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G. S. Chang
J. R. Parry

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MCNP Super Lattice Method for VHTR ORIGEN2.2 Nuclear Library Improvement Based on ENDF/B-VII

G. S. CHANG and J. R. PARRY
Idaho National Laboratory
Idaho Falls, Idaho 83415 – United States

The advanced Very High Temperature gas-cooled Reactor (VHTR) achieves simplification of safety through reliance on innovative features and passive systems. One of the VHTRs innovative features is the reliance on ceramic-coated fuel particles to retain the fission products under extreme accident conditions. The effect of the random fuel kernel distribution in the fuel prismatic block creates a double-heterogeneous lattice, which needs to be addressed through the use of the newly developed prismatic super Kernel-by-Kernel Fuel (KbKF) lattice model method. Based on the new ENDF/B-VII nuclear cross section evaluated data, the developed KbKF super lattice model was then used with MCNP to calculate the material isotopes neutron reaction rates, such as, (n,γ); (n,n'); (n,2n'); (n,f); (n,p); (n,α). Then, the MCNP-calculated results are rearranged to generate a set of new libraries "VHTRXS.lib," for the ORIGEN2.2 isotopes depletion and build-up analysis code. The libraries contain one group cross section data for the structural light elements, actinides, and fission products that can be applied in the VHTR related fuel burnup and material transmutation analysis codes. The efficiency and ease of use of the MCNP method to generate and update the ORIGEN2.2 one-group spectrum weighed cross section library for VHTR was demonstrated.

KEYWORDS: [VHTR MCNP MCWO ORIGEN2.2 Cross-Section Library]

I. Introduction

ORIGEN2.2[1,2] is one of the most widely used burnup codes for many purposes, such as analysis of transmutation of radioactive waste. It is because of its simple and user friendly input data, rich output file contents, and the existence of data libraries prepared for various reactor systems. However, ORIGEN2 generated one-group spectrum-weighted cross section (SWXS) libraries were mainly developed from the end of 1960's to early 1980's. The libraries in ORIGEN2 are generated from old neutron cross section (XS) libraries such as ENDF/B-IV[3], ENDF/B-V[4], and LENDL[5]. For the helium gas cooled reactor, ORIGEN2 did provided the High Temperature Gas-cooled Reactor (HTGR) and Modular High Temperature Gas-cooled Reactor (MHTGR) one-group SWXS libraries with only one specific ^{235}U enrichment and fuel loading fraction. The ^{235}U enrichment of the HTGRXS and MHTGRXS are 93 and 20 atom density percent (AD%), respectively. The current Very High Temperature gas-cooled Reactor (VHTR) with the ^{235}U enrichment varied from 10 to 20.0AD%. Because the VHTR burnup value of spent fuel has been increased today, suitable libraries for high burnup and different enrichment fuel for the ORIGEN2.2 code are needed. The VHTR one-group SWXS libraries of ORIGEN2.2 code based on the current reactor design are generated using the newest nuclear data file ENDF/B-VII[6] in this paper.

The integrated MCNP method was used to make "VHTRXS.lib based on ENDF/B-VII" one-group spectrum-weighted cross section (SWXS) libraries for VHTRs. The prepared one-group SWXS (in barns) depend upon the local neutron spectrum and the nuclide concentration (self-shielding). MCNP calculates the fuel actinides (ACT), and fission products (FP) one-group SWXS using the heterogeneous fuel kernel neutron spectrum for the ACT and FP. Because the MCNP method can generate the more realistic and softer neutron spectrum in structural light elements (SLE), in this study, the developed one-group SWXS generation method by using MCNP to show the differences of the SLE one-group SWXS based on the different neutron spectrum in a fuel kernel and in the graphite block. The old MHTGRXS set of library in ORIGEN2.2 was chosen as the reference case in this study. The MCNP method calculated one-group SWXS with respect to the fuel kernel and the graphite block neutron spectrum was validated and compared against the MHTGRXS. The MCNP method calculated one-group SWXS with respect to the fuel kernel and the graphite block neutron spectrum with different ^{235}U enrichments, which were validated and compared against each other and the MHTGRXS.lib.

In Section 2, method of development of the VHTR library with the developed MCNP method is presented. The objectives of the improved VHTR libraries based on ENDF/B-VII6 XS data are discussed in Section 3. Also, in Section 3, the updated ^{241}Am and ^{243}Am (n,γ) ground and exited XS data were compared and described. The results

* Corresponding Author, E-mail:gray.chang@inl.gov

and discussion and conclusions are presented in Section 4 and 5, respectively.

II. MCNP Super Lattice Method

The VHTR Kernel-by-Kernel Fuel triangular (KbKF-tri) lattice model[7] used in this study has a compact fuel zone with an outer diameter, OD = 1.261 cm and a helium coolant OD = 1.5875 cm, and is arranged in a unit graphite triangular block as shown in **Fig. 1**. To build the KbKF-hexagonal super lattice model from the triangular unit lattice model, first, the model fuel zone thickness is set to be 0.1356 cm with reflecting boundaries. Note the fuel particle outer diameter is 0.1148 cm. Then, the compact fuel zone (C-matrix) is cylindrically divided into 25 equal-volume shells, such that each sub-shell contains one fuel kernel to maintain a packing factor of 0.25 as shown in the Fig. 1. The pitch (center to center) of the hexagonal fuel channel is 1.88 cm. The graphite compact contains particle fuel kernel density of 10.8 g/cc. The main purpose of the KbKF-hex model is to have the capability to simulate the equilibrium fuel cycle analysis with a different fuel burnup in each of the KbKF-tri lattice. As a result, the MCNP method can use the KbKF-hex super lattice model to generate the burnup dependent XS library in the next phase of the study. The detailed verification of the KbKF-hex supper lattice model is reported in Ref. 7.

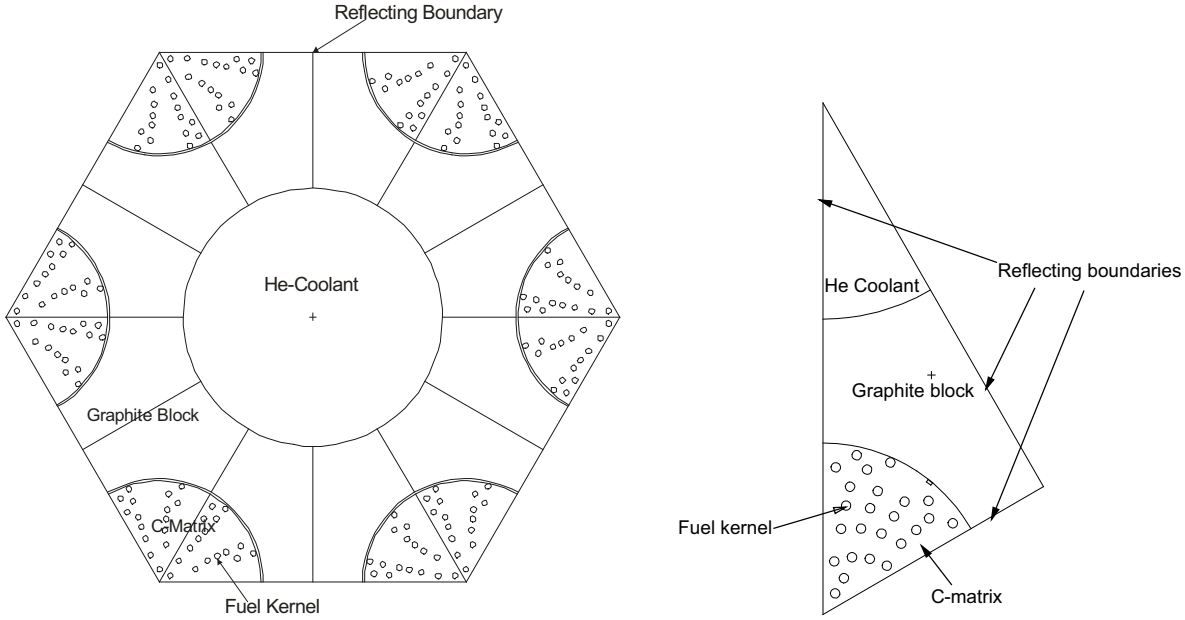

Fig. 1 Cross-section view of the double-heterogeneous super and triangular unit lattice models

The super lattice model consists of 12 triangular unit lattices in a hexagonal fuel block as shown in Fig.1. The major sources of uncertainty in the fuel burnup calculation come from burnup-dependent cross-section (XS), resonance treatment of neutron spectrum vs. fuel enrichment, and minor long-life actinide XS. The verified depletion tool, MCWO[8], (MCNP coupled With ORIGEN2) was used to analyze fuel cycle burnup characteristics. MCWO, which can update the actinide XS at the beginning of each time step, is a UNIX shell script that couples the MCNP and ORIGEN2 computer codes automatically from Beginning of Life (BOL) to End of Life (EOL) without the need for any manual interface. However, the investigation of the fuel burnup dependent XS library is out of the work scope in this paper. We only use a part of the MCWO process modules to convert the MCNP reaction tallies to ORIGEN2.2 one group SWXS library at the beginning of life.

III. VHTR Library Improvement Objectives by MCNP Method

A Data Library for the ORIGEN2.2 Code is compiled by the MCNP method for the current VHTR reactor systems based on ENDF/B-VII XS data. The library of decay constants, the photon spectrum data library and fission yield data are kept the same as in the original MHTGRXS.lib data. The MCNP-calculated reaction rates are integrated over the continuous-energy nuclear data to generate a one-group XS as specified in ORIGEN2.2. For SLE and FP, the MCNP-calculated one-group XS are (n,γ), (n,2n), (n,p), and (n,α). While for the fuel actinides (ACT) the MCNP-calculated one-group XS are (n,γ), (n,2n), (n,3n), and (n,f).

The MCNP-calculated SLE, ACT, and FP cross sections are compiled by the subroutines written in FORTRAN. The photon spectrum data library, constants, branching ratios of radioactive decay, recoverable energy of decay, and direct fission yield data, etc. are inherited from the ORIGEN-2.2

data. The main objective of the generated and improved XS library is to calculate isotopic compositions averaged over fuel and structural assemblies for the VHTR fuel burnup and spent fuel characteristics analysis. The improvements of MCNP method generated one group SWXS library are summarized as: (A) Improving VHTR One Group XS Library based on ENDF/B-VII; (B) Using state of the art KbKF-hex Super Lattice Model; (C) Generating the Graphite Block Neutron Spectrum for SLE SWXS Calculation; (D) Improving ^{241}Am and ^{243}Am Ground and Exited State XS Libraries; and (E) Updating the VHTR XS Libraries on-the-fly. A more detailed discussion of the graphite block neutron spectrum and its comparison with respect to the fuel kernel neutron spectrum is presented in the following.

1. MCNP-generated Fuel Kernel and Graphite Block Neutron Spectrum Comparison

As we know, the neutron spectrum in the structural (ST) graphite block is softer relative to the neutron spectrum (SP) in the fuel (F) kernel as shown in **Fig. 2**. Because the ^{235}U density is quite low, the difference between the F-SP and ST-SP is not quite noticeable. However, it clearly shows that the F-SP is lower than ST-SP at the thermal region. Yet, the F-SP is higher than ST-SP at the fast neutron region. The detailed fraction of the neutron flux 4 energy groups (0.0 < E < 0.625 eV), (0.625 eV < E < 0.1 MeV), (0.1 – 1.0 MeV), and (1.0 – 20 MeV) are summarized in **Table 1**. The fast neutron flux (E > 1.0 MeV) to thermal neutron flux (E < 0.625 eV) (F/T) ratio for the graphite block and fuel kernel for ^{235}U 10, 15, and 20.0AD%, are 0.3315 and 0.3489; 0.3518 and 0.3701; and 0.4658 and 0.4970, respectively. Table 1 consistently shows that the neutron spectrum in fuel kernel is harder than in graphite block.

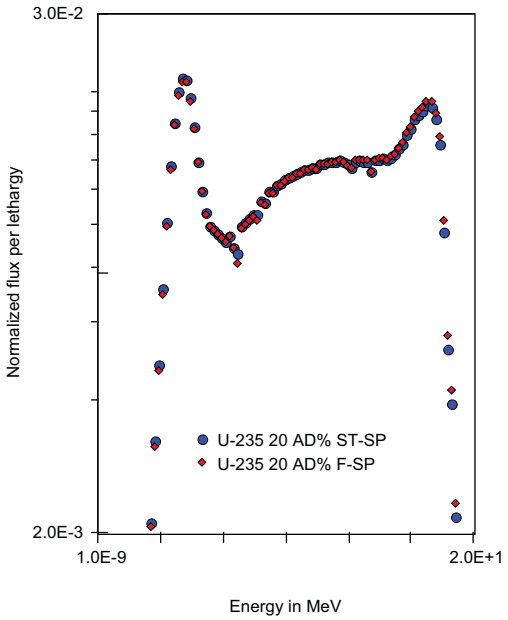

Fig. 2. MCNP-calculated neutron spectrum in fuel kernel and structural graphite block for ^{235}U 20.0AD% case.

Table 1 VHTR super lattice model calculated neutron flux fractions in 4 energy group and Fast (E > 1.0 MeV) to Thermal (E < 0.625 eV) neutron flux ratio

		Neutron flux fractions in 4 energy group				
		0 – 0.625eV	0.625eV – 0.1 MeV	0.1 – 1.0 MeV	1.0 – 20.0 MeV	F/T ratio
U-235 10.0AD%	ST-SP	0.2329	0.5516	0.1383	0.0772	0.3315
	F-SP	0.2301	0.5498	0.1399	0.0803	0.3489
U-235 15.0AD%	ST-SP	0.2230	0.5582	0.1402	0.0785	0.3518
	F-SP	0.2204	0.5566	0.1415	0.0816	0.3701
U-235 20.0AD%	ST-SP	0.1782	0.5880	0.1500	0.0837	0.4698
	F-SP	0.1755	0.5859	0.1514	0.0872	0.4970

IV. Results and Discussion

The ^{235}U enrichment varied from 10 to 20.0AD% is investigated in this paper. To make new libraries for use with VHTRs, the integrated MCNP method was used with the unit fuel lattice model. The one-group SWXS for the nuclides were updated with MCNP-calculated results. MCNP was run in KCODE mode, 100 cycles with 8500 source neutrons on Idaho National Laboratory (INL) High Performance Computing (HPC) workstations with 50 parallel CPUs. This calculation can achieve a one standard deviation (1σ) of less than 0.12% for the (n, γ) reaction tally. For comparison between SWAT and MCNP methods, the following nuclides of interest were chosen: Fe-54, Fe-56, Fe-57, and Fe-58 for SLE, Xe-135 and Sm-149 for SLE and FP; and U-235, U-238, Pu-238 to Pu-243, Am-241 to Am-244 for ACT. As we know, the neutron spectrum in the graphite block is quite soft relative to the neutron spectrum in the fuel kernel. The fraction of the thermal neutron flux ($E < 0.625$ eV) to the fast neutron flux ($E > 1.0$ MeV) for the graphite block and fuel kernel are 1.008 and 0.655, respectively. The SWAT and MCNP calculated one-group (n,γ) XS for the chosen SLE and FP nuclides are tabulated in Table 1.

To make new libraries for use with VHTRs, the integrated MCNP method was used with the KbKF-hex super lattice model. The one-group SWXS for the nuclides were updated with MCNP-calculated results based on the ENDF/B-VII XS data. MCNP was run in KCODE mode, 100 cycles with 8500 source neutrons on Idaho National Laboratory (INL) High Performance Computing (HPC) workstations with 30 parallel CPUs. This calculation can achieve a one standard deviation (1σ) of less than 0.12% for the (n, γ) reaction tally. For comparison of the MCNP method calculated results the following nuclides of interest were chosen: Fe-54, Fe-56, Fe-57, and Fe-58 for SLE, Xe-135 and Sm-149 for SLE and FP; and U-235, U-238, Pu-238 to Pu-243, Am-241 to Am-244 for ACT.

1. New ACT One Group SWXS and MHTGRXS.lib Comparison

The MCNP method calculated ACT new one group (n,γ) and (n,f) XS for ^{235}U 10, 15, and 20.0AD% cases and the original MHTGRXS.lib are summarized in **Table 2**. For the ^{235}U 10, 15, and 20.0AD% cases, due to the ^{235}U self-shielding effect, the (n,f) XS decrease from 64.73, 62.23, and 50.69 barn, respectively. The (n,γ) and (n,f) XS for ^{235}U 20.0AD% case are in a very good agreement with the MHTGRXS.lib. The ^{239}Pu and ^{241}Pu are assumed to be infinitely diluted in a homogenized unit lattice cell in MHTGRXS.lib, the (n,f) XS are 195.9b and 165.0b, which are relatively higher than the (n.f) XS for U-235 20.0AD% of 175.6b and 152.7b in the new VHTRXS.lib, respectively.

2. Selected SLE One Group SWXS on Fuel Kernel and Graphite Block Neutron Spectrum Comparison

Boron-10 commonly exists in the graphite block as an impurity with several ppms in quantity. The depletion of 10B can have impacts on the system Keff. The MCNP method calculated 10B (n,α) for 235U 10, 15, and 20.0AD% cases and the original MHTGRXS.lib are tabulated in **Table 3**. As expected, SWXS on the ST-SP, 10B (n,α) for 235U 10, 15, and 20.0AD% cases decrease from 462.6b, 444.5b, and 359.6b, respectively. If the SWXS on the harder F-SP, the 10B (n,α) for 235U 10, 15, and 20.0AD% cases decrease from 456.2b, 437.9b, and 353.3b, respectively. The 10B (n,α) XS in MHTGRXS.lib is 401.5b, which is about 13.6% higher than the corresponding 235U 20.0AD% case.

The MCNP method calculated Fe and Gd (n,γ) for 235U 10, 15, and 20.0AD% cases and the original MHTGRXS.lib are summarized in **Table 4**. Fe is the most commonly used structural material in the reactor system. The MCNP method calculated Fe (n,γ) reaction shows a consistently decreasing XS for 235U 10, 15, and 20.0AD% cases. Fe SWXS on the F-SP for the 235U 20.0AD% case shows a good agreement with respect to the original MHTGRXS.lib XS.

Gd is commonly used in the reactor as a burnable absorber. The MCNP method calculated Gd (n,γ) reaction also shows a consistently decreasing XS for 235U 10, 15, and 20.0AD% cases. Gd SWXS on the F-SP for the 235U 20.0AD% case shows a good agreement with respect to the original MHTGRXS.lib XS. However, 155Gd and 157Gd excited (n,γ) XS for 235U 10.0AD% agrees better with the original MHTGRXS.lib, which is not consistent with respect to the Fe SWXS comparison.

Table 2 MCNP-calculated (n,γ) and (n,f) for 235U 10, 15, and 20.0AD% cases compare to MHTGRXS.lib.

		U-235 10.0AD%		U-235 15.0AD%		U-235 20.0AD%		MHTGRXS.LIB	
	Isotope ID	(n, γ) barn	(n,f) barn	(n,γ) barn	(n,f) barn	(n, γ) barn	(n,f) barn	(n, γ) barn	(n,f) barn
U	922350	15.33	64.73	14.93	62.23	12.99	50.69	13.55	51.70
	922360	13.01	0.24	13.19	0.24	13.59	0.25	16.80	0.07
	922370	55.99	0.43	53.86	0.44	44.50	0.45	46.25	0.53
	922380	3.73	0.03	3.80	0.03	3.98	0.03	12.22	0.03
	922390	13.31	2.56	13.15	2.43	12.82	1.91	3.72	1.54
	922400	47.90	0.03	48.27	0.03	48.49	0.03	0.54	0.07
Np	932350	5.87	0.00	5.80	0.00	5.44	0.00	16.92	0.00
	932360	23.19	385.40	22.41	369.90	18.79	297.70	0.00	230.50
	932370	57.42	0.22	56.78	0.22	52.58	0.24	60.55	0.21
	932380	53.43	246.50	51.29	236.60	41.38	191.00	18.29	177.60
	932390	21.07	0.23	20.93	0.24	20.14	0.25	11.34	0.43
Pu	942360	12.90	51.88	12.75	51.30	12.40	49.08	24.81	25.28
	942370	62.12	255.40	59.53	245.50	47.55	199.40	49.19	206.70
	942380	45.48	2.51	43.43	2.46	34.33	2.25	32.57	2.02
	942390	133.60	221.40	129.30	213.90	107.00	175.60	122.90	195.90
	942400	378.20	0.32	374.00	0.32	367.40	0.33	381.90	0.35
	942410	74.64	195.20	71.98	188.10	58.57	152.70	57.74	165.00
	942420	48.02	0.17	48.39	0.17	48.63	0.18	56.45	0.17
	942430	18.57	37.80	18.32	37.27	16.78	34.09	17.49	35.58
	942440	4.81	0.00	4.74	0.00	4.94	0.00	4.52	0.14
	942450	17.55	0.00	17.55	0.00	17.55	0.00	17.55	0.00
Am	952410	200.20	1.52	195.50	1.49	169.80	1.33	191.20	1.32
	952421	189.50	984.50	181.10	941.50	141.70	739.50	159.50	798.20
	952420	38.76	346.50	37.45	333.30	31.05	270.30	20.13	179.90
	952430	3.94	0.23	3.97	0.23	3.91	0.24	4.24	0.15
	952441	73.61	292.60	70.92	281.90	58.12	231.00	0.00	147.20
	952440	80.01	314.90	76.89	302.70	62.36	245.80	0.00	211.50
Cm	962410	29.73	309.20	28.54	296.80	23.03	239.60	5.71	0.49
	962420	6.44	0.41	6.43	0.40	6.30	0.34	8.38	0.34
	962430	19.98	126.80	19.46	123.90	17.05	110.70	15.50	140.50
	962440	27.45	0.57	27.79	0.57	28.33	0.57	28.33	0.77

Table 3 The MCNP method calculated ^{10}B (n,α) for ^{235}U 10, 15, and 20.0AD% cases and the original MHTGRXS.lib comparison

		U-235 10.0AD%	U-235 15.0AD%	U-235 20.0AD%	MHTGRXS.LIB
	Isotopes	(n,α) barn	(n,α) barn	(n,α) barn	(n,α) barn
Boron-10 XS weighted on ST-SP					
	50100	462.6	444.5	359.6	
Boron-10 XS weighted on F-SP					
	50100	456.2	437.9	353.3	401.5
		U-235 10.0AD%	U-235 15.0AD%	U-235 20.0AD%	MHTGRXS.LIB

Table 4 Fe and Gd (n,γ) for ^{235}U 10, 15, and 20.0AD% cases and the original MHTGRXS.lib Comparison

		U-235 10.0AD%	U-235 15.0AD%	U-235 20.0AD%	MHTGRXS.LIB
		(n, γ) barn	(n, γ) barn	(n, γ) barn	(n, γ) barn
Fe XS weighted on STR-SP					
	260540	0.281	0.271	0.222	
	260560	0.321	0.309	0.253	
	260570	0.311	0.300	0.247	
	260580	0.186	0.182	0.160	
Fe XS weighted on F-SP					
	260540	0.278	0.267	0.218	0.212
	260560	0.317	0.305	0.249	0.268
	260570	0.307	0.295	0.243	0.233
	260580	0.184	0.180	0.157	0.122
Gd XS weighted on ST-SP					
	641520	94.790	91.560	76.230	
	641530	807.000	761.000	558.500	
	641540	17.770	17.500	16.180	
	641550	2649.000	2499.000	1836.000	
	641560	5.139	5.165	5.411	
	641570	11260.000	10610.000	7735.000	
	641580	3.260	3.286	3.364	
	641600	0.540	0.541	0.532	
	641610	0.371	0.371	0.371	
Gd XS weighted on F-SP					
	641520	92.630	89.300	74.070	162.800
	641530	789.100	741.800	542.800	0.000
	641540	17.620	17.370	16.120	13.480
	641550	2592.000	2438.000	1785.000	2757.000
	641560	5.114	5.108	5.374	3.770
	641570	11020.000	10350.000	7523.000	11720.000
	641580	3.246	3.271	3.386	1.795
	641600	0.533	0.537	0.528	0.371
	641610	2851.000	2851.000	2851.000	2851.000

3. 241Am and 243Am Ground and Exited State One Group XS Comparison

The Monte Carlo fuel burnup analysis codes, such as, MCWO and MOCUP9, which are developed at Idaho National Laboratory (INL) did not update the ^{241}Am and ^{243}Am excited state XS in fifth column of the original MHTGRXS.lib XS format. The one group XS library format is (n,γ); (n,n'); (n,2n'); (n,f); Exited state XS (fifth column). By definition, the exited state XS is the ratio of Exited XS / (Exited and Ground XS) (exR) multiply by the MCNP-calculated (n,γ) XS. The exR for ^{241}Am and ^{243}Am in the original MHTGRXS.lib are 0.11 and 0.95, respectively. MCNP-calculated (n,γ) reaction rate is the sum of the ground and exited state XS. If we do not treat the fifth column XS – exited state (n,γ) XS properly, we will over-estimate the ^{241}Am and ^{243}Am (n,γ) transmutation rate. The MCNP-calculated ^{241}Am and ^{243}Am (n,γ) XS and the original MHTGRXS.lib exited state XS are tabulated in **Table 5**. It is interesting to see that the excited XS of the U-235 15.0AD% case agrees better with the original MHTGRXS.lib.

Table 5 MCNP-calculated ^{241}Am and ^{243}Am (n,γ) and the original MHTGRXS.lib exited state XS

		Exited state XS (barn)			
		U-235 10.0AD%	U-235 15.0AD%	U-235 20.0AD%	MHTGRXS.LIB
Am	952410	24.74	24.17	20.99	23.63
	Exited XS ratio	0.11	0.11	0.11	0.11
Am	952430	74.87	75.41	74.28	80.50
	Exited XS ratio	0.95	0.95	0.95	0.95

V. Conclusion

The set of new libraries for ORIGEN2.2 code "VHTRXS.lib" was developed based on ENDF/B-VII using the latest VHTR core parameters. To make new libraries for VHTR, the integrated MCNP method code was used adopting the KbKF-hex supper lattice model. The improvement of the new VHTRXS.lib by MCNP method is clearer.

The MCNP method used in this study can handle the complex spectral transitions at the boundaries between the fuel kernel, graphite block, and helium coolant in a straight-forward manner and treat the entire super lattice at once. The results from this study indicate that the MCNP method has good agreement with respect to the original MHTGRXS.lib. The MCNP method can calculate the neutron SWXS in fuel kernels and the graphite block efficiently, which can improve the SLE one group SWXS by 2%. Because of the very simple streaming process in compiling the MCNP method calculated reaction tallies into one group SWXS ORIGEN2.2 library, the method can be used to generated a new specific fuel design and burnup dependent SWXS on-the-fly. The same MCNP method approach to accurately calculate the ORIGEN2.2 one group SWXS can also be used in the Advanced Fuel Cycle Initiative (AFCI), Reduced Enrichment for Research and Test Reactors (RERTR), and Advanced Gas-cooled Reactor (AGR) fuel research and development programs.

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