range of results. Corrected values and trends for ^{235}U are shown in Figure 3. For practicality, Serpent results are compared against the average of two (very similar) OpenMC sets of results; while appearing to use one set as a reference solution, this does not imply better accuracy of either OpenMC or Serpent results.

After the corrections, the VCU/BNL results are in close agreement with OpenMC results for the first half of the cycle. The CVREZ results are presented with a modified x-axis in order to make a true comparison and the relative percent difference compared to the OpenMC results strongly follows that of the VCU/BNL trend. Furthermore, it can be observed that the differences between codes mainly increase once the depletion step length increases which presents the possibility that the differences later in the cycle might be attributed to the depletion algorithm used in each code. This behavior and discrepancy will be further discussed and evaluated in the next section.

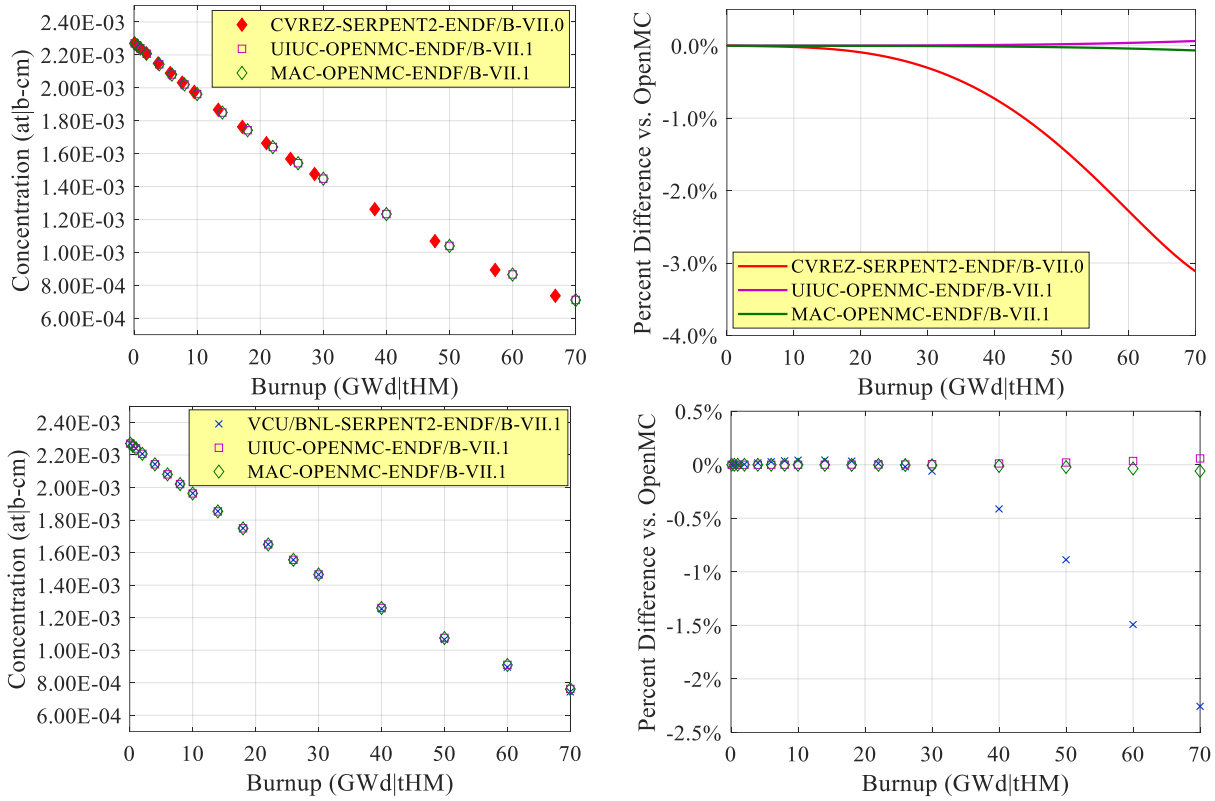

Figure 3. ^{235}U number densities (left column) and percent difference relative to OpenMC (right column) after corrections for Case I-B-1 (top) and I-B-4 (bottom).

2.4. OpenMC and SCALE6.2.4 Results after Energy per Fission Correction

OpenMC participants corrected the energy per fission by modifying the fission Q values in the depletion chain file to match the Serpent 2 recoverable energy treatment. Q values of Uranium and Plutonium isotopes were modified to match the recoverable energy of fission based on the Serpent 2 methodology with E_R values calculated using fission Q values and a reference ^{235}U heating value of 202.27 MeV. In order to match the Serpent 2 depletion rate, SCALE6.2.4 users directly modified the capture energy resource in SCALE's source code such that all values of κ_c were set to zero. Furthermore, the same Q values used by OpenMC were used as SCALE's values of κ_f to create a consistent energy resource between codes. To test whether the predictor scheme originally used by OpenMC was a cause for the difference in results, a modified number of burnup steps as well

as the more accurate LE/QI [9] predictor-corrector scheme was used for Case I-B-1 simulations. The CE/CM predictor-corrector scheme [5], which is different than SCALE's Ce/CM scheme despite the similar name, was used for I-B-4 OpenMC simulations. Since SCALE only uses a Ce/CM scheme, only a single case with modified κ values was performed for I-B-I. The case labels and burnup steps are listed in Table I. ^{235}U comparisons to GT Serpent 2 results for each case are shown in Figure 4 and various isotopes are compared for each case in Tables II and III.

Table I. Simulation cases: Description of the various depletion cases used and their associated algorithms, codes, and burnup steps.

Group-#Steps-Algorithm-Case	Algorithm (Code)	BU Steps (Number of Steps × GWd|tHM)
McMaster-17-PI-B1	Predictor (OpenMC)	1×0.1, 1×0.4, 1×0.5, 1×1, 4×2, 5×4, 4×10
McMaster-34-PI-B1	Predictor (OpenMC)	1×0.1, 1×0.4, 1×0.5, 1×1, 14×2, 16×2.5
McMaster-17-LEQI-B1	LE/QI (OpenMC)	1×0.1, 1×0.4, 1×0.5, 1×1, 4×2, 5×4, 4×10
UIUC-34-PI-B1	Predictor (OpenMC)	1×0.1, 1×0.4, 1×0.5, 1×1, 14×2, 16×2.5
GT-17-CeCM-B1	Ce/CM (SCALE6.2.4)	1×0.1, 1×0.4, 1×0.5, 1×1, 4×2, 5×4, 4×10
McMaster-17-CECM-B4	CE/CM (OpenMC)	1×0.1, 1×0.4, 1×0.5, 1×1, 4×2, 5×4, 4×10
UIUC-17-CECM-B4	CE/CM (OpenMC)	1×0.1, 1×0.4, 1×0.5, 1×1, 4×2, 5×4, 4×10
GT-17-CeCM-B4	Ce/CM (SCALE6.2.4)	1×0.1, 1×0.4, 1×0.5, 1×1, 4×2, 5×4, 4×10

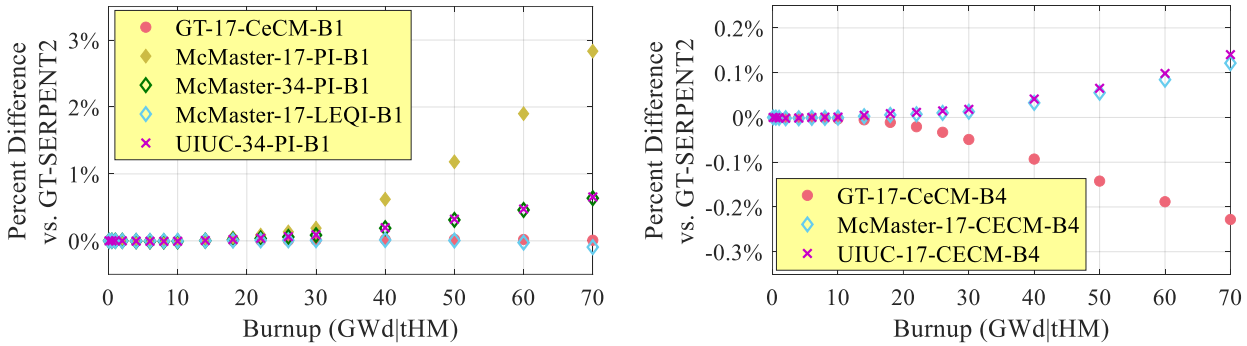

Figure 4. ^{235}U percent difference relative to Original GT-Serpent 2 results for Case I-B-1 (left) and Case I-B-4 (right).

^{235}U differences with corrected recoverable energy from OpenMC were found to still deviate from the Serpent 2 results by greater than 2.5% when using the predictor scheme in Case I-B-1. However, once burnup steps were refined, differences between results are greatly reduced. Using the LE/QI algorithm, the differences reduce even further and the agreement between Serpent 2 and OpenMC is nearly exact. When SCALE6.2.4 κ values are internally modified, the agreement with Serpent 2 is also nearly exact for ^{235}U in Case I-B-1. Also presented in Tables II and III are relative differences for a variety of select isotopes in each different case. The proposed corrections to the energy resource reduce the overall difference from GT-Serpent 2 results for most isotopes.

When depleting with the corrected recoverable energy and the CE/CM scheme, differences were again greatly reduced for OpenMC. For Case I-B-4, SCALE6.2.4 results are seen to behave very differently and there is little improvement in agreement once the energy resource is corrected. It is noted that SCALE6.2.4 Europium results show much better agreement with Serpent 2 once corrections are made but the differences in both the uncorrected and corrected results do raise further questions due to the magnitude of the overall percent difference. OpenMC results become more consistent with Serpent 2 results for ^{153}Eu but there are still significant differences for ^{151}Eu. When comparing ^{151}Eu results between codes, it is found that there is a large spread in results without any strong indications of consistency between codes or even cross section libraries. Since the main driver of original differences was eliminated by using a predictor corrector algorithm with a modified energy resource, the differences seen are believed to be more representative of differences between codes, depletion chains, cross sections, or statistical noise during the transport steps.

Table II. I-B-1 percent differences: Percent differences at end of life compared to GT Serpent 2 results for various isotopes for Case I-B-1 before and after corrections to recoverable energy. Cases marked "Original" are original benchmark results before corrections.

Depletion Case	^{235}U	^{238}U	^{239}Pu	^{240}Pu	^{241}Pu	^{135}Xe	^{149}Sm	^{151}Sm	^{137}Cs
McMaster-Original-B1	-3.43	-0.12	-0.50	0.047	2.77	-0.86	-28.11	-5.72	1.71
McMaster-17-PI-B1	2.83	0.10	0.54	-2.12	-0.20	1.53	1.54	0.21	-2.61
McMaster-34-PI-B1	0.64	0.028	-0.49	-0.09	-0.0053	0.24	-0.32	-0.33	-1.13
McMaster-17-LEQI-B1	-0.14	-0.00029	-0.54	0.21	0.43	-0.068	-0.46	-0.21	-0.59
UIUC-Original-B1	-3.31	-0.13	0.16	0.24	3.17	-0.37	0.53	1.17	1.74
UIUC-34-PI-B1	0.66	0.028	-0.47	-0.012	-0.064	0.22	-0.37	-0.39	-1.13
GT-SCALE-Original-B1	-0.68	-0.050	1.14	1.01	1.67	-0.11	-0.15	-0.31	0.59
GT-17-CeCM-B1	0.0087	-0.027	1.25	0.76	1.37	0.30	0.031	-0.37	0.11
VCU-Original-B1	-0.034	0.0046	-0.082	-0.039	-0.10	0.060	0.010	-0.045	0.0018
CVREZ-Original-B1	0.10	-0.0018	0.084	0.33	-0.064	-0.10	-31.24	-7.38	0.0018

Table III. I-B-4 percent differences: Percent differences at end of life compared to GT Serpent 2 results for various isotopes for Case I-B-4 before and after corrections to recoverable energy. Cases marked "Original" are original benchmark results before corrections.

Depletion Case	^{235}U	^{238}U	^{239}Pu	^{240}Pu	^{241}Pu	^{135}Xe	^{151}Sm	^{151}Eu	^{153}Eu
McMaster-Original-B4	-3.57	-0.17	0.08	0.35	3.80	-0.22	-4.86	-6.47	-4.45
McMaster-17-CECM-B4	0.12	-0.0093	0.12	0.31	1.05	0.53	0.31	7.84	-2.24
UIUC-Original-B4	-3.46	-0.18	0.66	0.46	4.19	0.27	1.82	-8.47	-3.83
UIUC-17-CECM-B4	0.14	-0.010	0.19	0.33	1.03	0.52	0.25	5.30	-2.36
GT-SCALE-Original-B4	-0.29	0.014	1.06	0.13	0.57	0.17	-0.49	-71.41	-22.79
GT-17-CeCM-B4	-0.23	-0.013	0.97	0.34	0.96	0.15	-0.38	13.61	-16.18
VCU-Original-B4	-0.044	0.0055	-0.14	-0.056	-0.11	-0.014	-0.11	-4.57	0.65
CVREZ-Original-B4	0.11	-0.0042	0.15	0.34	0.018	-0.050	-7.07	12.78	0.76

2.5. OpenMC Neutron-Gamma Coupled Depletion

The most accurate method to simulate the depletion of fuel in the infinite assembly is to simulate the gamma energy deposition in a neutron-gamma calculation. The FHR assembly is expected to contain a high fraction of non-fuel energy deposition due to its small volumetric fuel content and large graphite content. Therefore, it is important to quantify the fuel depletion and energy deposition using the most accurate available option. A coupled neutron-gamma simulation using the CE/CM depletion algorithm in OpenMC was therefore performed for Case I-B-1. Since there is no reference solution or other benchmark comparisons, the OpenMC neutron-gamma simulation is used as the reference solution while comparing other McMaster results and SCALE6.2.4 results. The SCALE6.2.4 comparison is made since there is interest to compare how well SCALE6.2.4 depletes when using the default κ_c and κ_f values as the energy resource. Comparisons are made in Table IV. As shown, the ^{235}U depletion rate is nearly identical between the original SCALE6.2.4 simulation and the neutron-gamma simulation. All isotopes except for ^{239}Pu are within 1% difference when compared. SCALE's inclusion of the κ_c values therefore does very well at capturing the correct depletion behavior for the infinite assembly. For a finite problem, gamma particles leaving the core are expected to have a larger impact on the power normalization and subsequent fuel depletion rate depending on core and reactor size.

Table IV. I-B-1 neutron-gamma percent differences: End of life percent difference comparison of various cases to the neutron-gamma coupled depletion calculation in OpenMC.

	^{235}U	^{238}U	^{239}Pu	^{240}Pu	^{241}Pu	^{135}Xe	^{149}Sm	^{151}Sm	^{137}Cs
McMaster-Original-B1	-2.75	-0.09	-0.093	-0.56	1.66	-0.69	-28.17	-5.80	1.85
McMaster-17-LEQI-B1	0.61	0.025	-0.30	0.050	-0.77	0.058	-0.61	-0.41	-0.43
GT-SCALE-Original-B1	0.017	-0.022	1.56	0.40	0.57	0.070	-0.24	-0.39	0.72

3. CONCLUSIONS

Depletion analysis of a plate type FHR assembly, as defined in NEA Benchmark, was performed by SCALE6.2.4, Serpent 2, and OpenMC. The major culprit for the initial differences between results was found to be the recoverable energy per fission used by each code. The magnitude of differences is representative of what a typical user might obtain using default options. Benchmark participants then attempted to correct for differences due to recoverable energy per fission by modifying the power normalization or energy resource in each code or input. Accounting for this difference through power adjustment results in extremely good agreement for U-235 for approximately half of the cycle; the results then diverge as Plutonium builds and recoverable energy per fission changes and as the used depletion steps became longer. Correcting differences by modification of the energy resource in addition to using more accurate predictor-corrector algorithms in each code was seen to result in even better, and in some cases, nearly exact agreement. Despite agreement seen when there was no burnable absorber present, comparisons for SCALE6.2.4 results leave future motivation to further investigate the disagreement seen when there were burnable absorbers present during depletion. The results from this benchmarking study

will be used to support future benchmarking objectives to understand and facilitate eliminating discrepancies between results obtained by various codes used by various users.

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