VVER AND RBMK CROSS SECTION LIBRARIES FOR ORIGEN-ARP

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Introduction

An accurate treatment of neutron transport and depletion in modern fuel assemblies characterized by heterogeneous, complex designs, such as the VVER or RBMK assembly configurations, requires the use of advanced computational tools capable of simulating multi-dimensional geometries. The depletion module TRITON [1], which is part of the SCALE code system [2] that was developed and is maintained at the Oak Ridge National Laboratory (ORNL), allows the depletion simulation of two- or three-dimensional assembly configurations and the generation of burnup-dependent cross section libraries. These libraries can be saved for subsequent use with the ORIGEN-ARP module in SCALE. This later module is a faster alternative to TRITON for fuel depletion, decay, and source term analyses at an accuracy level comparable to that of a direct TRITON simulation.

This paper summarizes the methodology used to generate cross section libraries for VVER and RBMK assembly configurations that can be employed in ORIGEN-ARP depletion and decay simulations. It briefly describes the computational tools and provides details of the steps involved. Results of validation studies for some of the libraries, which were performed using isotopic assay measurement data for spent fuel, are provided and discussed.

Cross section libraries for ORIGEN-ARP

Methodology

The TRITON capability to perform depletion simulations for two-dimensional (2-D) configurations was implemented by coupling of the 2-D transport code NEWT with the point depletion and decay code ORIGEN-S. NEWT solves the transport equation on a 2-D arbitrary geometry grid by using an S_N approach, with a treatment of the spatial variable that is based on an extended step characteristic method [3]. The flux solution from the transport calculation serves for updating, at each depletion step, the effective cross sections used by ORIGEN-S in the depletion calculation. The nuclide composition provided by ORIGEN-S is applied to a subsequent transport calculation, and the process continues in an iterative manner until all the depletion steps are simulated. At the end of each NEWT transport calculation, weighted cross sections and fluxes are obtained, which are subsequently used in the COUPLE code to calculate one-group effective cross sections required in the ORIGEN-S calculations. More details on the components, functionality, and capabilities of TRITON can be found in Ref. [4].

The cross sections used in the NEWT transport calculation in this work were from a SCALE 44-group ENDF/B-V transport library; the BONAMI and NITAWL modules were used to correct the cross sections for temperature and resonance effects. Note that the current default option for resonance self-shielding treatment in SCALE 5.1 is CENTRM/PMC. CENTRM is a code that solves the transport equation in a one-dimensional (1-D) cell by using a combination of point-wise and multigroup cross section data, and provides a quasi-continuous problem-dependent energy flux spectrum; this flux is used by the PMC module to generate self-shielded multigroup cross sections for the transport calculation. However, the CENTRM/PMC methodology was not used for the work reported in this paper due to limited experience with its use for reactor operating conditions.

The ORIGEN-ARP sequence in SCALE includes a Windows graphical user interface and permits the user to create and execute depletion and decay cases with minimal effort, and to generate tables and plots showing the calculated data in a fast and user-friendly fashion. ORIGEN-ARP has three main components: (1) the ARP code to interpolate on a set of pre-generated burnup-dependent cross sections to obtain cross sections for use with ORIGEN-S; (2) the ORIGEN-S code to perform depletion and decay simulations; and (3) the OPUS/PlotOPUS codes to extract and plot

the calculated results. The interpolation in ARP, which is based on Lagrange polynomials, can be carried out in the case of a uranium dioxide fuel for three interpolation parameters: burnup, fuel enrichment, and moderator density.

The main computational steps used in this work to obtain the cross sections for use with ORIGEN-ARP consisted of the following. (1) For each unique assembly configuration, and for combinations of discrete values of enrichment and moderator density, TRITON depletion simulations were carried out for a given number of depletion steps to generate burnup-dependent cross sections for use with ORIGEN-S. (2) The number of cross sections sets in each library file was reduced by using the ARPLIB utility code in SCALE, in order to decrease the library size; the thinning of a library file was performed by removing the cross section data for those burnup points in the range where the cross sections exhibit a slow variation with burnup.

VVER assemblies

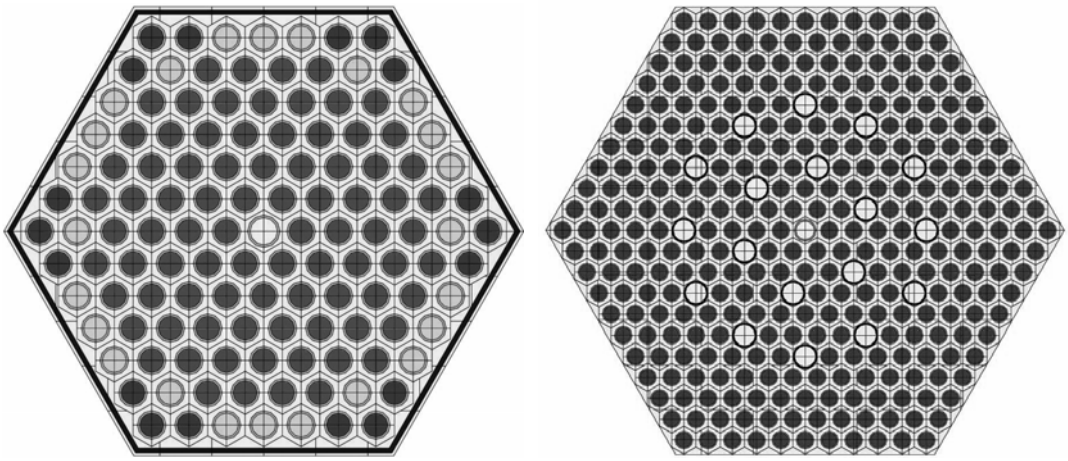
The generation of the VVER libraries was carried out to provide data for modern assembly designs that are currently used in the nuclear industry. The cross section libraries, which are briefly described in Table 1, were created for five representative VVER assembly configurations—one VVER-1000 and four VVER-440 configurations—and cover a burnup range up to 70.5 GWd/MTU. The burnup values corresponding to data in each library are 0, 1.5, 4.5, 7.5, 10.5, 13.5, 16.5, 31.5, 46.5, 58.5, and 70.5 GWd/MTU.

Three of the four VVER-440 configurations are characterized by an enrichment zoning with an assembly average enrichment of 3.82, 4.25, and 4.38 wt % ^{235}U; two of these designs contain burnable absorber rods. The other VVER-440 design considered is characterized by a flat enrichment; in this case, libraries were generated for three enrichment values: 1.6, 2.4, and 3.6 wt % ^{235}U. The VVER-1000 libraries were generated for six fuel enrichment values: 1.5, 2.0, 3.0, 4.0, 5.0, and 6.0 wt % ^{235}U. A core-average value of 0.75 g/cm^3 was used for the moderator density in all cases. The level of detail in the TRITON models is illustrated in Figure 1 for a VVER-440 assembly design with 3.82 wt % ^{235}U average enrichment and also for a VVER-1000 design. The detailed assembly data and reactor operating data used to generate the libraries can be found in the SCALE 5.1 manual.

The VVER libraries previously released with SCALE 5.0 were generated using the 1-D depletion sequence of SAS2. The former VVER-440 libraries were shown in a previous study to provide sufficiently accurate results for actinides as compared to measured isotopic assay data [5].

Table 1. Description of the VVER libraries for ORIGEN-ARP in SCALE 5.1

Assembly design	Name of library	Enrichment profile	Enrichment value(s) (wt % ^{235}U)
VVER-440	vver440(3.6)	flat	1.6, 2.4, 3.6
VVER-440	vver440(3.82)	zoned	average 3.82
VVER-440	vver440(4.25)	zoned	average 4.25
VVER-440	vver440(4.38)	zoned	average 4.38
VVER-1000	vver1000	flat	1.5, 2.0, 3.0, 4.0, 5.0, 6.0



(a) VVER-440 (3.82) (b) VVER-1000

Figure 1. TRITON models for VVER assemblies.

RBMK assembly

The RBMK libraries were generated based on design data representative of the Chernobyl Unit 4 reactor. They were obtained by using a TRITON model as illustrated in Figure 2 that shows a single fuel assembly and surrounding graphite moderator. The assembly fuel rods are surrounded by coolant water within a zirconium cylindrical container in the graphite moderator. The coolant water also acts as a moderator. The RBMK libraries developed are representative of the average assembly. For illustrative purposes, the model in Figure 2 distinguishes between the inner and outer rings of fuel rods to illustrate that separate libraries representative of either the inner or outer fuel can be created in addition to those representative of the average assembly.

Cross sections for a burnup range up to approximately 25 GWd/MTU were generated for each combination of values from a set of fuel enrichments and coolant densities. In contrast to a VVER reactor, for which the use of an average coolant density is sufficiently adequate given its small variation axially, the RBMK configuration has a boiling water coolant and therefore an axial void-fraction profile. Libraries were prepared for three enrichments (1.8, 2.0, and 2.2 wt % ^{235}U) and six coolant densities (0.15, 0.28, 0.41, 0.54, 0.67, and 0.80 g/cm^3). The libraries were provided for fresh fuel (zero burnup) and for twenty other burnup values between 0.625 and 24.375 GWd/MTU with a burnup step of 1.25 GWd/MTU.

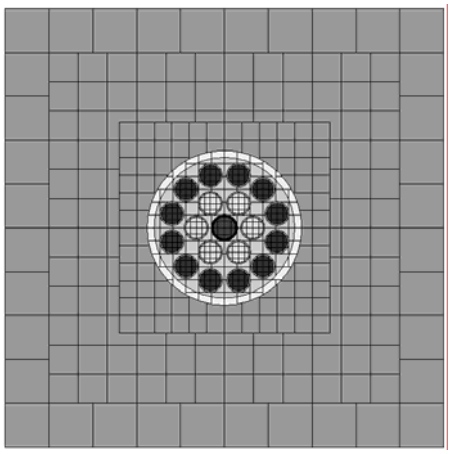


Figure 2. TRITON model for RBMK assembly.

Validation studies

Validation studies of the libraries were performed by comparison to available experimental data from selected isotopic assay measurements for VVER and RBMK spent fuel.

VVER libraries

Validation studies for the VVER libraries were carried out by using isotopic assay measurement data for spent fuel from experiments performed at the Khlopin Radium Institute (KRI) in Russia [6,7,8]. The measured samples included in the present analysis were selected from VVER-440 and VVER-1000 fuel assemblies that were irradiated in reactors operated at the Novo-Voronezh and Kalinin nuclear power plants. The initial fuel enrichment was 3.6 wt % ^{235}U and 4.4 wt % ^{235}U for the samples from VVER-440 and VVER-1000 fuel, respectively. In both cases, a flat enrichment was modeled. The analysis in this work included twenty VVER-440 fuel samples with burnups in the range 20–43 GWd/MTU and thirteen samples from VVER-1000 fuel with burnups between 14 and 52 GWd/MTU. Note that the reported burnup values were determined based on measured values of three burnup monitors: ^{148}Nd, $^{145+146}$Nd, and ^{137}Cs. The decay time, from discharge to the time the measurements were performed, was about 3 to 4 years in the case of the VVER-440 fuel samples and between about 7 and 10 years for the VVER-1000 fuel samples. However, the measured nuclide concentrations were back calculated or adjusted and reported at discharge time. The isotopes for which measurement data are available include ^{234,235,236,238}U, ^{238,239,240,241}Pu, ^{237}Np, ^{243}Am, ^{244}Cm, ^{148}Nd, and ^{137}Cs. The last five of these nuclides were not measured in all samples. In particular, ^{137}Cs was not measured in the VVER-440 fuel samples, and ^{237}Np was not measured in any of the VVER-1000 samples.

Simulations with ORIGEN-ARP were carried out for each of the 33 samples considered by using the libraries generated as described earlier in this paper. The only information available with respect to the irradiation history of the samples consisted of the total irradiation time and the reported sample burnup. The power used in simulations was calculated as a ratio of the sample burnup to the total irradiation time. For simulation purposes, the total irradiation time was divided into cycle lengths of 100 to 200 days, and cross section values were updated in each cycle. No information was available with respect to the initial concentration of ^{234}U and ^{236}U in fuel; these values were approximated based on the initial enrichment [9]. The results of the comparison of the predicted and the measured nuclide concentrations are summarized in Table 2 and illustrated in Figures 3 and 4 for the VVER-440 and VVER-1000 cases, respectively. For each measured isotope, an average (mean value) over all measured samples of the calculated-to-experimental concentration ratio (C/E) is shown in Table 2, along with the corresponding relative standard deviation (RSD).

Table 2. Comparison of calculated and measured nuclide concentrations for VVER

	VVER-440			VVER-1000		
	# samples	$(C/E)_{avg}$	RSD (%)	# samples	$(C/E)_{avg}$	RSD (%)
^{234}U	20	0.89	4.3	13	0.91	18.1
^{235}U	20	1.04	5.1	13	0.93	6.5
^{236}U	20	1.00	1.7	13	0.97	3.2
^{238}U	20	1.00	0.1	13	1.00	0.2
^{238}Pu	20	0.95	6.5	13	0.83	14.7
^{239}Pu	19	1.06	5.3	13	0.95	9.5
^{240}Pu	20	1.04	3.5	13	0.96	7.6
^{241}Pu	19	1.03	4.4	13	0.95	13.0
^{242}Pu	20	1.07	6.5	13	0.99	13.5
^{237}Np	10	1.18	23.6			
^{243}Am	19	1.33	13.7	7	1.08	24.7
^{244}Cm	19	1.17	16.7	7	0.93	24.9
^{148}Nd	6	0.98	1.5	7	1.05	8.8
^{137}Cs				10	1.01	2.4

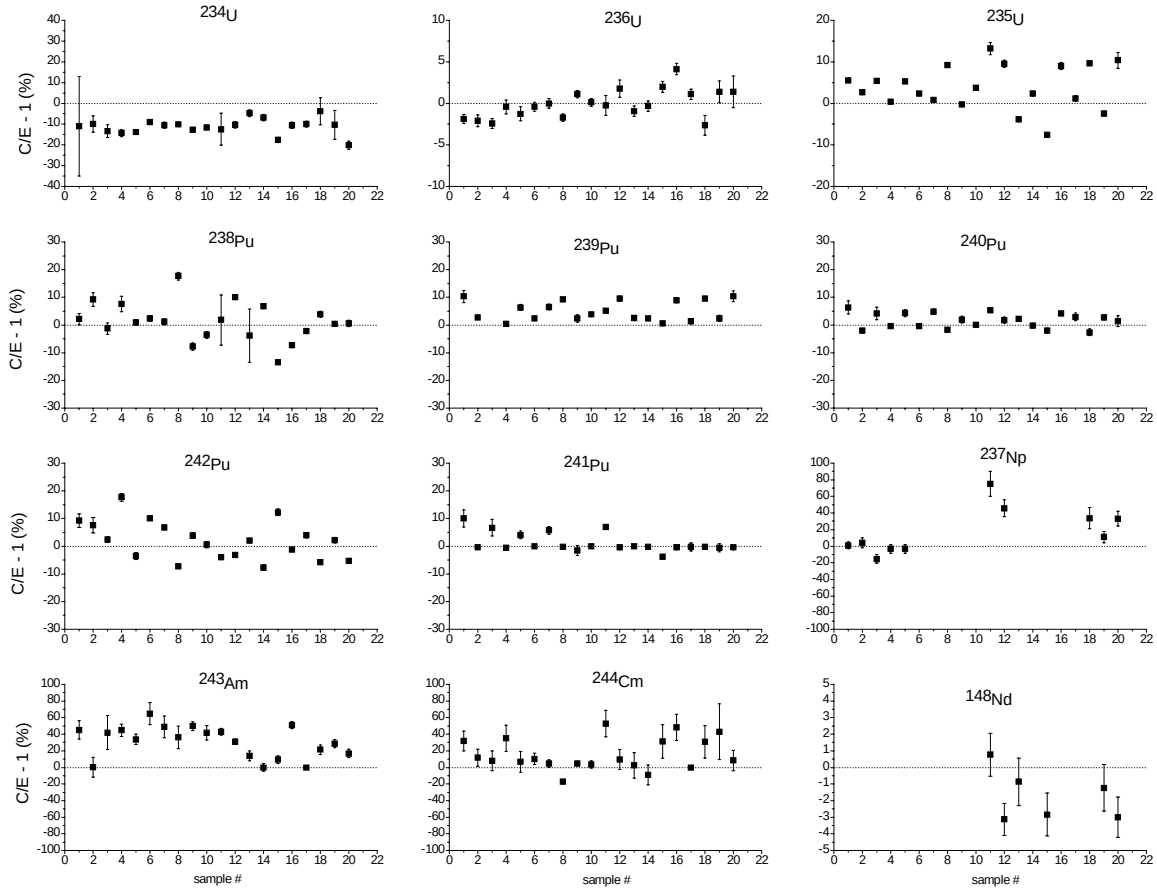


Figure 3. Comparison of calculated and measured isotopic data for VVER-440 samples.

The results of the comparison show good agreement between calculations and measurements, especially if one accounts for the fact that these libraries were generated for typical configurations and are representative of the assembly as a whole. The user needs be cautioned that the use of these libraries for simulations of single fuel pins located in an environment with physics characteristics that are not similar to those of the average assembly, such as stronger absorption (i.e., close to gadolinia-bearing pins), may not be appropriate. In such particular cases, depending on the accuracy level desired, the user may generate cross-section libraries for specific fuel locations in an assembly by following the procedure explained in detail in the SCALE manual.

As shown in Table 2 and illustrated in Figure 3, the VVER-440 results for uranium nuclides are good, with ^{235}U overpredicted by 4% on average and ^{236}U calculated within less than 1% of measurement. With the exception of ^{238}Pu, which is underestimated by 5%, the other plutonium nuclides are overpredicted, with the overestimation values in the range 3 to 7%. The minor actinides ^{237}Np, ^{243}Am, and ^{244}Cm are overpredicted by 18%, 33%, and 17% on average, respectively (a large variation around the mean value is observed for these isotopes), whereas the burnup-indicator nuclide ^{148}Nd is underestimated by 2%.

Note that the effects of the irradiation history details on the calculated concentration were not accurately accounted for, as detailed irradiation data were not available. Also, eight of the twenty samples of VVER-440 fuel (identified by numbers 1 to 5, 10, 11, and 20 in the plots in Figure 3) were selected from fuel pins located at the edge of the assembly, and therefore subject to more moderation than the average pin in the assembly. In the case of some isotopes, it is the contributions of these peripheral pins that cause the C/E ratio of all twenty samples to be overestimated; for example, the C/E averaged over the eight peripheral pins for ^{235}U and ^{239}Pu is 7%

and 10%, respectively. In assessing the performance of the libraries, one must also account for the reported experimental uncertainties, because these uncertainties can be significant for some isotopes that are difficult to measure. In the cases studied here, the average reported measurement errors (1σ) for the minor actinides ^{237}Np, ^{243}Am, and ^{244}Cm were 7%, 6%, and 10%, respectively.

In the case of the VVER-1000 comparison, as shown in Table 2 and illustrated in Figure 4, the agreement is also good. All major actinides except for ^{238}U are underpredicted. The minor actinides ^{243}Am and ^{244}Cm are on average predicted within 8% of the measured values. Note that for these two isotopes, as compared to the measurements for the VVER-440 fuel samples, the reported experimental uncertainties are smaller: 7% and 4% on average, respectively. The important major actinides ^{235}U and ^{239}Pu are underestimated on average by 7% and 5%, respectively. This underestimation can be correlated to the overestimation of the burnup-indicating isotope ^{148}Nd, which is underpredicted by 5% on average, suggesting that the reported burnup for these samples may be too large. An alternative computational approach would be to adjust the reported burnup value to be used in calculations such that the calculated ^{148}Nd concentration is consistent with the measured value, and in this way the total number of fissions in the calculation is consistent with that corresponding to the measured ^{148}Nd. Unfortunately, ^{148}Nd measurement data was not reported for all samples.

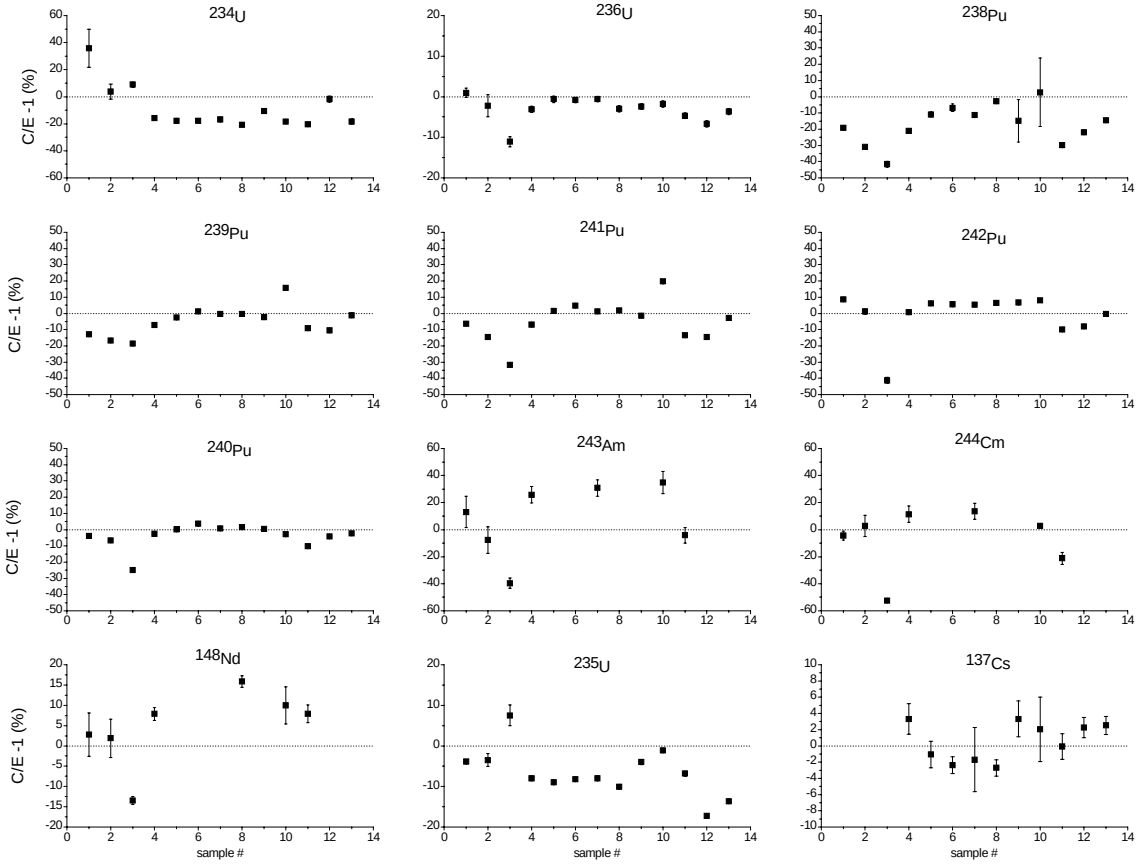


Figure 4. Comparison of calculated and measured isotopic data for VVER-1000 samples.

RBMK libraries

The performance of the RBMK libraries was assessed by comparison of calculations to isotopic assay measurement data for spent fuel. The experimental data used for this study are results of measurements performed by KRI [10,11] on spent fuel samples selected from ten RBMK-1000 assemblies irradiated in reactors operated at the Leningrad nuclear power plant. A set of fifteen

spent fuel samples were considered for this comparison. The samples had initial enrichments of 1.80, 2.00, 2.02, and 2.09 wt % ^{235}U, and reported burnups in the range 6–23 GWd/MTU. The measurements carried out at KRI included uranium, plutonium, curium, americium, cesium, and neodymium isotopes, and the measured concentrations were adjusted by calculation and reported at discharge time. No detailed information on the irradiation history was available, but the total irradiation time, the sample burnup, and the axial height of the sample along the fuel rod were available. The coolant density was not available and was estimated as described in Ref. [11].

The results of the calculation-experiment comparison are summarized in Table 3, which shows for each nuclide the number of samples measured, the average C/E ratio, and the corresponding RSD. As observed from the table, the major actinides are well predicted. The important major actinides ^{235}U and ^{239}Pu are predicted on average within 2% of the measurement. The curium nuclides ^{242}Cm and ^{244}Cm are predicted within 10%. The difference seen for ^{243}Am is quite large; it is suspected that this discrepancy is largely due to difficulties in the measurements. The average reported experimental error (1σ) for ^{244}Cm and ^{243}Am is about 10%. It also needs to be noted that the estimated values for the coolant densities are probably subject to significant uncertainties, as no actual data were available and estimations were made based on data for typical BWR axial void profiles and not for the actual RBMK configuration.

Table 3. Comparison of calculated and measured nuclide concentrations for RBMK

Nuclide	# samples	C/E_{avg}	RSD (%)	Nuclide	# samples	C/E_{avg}	RSD (%)
^{234}U	15	0.96	24.1	^{242}Pu	15	1.15	21.5
^{235}U	15	0.98	8.7	^{237}Np	15	0.79	32.8
^{236}U	15	0.90	20.3	^{243}Am	14	1.67	124.1
^{238}U	15	1.00	0.5	^{242}Cm	14	0.90	29.9
^{238}Pu	15	0.83	21.4	^{244}Cm	14	0.90	30.2
^{239}Pu	15	0.98	8.7	^{137}Cs	13	1.03	4.0
^{240}Pu	15	1.07	10.1	^{148}Nd	15	1.04	3.7
^{241}Pu	15	1.05	10.6				

Conclusions

VVER-440, VVER-1000, and RBMK-1000 cross section libraries for ORIGEN-ARP have been generated using the 2-D depletion module TRITON of the SCALE code system. Four assembly configurations were considered for the VVER-440 design, one with a flat enrichment and three with a more modern design characterized by enrichment zoning and the presence of burnable absorbers. One assembly configuration was considered in the case of the VVER-1000 or RBMK design. The ORIGEN-ARP libraries cover burnups up to approximately 70.5 GWd/MTU in the case of the VVER design and 25 GWd/MTU in the case of the RBMK design. The VVER libraries are included in the recent release of the SCALE 5.1 code system. Validation studies of the libraries were performed by comparison to isotopic assay experimental data for spent fuel. These studies showed good agreement between the measured data and the ORIGEN-ARP results.

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