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ON SCALE VALIDATION FOR PBR ANALYSIS

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ABSTRACT

Studies were performed to assess the capabilities of the SCALE code system to provide accurate cross sections for analyses of pebble bed reactor configurations. The analyzed configurations are representative of fuel in the HTR-10 reactor in the first critical core and at full power operation conditions. Relevant parameters—multiplication constant, spectral indices, few-group cross sections—are calculated with SCALE for the considered configurations. The results are compared to results obtained with corresponding consistent MCNP models. The code-to-code comparison shows good agreement at both room and operating temperatures, indicating a good performance of SCALE for analysis of doubly heterogeneous fuel configurations.

Key Words: pebble bed reactor, cross sections, SCALE, MCNP, HTR-10

1. INTRODUCTION

The development of advanced methods and computational tools for the analysis of pebble bed reactor (PBR) configurations has been a research area of renewed interest for the international community during recent decades. The PBR, which is a High Temperature Gas Cooled Reactor (HTGR) system, represents one of the potential candidates for future deployment throughout the world of reactor systems that would meet the increased requirements of efficiency, safety, and proliferation resistance and would support other applications such as hydrogen production or nuclear waste recycling. In the U.S, the pebble bed design is one of the two designs under consideration by the Next Generation Nuclear Plant (NGNP) Program [1].

The primary challenge in the design and analysis of HTGR configurations is the modeling of the fuel, which has characteristics very different from those of conventional light water reactor (LWR) fuel. The HTGR fuel is composed of a large number of tiny TRISO (tristructural-isotropic) fuel particles embedded in a graphite matrix and shaped into spherical or cylindrical fuel elements. Each fuel particle has a spherical fuel kernel with a radius of about 0.025 cm that is covered by carbon-based layers for a total radius of about 0.045 cm. The fuel element for a PBR, usually referred to as a fuel pebble, is spherical and about the size of a tennis ball. A fuel pebble has a spherical inner fuel zone with a radius of about 2.5 cm that contains the fuel particles in a graphite matrix and is covered by a graphite shell about 0.5 cm thick. The inherent double heterogeneity of such a fuel makes it more difficult to model and requires methods different from those used for a typical LWR fuel. The first level of heterogeneity concerns the random distribution of the large number of fuel particles inside the fuel pebble. The second level of heterogeneity refers to the random distribution of the fuel pebbles inside the reactor core. The reactor core might contain, in addition to fuel pebbles, graphite moderator pebbles of similar size and also randomly distributed throughout the core. The movement of the fuel and moderator pebbles during the reactor operation adds another level of complexity.

Recent improvements in the SCALE [2] code system, developed and maintained by Oak Ridge National Laboratory (ORNL), have focused on addressing the particular needs for the design and analysis of HTGR configurations. As discussed in a later section, improved physics approximations and numerical techniques to perform resonance self-shielding of the cross sections and treat doubly heterogeneous systems [3] have been introduced in the 5.1 release of SCALE. Later, this cross-section processing methodology has been folded into the TRITON depletion sequence [4] in SCALE to permit burnup simulation of doubly heterogeneous fuels [5]. In addition to the development work, there has been an ongoing effort to qualify and validate the SCALE models, methodologies, and associated nuclear data for use with doubly heterogeneous configurations. SCALE has been shown to provide very good results for HTGRs that use a prismatic assembly design; the code system has been benchmarked against measurement data from the start-up core physics tests for Japan's High Temperature Test Reactor (HTTR) [6]. Recently, preliminary results of depletion studies [7] for a conceptual prismatic HTGR fuel assembly have shown good agreement of the system multiplication constant (k_{eff}) as a function of burnup between SCALE 6 and the Monte Carlo burnup code Serpent [8]. Also recently and as presented in another paper at this conference [9], SCALE has been successfully used to model the initial critical core of the HTR-10 PBR that is operated in China; a full core three-dimensional (3-D) SCALE model based on the benchmark specifications as included in the 2009 release of the OECD/NEA International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhE) [10] showed very good agreement with a corresponding consistent MCNP core model, with a difference in k_{eff} obtained with the two codes of 62 ± 34 pcm.

An ongoing study at ORNL is focused on developing nuclear data libraries for use with the ORIGEN-S isotope depletion and decay code [11] in SCALE that are suitable for characterizing the isotopic inventory and radiation source terms for spent fuel from the HTR-10 reactor. Generation of this library will enable enhancing the computational capabilities for analyzing spent fuel discharged from HTR-10 as well as establishing an analysis methodology applicable to analysis of other PBR fuels. As one of the steps for generating highly accurate and reliable burnup-dependent cross sections for ORIGEN, studies were carried out to assess the ability of SCALE to provide accurate cross sections for PBR analysis. The models used for these studies and the results obtained are presented in this paper.

2. COMPUTATIONAL MODELS

Different configurations representative of the HTR-10 fuel are analyzed and two operating conditions are considered: one corresponding to the initial critical core and the other to the full power operating core of the HTR-10. A model representative of the HTR-10 initial core fuel, which consisted of a mixture of fuel and moderator pebbles, consisted of a hexagonal prism containing both fuel and moderator pebbles in a ratio that would conserve the actual ratio of fuel-to-moderator pebbles in the first core. Calculations were carried out for this configuration using SCALE and MCNP5 [12].

At nominal power operating condition, the fuel core includes only fuel pebbles. A configuration consisting of a simple unit cell with a single fuel pebble surrounded by coolant was considered for this condition. This configuration was analyzed with MCNP5 and SCALE at an operating temperature and for a fresh fuel composition. To assess how the results obtained would depend on temperature, the same unit cell was also studied at a temperature of 300 K.

2.1. Configuration typical of first critical core fuel

This model consists of a hexagonal prism containing a mixture of fuel and moderator pebbles in a 53:47 ratio, characteristic of the actual first critical core, with saturated air surrounding the pebbles. The material composition and geometry data are based on the benchmark specifications for the HTR-10 initial core as included in the IRPhE Handbook [10]. The fuel pebble has an inner region of 2.5 cm radius, which includes 8,335 fuel particles in a graphite matrix, and a graphite shell of 0.5 cm thickness. The packing fraction of the fuel and moderator pebbles in the core is 61%. Each fuel particle has a 0.025 cm radius kernel that contains uranium dioxide and is surrounded by four carbon-based layers, for a total outer radius of 0.0455 cm.

This configuration was modeled with both MCNP5 using continuous energy cross sections and with the KENO-VI Monte Carlo transport code in SCALE using 238-group cross section libraries. In both cases, the libraries were based on ENDF/B-VII data at 300 K temperature. The KENO model of the hexagonal fuel cell is illustrated in Fig. 1, which shows the whole cell, the cell at half height, and the pebbles' arrangement in three layers inside the hexagonal prism. This KENO model served as a building block to represent the fuel zone in the 3-D model of the HTR-10 as discussed by Sunny and Ilas [9]. The MCNP model of the hexagonal fuel cell is similar to the model used by Seker and Colak [13]. A cross section of the MCNP5 model at half height of the cell is illustrated in Fig. 2. The MCNP5 model explicitly represents the fuel particles inside the fuel pebbles using a lattice representation that ensures the fuel particles do not intersect the interface of the graphite matrix with the pebble shell. The fuel particles are not explicitly modeled with KENO. However, the doubly heterogeneous nature of the fuel is accounted for through the way the cross sections for the fuel zone inside the pebble are calculated, as further discussed.

(a) hexagonal fuel cell (b) half of fuel cell (c) pebbles' arrangement

Figure 1. KENO-VI model of hexagonal fuel cell.

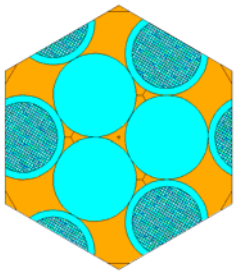


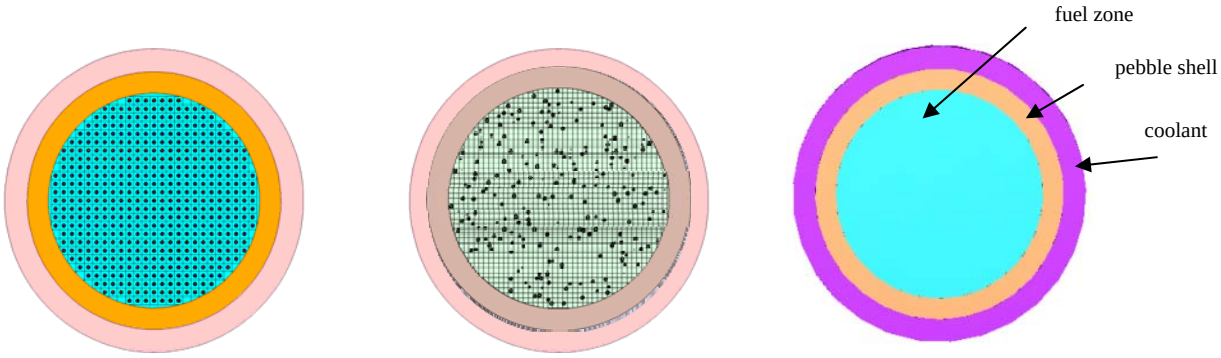
Figure 2. MCNP model of hexagonal fuel cell—cross section at half height.

2.2. Configuration typical of full power core fuel

This configuration is a spherical cell that includes a single fuel pebble surrounded by helium coolant. The radius of the spherical cell, 3.53735 cm, was calculated to correspond to the 61% packing fraction of the fuel pebbles in the core, knowing that there are 27,000 fuel pebbles and no moderator pebbles [14] in the full power core. The geometry and material data for the fuel pebble were the same as used for the first critical core [10]. However, in this case the saturated air coolant was replaced by helium at 861.05 K temperature [14]; the helium atomic density was calculated based on temperature and pressure (3 MPa) values [15].

The configuration is modeled with both SCALE and MCNP5 at a fresh fuel composition of the fuel pebble. The cross sections for fuel pebble materials are considered at 1200 K and the cross sections for the coolant at 900 K, to facilitate a comparison of the results obtained with the two codes. These two temperature values are selected to be close to the actual operating temperatures reported in literature and to be consistent with the temperatures for which cross section data are available with MCNP5.

The single pebble unit cell was modeled with MCNP5 using two approaches for representing the distribution of the fuel particles in the pebble. In the first approach, the fuel particles were modeled as used by Seker [13], as a lattice of particles but avoiding the intersection of the particles with the pebble shell inner surface. In the second approach, the fuel particles were modeled as randomly distributed inside the pebble. The models for the pebble cell are illustrated in Fig. 3.



(a) MCNP5 model 1 (b) MCNP5 model 2 (c) SCALE model

Figure 3. Pebble cell model.

2.3. Modeling doubly heterogeneous fuel in SCALE

The double heterogeneity of the fuel can be modeled in SCALE using the DOUBLEHET option for cross section processing, which combines the treatment of the first level of heterogeneity (fuel particles in the fuel compact—either sphere or cylinder) with the treatment of the second level of heterogeneity (pebbles inside the core for a PBR or cylindrical fuel compacts inside a prismatic fuel assembly for a prismatic HTGR). Though the fuel particles inside the fuel pebble are not explicitly modeled in the pebble unit cell shown in Fig. 3(c), the doubly heterogeneous nature of the fuel is accounted for through the way the cross sections for the fuel zone inside the pebble are calculated, which is illustrated in Fig. 4.

Problem-dependent multigroup cross sections for transport calculations are determined in SCALE using the CENTRM/PMC cross section processing methodology. For fuels with no double heterogeneity, the

CENTRM code solves the 1-D neutron transport equation for a simple building block (such as a fuel pin in an LWR assembly) using pointwise cross sections and calculates the flux solution on a fine grid (about 50,000 to 70,000 points). This flux is used by the PMC code to weight pointwise cross sections for obtaining self-shielded multigroup cross sections for transport calculations with the XSDRNPM (1-D), NEWT (2-D), or KENO (3-D) transport code in SCALE. For doubly heterogeneous fuel, the DOUBLEHET option sequentially applies the CENTRM/PMC methodology to the two levels of heterogeneity of such a fuel. On the first level of heterogeneity, the fuel particles inside the pebble (see Fig. 4), pointwise flux disadvantage factors are calculated and used to generate zone-weighted pointwise cross sections for the homogenized fuel region inside the pebble (radius 2.5 cm). These pointwise cross sections are used on the second level of heterogeneity calculations, the pebble in a lattice of pebbles, to determine with CENTRM the flux distribution that is used then by PMC to determine multigroup problem-dependent cross section data for the fuel element (i.e., pebble).

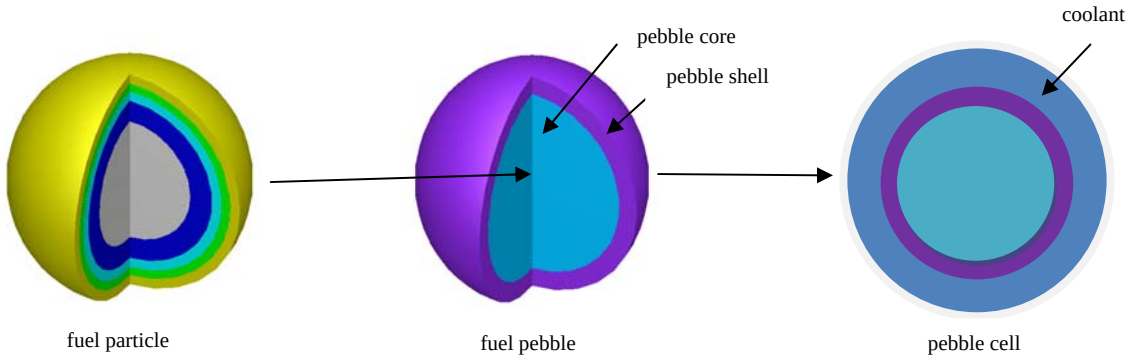


Figure 4. Double-heterogeneity model for cross sections in SCALE.

3. RESULTS

Relevant parameters for the configurations presented in Section 2 were calculated with SCALE and compared to corresponding data calculated with MCNP. The values of the infinite medium multiplication factor (k_{inf}) for the hexagonal prism fuel cell models illustrated in Figs. 1 and 2, as calculated with SCALE (KENO-VI) and MCNP5, are presented in Table I. As seen, the KENO-VI k_{inf} value is within 2 mk (or 0.1%) of the MCNP5 value.

Table I. Comparison of k_{inf} for hexagonal prism fuel cell

Code	Cross section data	k_{inf}	σ	Difference (mk[a])
MCNP5	CE[b] ENDF/B-VII	1.74949	0.00028	
KENO-VI	238-gr ENDF/B-VII	1.75138	0.00017	1.9 ± 0.3

[a] 1 mk = 10^{-3}
[b] continuous energy data

A comparison of the spectral indices and k_{inf} for the pebble cell unit models illustrated in Fig. 3 (a) and (c) are shown in Table II; all cross sections were considered at 300 K for this case. The cross sections from the unit cell calculation were collapsed to a two-group structure to determine spectral indices, with the boundary between thermal and fast energy groups at 0.625 eV. The SCALE values shown in Table II were obtained using a 1-D spherical geometry transport calculation for the flux and eigenvalue solution in

the pebble unit cell; however, the multigroup cross sections in the 1-D transport calculation accounted for the double heterogeneity of the fuel as the DOUBLEHET option was used for cross section self-shielding. Compared with the 3-D detailed MCNP model, the 1-D SCALE model performs remarkably well and, inherent to the approach used for neutron transport, is very fast, requiring about 2 minutes to complete on a single CPU vs. the 9 hours to run MCNP in parallel on 10 CPUs. The difference of the spectral indices in Table II calculated with SCALE compared to the MCNP values as a reference is less than 2%.

Table II. Spectral indices for single fuel pebble cell (at 300 K)

Parameter	Significance	MCNP5 [a]	SCALE	Diff [b] (%)
ρ_{28}	fast-to-thermal ^{238}U capture ratio	8.028 (0.004)	8.159	1.6
$\delta_{25} \times 10^2$	fast-to-thermal ^{235}U fission ratio	11.081 (0.004)	11.048	-0.3
$\delta_{28} \times 10^4$	^{238}U fission to ^{235}U fission ratio	14.117 (0.005)	13.890	-1.6
C^*	^{238}U capture to ^{235}U fission ratio	0.196 (<0.0005)	0.199	1.5
k_{inf}	multiplication constant	1.6596 (0.0001)	1.6553	-0.3

[a] value in parentheses represents the standard deviation
[b] calculated as $100*(value_{SCALE} - value_{MCNP})/value_{MCNP}$

The pebble unit cell total, fission, and absorption microscopic cross sections for ^{235}U and ^{238}U in a four-group structure are shown in Tables III and IV. The four-group structure is as used in the VSOP code [16]. The ^{235}U cross sections are estimated by SCALE within 1% of the MCNP reference, except for those in group 3. The fission cross section in group 3 is underestimated by about 1.7%; note, however, that this group contributes only 4% of the total number of fissions in the system. The largest difference for ^{238}U cross sections is seen for the absorption cross section in group 3 that is underestimated by 1.2%; note that the absorption in group 3 accounts for about 60% of total absorptions in ^{238}U.

Table III. ^{235}U cross sections for single fuel pebble cell (at 300 K)

Group	Upper energy (eV)	σ_{tot} (b)				σ_{fiss} (b)				σ_{abs} (b)			
		MCNP	σ_{MCNP} (%)	SCALE	Diff[a] (%)	MCNP	σ_{MCNP} (%)	SCALE	Diff (%)	MCNP	σ_{MCNP} (%)	SCALE	Diff (%)
1	2 x 10^7	8.86	0.01	8.80	-0.7	1.31	0.01	1.30	-1.0	1.49	0.01	1.47	-0.8
2	1 x 10^5	29.39	0.01	29.36	-0.1	11.81	0.02	11.81	0.0	17.79	0.02	17.78	0.0
3	29.0	73.39	0.02	72.38	-1.4	35.41	0.03	34.81	-1.7	61.91	0.03	60.95	-1.5
4	1.87	342.80	0.03	341.22	-0.5	280.27	0.03	278.98	-0.5	328.62	0.03	327.13	-0.5

Table IV. ^{238}U cross sections for single fuel pebble cell (at 300 K)

Group	Upper energy (eV)	σ_{tot} (b)				σ_{fiss} (b)				σ_{abs} (b)			
		MCNP	σ_{MCNP} (%)	SCALE	Diff[a] (%)	MCNP	σ_{MCNP} (%)	SCALE	Diff (%)	MCNP	σ_{MCNP} (%)	SCALE	Diff (%)
1	2 x 10^7	9.04	0.01	9.05	0.1	1.5E-1	0.03	1.5E-1	-3.2	0.26	0.02	0.25	-2.2
2	1 x 10^5	23.64	0.03	23.98	1.4	2.5E-4	0.28	2.5E-4	0.5	3.96	0.06	4.05	2.2
3	29.0	33.78	0.06	33.89	0.3	2.4E-5	0.10	2.4E-5	1.3	21.29	0.08	21.37	0.4
4	1.87	10.46	0.03	10.40	-0.6	8.9E-6	0.03	8.9E-6	-0.5	1.43	0.03	1.43	-0.5

For assessing the effect of accuracy in the multigroup cross section data on the system behavior, it would be useful to quantify the contribution of particular groups to the system capture, fission, etc. Table V lists this type of information as estimated with the MCNP model illustrated in Fig. 3(a). This facilitates estimating the effect of uncertainty in the cross section for a particular energy group and nuclide to the uncertainty in the analyzed system reaction rates. For example, as the largest contribution to the fission rate in the system is due to thermal neutrons (group 4) fission in ^{235}U (as expected, as this is a thermal system), it is desirable to estimate the fission cross section in this group as accurately as possible. Regarding the contribution of ^{238}U to the total capture in the system, it is seen that the largest contribution is due to neutrons in the intermediate energy range (groups 2 and 3).

Table V. Group contributions to reaction rates in U—single fuel pebble cell (at 300 K)

Group	Upper energy (eV)	Total reaction rate U		Fission rate U [a]	Capture rate U	
		^{235}U (%)	^{238}U (%)	^{235}U (%)	^{235}U (%)	^{238}U (%)
1	2×10^7	1.1	1.2	0.3	0.1	0.1
2	1×10^5	6.9	5.5	4.1	8.4	5.6
3	29.0	5.0	2.3	3.6	10.9	8.7
4	1.87	75.6	2.3	92.0	64.2	1.9
	total	88.7	11.3	100.0	83.7	16.3

[a] fission rate in ^{238}U contributes less than 0.1% to the fission rate in U

The comparison of the results obtained with SCALE and MCNP5 for the single pebble unit cell at operating temperatures is shown in Table VI for spectral indices and in Tables VII and VII for the unit cell cross sections of ^{235}U and ^{238}U, respectively. The differences observed for k_{inf} and spectral indices in this case are consistent with those seen for the same configuration at 300 K. The differences in spectral indices are practically the same at the two temperature conditions, with the exception of δ_{28}, for which the difference is 1.6% larger at operating temperature compared to 300 K. This latter difference is mainly due to the increased underestimation of the ^{238}U fission cross section in the fast energy range at operating temperature compared to 300 K; note that this increased underestimation does not significantly impact the total fission in the system, as the ^{238}U contribution to the total fission rate in the system is less than 0.1%.

Table VI. Spectral indices for single fuel pebble cell (operating temperatures)

Parameter	Significance	MCNP5 [a]	SCALE	Diff [b] (%)
ρ_{28}	fast-to-thermal ^{238}U capture ratio	10.218 (0.006)	10.414	1.9
$\delta_{25} \times 10^2$	fast-to-thermal ^{235}U fission ratio	12.319 (0.004)	12.279	-0.3
$\delta_{28} \times 10^4$	^{238}U fission to ^{235}U fission ratio	14.519 (0.005)	14.058	-3.2
C^*	^{238}U capture to ^{235}U fission ratio	0.254 (<0.0005)	0.258	1.7
k_{inf}	multiplication constant	1.6081 (0.0002)	1.6034	-0.3

[a] value in parentheses represents the standard deviation
[b] calculated as $100*(value_{SCALE} - value_{MCNP})/value_{MCNP}$

With respect to the cross sections comparison, the only cases for which the absolute difference between the SCALE and the MCNP values changes by more than 0.5% are ^{235}U fission in group 1 and ^{238}U absorption in groups 1 and 3. As the contribution of ^{235}U fission or ^{238}U absorption in group 1 to the total fission or absorption rate in the system is negligible, a slightly increased underestimation or

overestimation of the corresponding cross sections would not have significant effect on the system properties. In the case of the ^{238}U absorption cross section in group 3, given that the absorption rate in this group contributes about 2–3% to the total absorption rate in the system, an increased overestimation of this cross section would have some effect on the system behavior. However, the magnitude of the overestimation (SCALE vs. MCNP) is not large, the value being 1.2%. The 238-group flux for the unit cell calculated with SCALE compares well with the corresponding one calculated with MCNP, as illustrated in Fig. 5. The group structure employed to calculate the flux shown in the plot is that used with the ENDF/B-VII 238-group cross section library in SCALE.

Table VII. ^{235}U cross sections for single fuel pebble cell (operating temperatures)

Group	Upper energy (eV)	σ_{tot} (b)				σ_{fiss} (b)				σ_{abs} (b)			
		MCNP	σ_{MCNP} (%)	SCALE	Diff[a] (%)	MCNP	σ_{MCNP} (%)	SCALE	Diff (%)	MCNP	σ_{MCNP} (%)	SCALE	Diff (%)
1	2×10^7	8.87	0.01	8.71	-1.8	1.31	0.01	1.29	-2.1	1.49	0.01	1.46	-1.9
2	1×10^5	29.39	0.01	29.34	-0.2	11.81	0.02	11.79	-0.2	17.79	0.02	17.75	-0.2
3	29.0	73.26	0.02	72.24	-1.4	35.50	0.03	34.86	-1.8	61.81	0.03	60.79	-1.6
4	1.87	242.09	0.04	244.08	-0.8	192.47	0.04	194.20	0.9	228.00	0.04	229.97	0.9

[a] calculated as $100*(value_{SCALE} - value_{MCNP})/ value_{MCNP}$

Table VIII. ^{238}U cross sections for single fuel pebble cell (operating temperatures)

Group	Upper energy (eV)	σ_{tot} (b)				σ_{fiss} (b)				σ_{abs} (b)			
		MCNP	σ_{MCNP} (%)	SCALE	Diff[a] (%)	MCNP	σ_{MCNP} (%)	SCALE	Diff (%)	MCNP	σ_{MCNP} (%)	SCALE	Diff (%)
1	2 x 10^7	9.04	0.01	8.95	-1.0	1.5E-1	0.03	1.4E-1	-5.2	0.26	0.02	0.25	-3.8
2	1 x 10^5	26.46	0.03	26.78	1.2	2.6E-4	0.20	2.6E-4	-0.3	4.95	0.06	5.03	1.8
3	29.0	42.26	0.06	42.69	1.0	3.2E-5	0.08	3.3E-5	1.8	28.27	0.07	28.61	1.2
4	1.87	10.13	0.03	10.16	0.3	6.4E-6	0.04	6.5E-6	0.8	1.04	0.03	1.06	0.8

[a] calculated as $100*(value_{SCALE} - value_{MCNP})/value_{MCNP}$

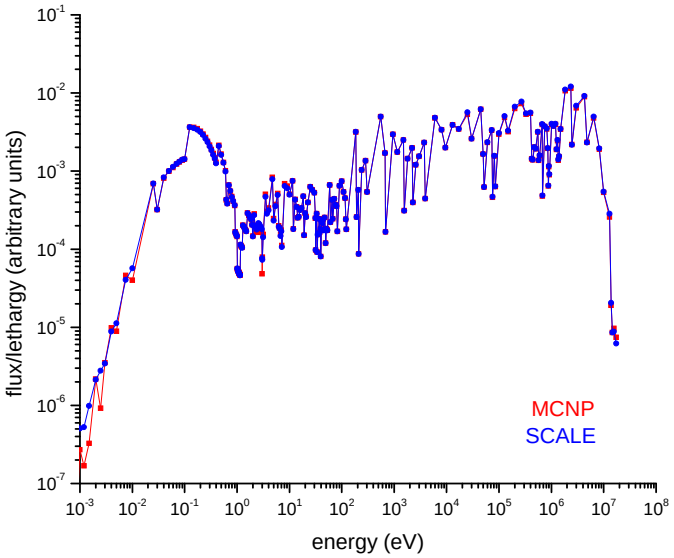


Figure 5. Comparison of 238-group flux for the unit cell (operating temperatures).

Work on studying the effect of fuel particle representation (regular lattice vs. random distribution) on the cross sections for the analyzed configurations is in progress, based on the model illustrated in Fig. 3(c). Currently available results for this model indicate that k_{inf} increases by about 2 mk when the fuel particles are represented as randomly distributed in the graphite matrix; the value of k_{inf} corresponding to the average of ten realizations of the random particle distribution is 1.61028 (σ = 0.00020). The observed difference in k_{inf} is consistent with other results reported in the literature [17, 18, 19]. Progress has also been made on studying the depletion with SCALE of the PBR unit cell configurations discussed in this paper, using both 1-D and 3-D depletion sequences available in SCALE.

4. CONCLUSIONS

Ongoing studies at ORNL are focused on validation of the methods and associated data in SCALE for use in applications involving PBR configurations. As shown previously, SCALE has been successfully benchmarked for the initial critical core of the HTR-10 based on benchmark specifications included in the IRPhE Handbook. Of particular interest at this time is the development of highly accurate and reliable burnup-dependent cross sections for use with the ORIGEN-S isotope depletion and decay code in SCALE which are suitable for characterizing the isotopic inventory and radiation source terms for spent fuel from PBRs. As one of the steps in this direction, work was performed to assess the ability of SCALE to provide accurate cross sections for PBR analysis.

The analyzed configurations discussed in this paper are representative of fuel in the HTR-10 reactor in the first critical core and at full power operation conditions. The material composition and geometry data are based on the IRPhE Handbook benchmark specifications. Relevant parameters—multiplication constant, spectral indices, few-group cross sections—are determined with SCALE for the considered configurations. The results obtained with SCALE are compared to results obtained with corresponding consistent MCNP models. The code-to-code comparison shows good agreement, at both room and operating temperatures, indicating a good performance of SCALE for treatment of doubly heterogeneous fuel configurations.

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