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ORIGEN-ARP Cross-Section Libraries for the RBMK-1000 System

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Nuclear Science and Technology Division

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ABSTRACT

This report describes the generation of RBMK-1000 cross-section libraries for use with the ORIGEN-ARP isotope burnup and decay code. The work was performed for the International Atomic energy Agency (IAEA) to support characterization and safeguards of irradiated nuclear material from the Chernobyl Unit 4 reactor using gamma-ray signatures of fission products in the materials. Although the libraries are based on the Chernobyl Unit 4 reactor design, they are applicable to other RBMK systems, and can be used to predict the uranium, plutonium, higher actinide, and fission-product inventories in the spent fuel. The ORIGEN-ARP code sequence allows rapid simulation of reactor burnup by using reactor-specific and burnup-specific cross-section libraries that are prepared in advance using detailed reactor-analysis codes in the Oak Ridge National Laboratory (ORNL) Standard Computation Analysis for Licensing Evaluation (SCALE) system. The simulation model used in developing the libraries was validated by comparing its predictions with the results of laboratory nuclide-assay studies on RBMK-1000 spent fuel that were carried out by Russian researchers. The assay studies were performed on isotopes of uranium, neptunium, plutonium, americium, curium, cesium, and neodymium. This work was supported by the U. S. Department of Energy, International Safeguards Project office under IAEA support task USA-A931 (POTAS Task A.252).

1. INTRODUCTION

With ORIGEN-ARP (1) one can carry out rapid simulations of reactor burnup by using reactor-specific and burnup-specific cross-section libraries that are prepared in advance. These types of calculations apply to a particular reactor configuration and therefore do not require a full reactor-analysis simulation for every burnup scenario. However, one must first prepare cross-section libraries for the reactor configuration using the more detailed reactor-analysis codes contained in the Oak Ridge National Laboratory (ORNL) Standard Computation Analysis for Licensing Evaluation (SCALE) system. A large variety of reactor-specific libraries have been prepared in this manner for use with ORIGEN-ARP. In this work we describe the preparation of burnup cross-section libraries for the RBMK-1000 system. In preparing these RBMK-1000 cross-section libraries, ORNL performed simulation studies that allowed comparisons to nuclide-assay measurements on spent-fuel samples from a Russian RBMK-1000 reactor (Leningrad Nuclear Power Plant). The assay work was performed at the Khlopin Radium Institute in St. Petersburg, Russia. These assay studies cover isotopes of uranium, neptunium, plutonium, americium, curium, cesium, and neodymium. The comparisons serve as calibrations on the models used to generate the cross-section libraries.

The RBMK libraries are intended for use with ORIGEN-ARP. The libraries were generated using the TRITON/NEWT two-dimensional burnup-simulation code that is part of the ORNL SCALE-5 system. RBMK units have not been studied to any great extent with the SCALE system at ORNL, although a small modeling effort involving the use of SAS2 was undertaken during a workshop held at ORNL. SAS2 is designed to handle reactors such as the common pressurized-water reactor (PWR) and boiling-water reactor (BWR) configurations, although it has been used to model Magnox and advanced gas-cooled reactors and was deemed to be reasonably successful in those efforts (2). Nevertheless, SAS2 performs best with pin-cell configurations that are common to U. S. reactor types. With the availability of a code such as TRITON, a considerably truer rendition of the geometry of the RBMK is possible.

2. DESCRIPTION OF THE RBMK

Data and descriptions for RBMK design and operation were obtained from numerous sources. Many of the choices in the simulations described here were made using data that combined information gleaned from these multiple sources. References 3 and 4, cited in the reference section at the end of this report, are two generally useful sources on the RBMK. Helpful information was also obtained from personal communications with Ludovic Bourva and Victoria Pratt in the Department of Safeguards at the International Atomic Energy Agency (IAEA), Vienna (5). A description of the analysis of RBMKs using SAS2 was also found to be useful in determining values for dimensions and operational parameters (6). Useful information was obtained in personal communications with Arturas Plukis at the Institute of Physics in Vilnius, Lithuania (7).

The RBMK-1000 system uses uranium oxide fuel and has a graphite-moderated water-cooled core. The water-cooled fuel assemblies are contained in vertical channels in the graphite moderator. Figure 1 shows a single assembly with its surrounding graphite moderator. The reactor core itself is cylindrical with a diameter of 11.8 m and a height of 7.0 m. The central portion of the core is fueled and the periphery acts

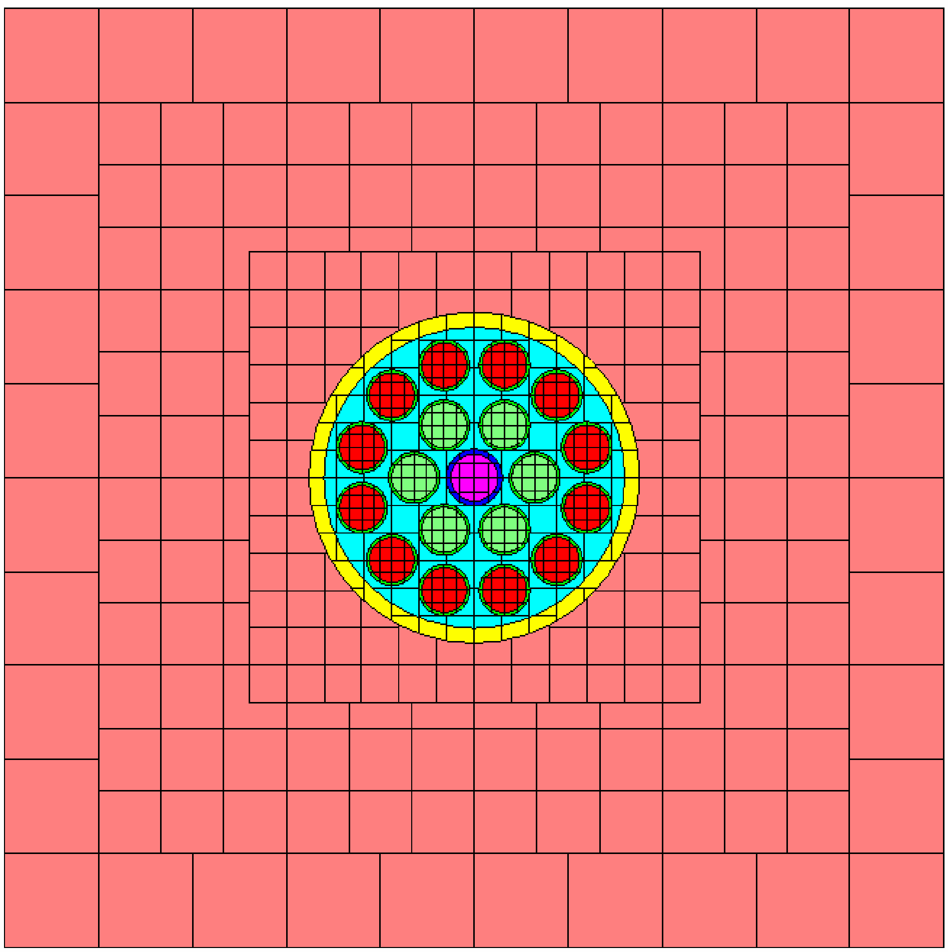

Fig. 1. TRITON/NEWT model for one RBMK assembly containing a central carrying rod, 6 inner fuel rods and 12 outer fuel rods and surrounded by a 4-mm thickness of clad plus the graphite moderator.

as a reflector. Above and below the active core there is 0.5 m of graphite reflector. There are 2488 vertical columns of 25- by 25-cm graphite blocks. There are 1661 channels in the core that contain fuel assemblies. The central (i.e., non-reflector) part of the core contains 1884 channels. The 1661 channels that are fueled are referred to as "technological channels," whereas the rest of the channels in the central part of the core are referred to as "control channels."

A fuel assembly contains 18 zirconium-alloy-clad UO_2 fuel rods. As can be seen in Fig. 1, the fuel rods are located on two concentric rings and there is a central carrying rod. When using the TRITON module one can distinguish between the inner and outer fuel rods. The central rod can be of solid metal, but more likely, it is hollow and does not contain water. The light-water coolant enters at the bottom of the assembly and flows up through the assembly. It begins to boil at about 2.5 m from the bottom of the active fuel zone, and at the top of the active fuel zone the average steam quality is 14.5%. As the name implies, the RBMK-1000 is a 1000 MW(e) core and is rated as slightly greater than 3000 MW(t). Although most of the reactor's thermal energy originates in the fuel rods, about 6% is generated in the graphite moderator. When at normal operating power, the average temperature of the graphite is about 873 K.

Table 1 gives design parameters for the RBMK-1000. All dimensions that apply to the assembly and core construction are exact values. Temperatures, however, are considered to be typical and can vary. The fuel pellets have a density of 10.4 g/cc. The pellets are chamfered and there is a gap between the outside of the pellet and the inside of the cladding. Each fuel rod consists of two 3.43 m segments of fuel pellets with an empty region between them. These two segments cover a total height of 7.0 m. The effective fuel density was determined by assuming that the fuel material is evenly distributed over the volume to the inside of the cladding (i.e., no gap) and over the active fuel length.

Because the cooling water boils, there will be a void-fraction profile along the vertical axis of the assembly. In this way, the RBMK has some similarity to a BWR. Cross-section libraries should therefore be prepared for a range of coolant densities. The effective axially-averaged cooling-water density for a currently operating RBMK is about 0.5 g/cc, but the libraries should allow the user to choose densities from a range of possible values. Of course the graphite provides the bulk of the moderation, but the cooling water is close to the fuel pins and its moderating effect is not insignificant.

Another version of the RBMK exists. It is known as the RBMK-1500 and is rated at 1500 MW(e). Many of its characteristics are similar to the RBMK-1000. It is likely that the libraries developed here could be applied to the RBMK-1500. However, more representative libraries for the RBMK-1500 could be produced using the models developed here with some modifications to the input parameters.

Table 1. Design parameters for the RBMK

Fuel pin	
Fuel pellet radius (cm)	0.575
Fuel pellet density (g/cc)	10.4
Effective fuel density (g/cc)	9.393
Clad inner radius (cm)	0.5975
Clad outer radius (cm)	0.68
Clad density (g/cc)	6.45
Clad composition (wt %)	Zr: 98.97; Nb: 1.0; Hf: 0.03.
Core height/bottom to top of fuel. (cm)	700
Active fuel length (cm)	2 by 343
Central tube	
Inner radius (cm)	0.625
Outer radius (cm)	0.75
Tube density (g/cc)	6.45
Tube clad composition (wt %)	Zr:97.47; Nb:2.5; Hf:0.03
Assembly	
Outside radius (cm)	4.4
Clad thickness (cm)	0.4
Assembly clad composition (wt %)	Zr: 97.5; Nb: 2.5.
Radius of outer fuel pin circle (cm)	3.101
Radius of inner fuel pin circle (cm)	1.605
Fuel Temperature (K)	1005
Coolant temperature (K)	560
Graphite temperature (K)	873
Graphite density (g/cc)	1.65
Maximum coolant density (g/cc)	0.757

3. COMPARISON CHECKS WITH THE TRITON RBMK MODEL

The Khlopin Radium Institute in St. Petersburg has reported on the analysis of spent-fuel samples from a group of RBMK-1000 assemblies (8). In all there were 41 spent-fuel samples, and we have chosen a subset of 15 of these to study. These 15 samples represent a range of burnup values and have initial enrichments of 1.80, 2.00, 2.02, and 2.09 wt%. Twelve of the fifteen samples were obtained from pins in an outer fuel ring with the remaining three samples being from inner-ring fuel pins. Table 2 lists some details about the samples. In the table, the samples are listed in order of increasing burnup. The columns of the table refer respectively to the Khlopin Institute sample number, enrichment, estimated coolant density, inner/outer sample ring, irradiation (burn) days, power, and burnup. The axial positions of the assayed samples were available, and the moderator density was therefore separately estimated for each simulation. In line with the operating criteria described above, the coolant was assumed to start boiling at 2.5 m above the bottom of the active fuel zone and the steam quality at the top of the fuel rod was assumed to be 14.5%. These facts are also reflected in a report from the Slavutych Laboratory of International Research and Technology (9). Reference 9 reports a coolant density of 0.423 g/cc at the top of the channel, and on this basis, a cooling water density profile was developed. The profile is shown in Fig. 2. The shape of the profile over the part of the fuel rod where the water is boiling was developed from examples of BWR void profiles supplied with Swedish BWR data used at ORNL in decay-heat validation studies (10). We would caution that estimates of coolant density are probably subject to more uncertainty than are most other input data. This is particularly the case towards the top of the coolant channel.

Table 2. Details of the 15 RBMK-1000 spent fuel samples

Sample no.	^{235}U Enrichment (wt %)	Coolant density	Sample ring	Burn (days)	Power MW/t	Burnup GWd/t
20	2.00	0.45	outer	278	20.91	5.81
25	2.00	0.45	inner	278	25.05	6.96
41	2.09	0.44	inner	1233	7.59	9.36
11	1.80	0.42	inner	1390	6.78	9.43
28	2.02	0.43	outer	1413	6.75	9.54
9	1.80	0.50	outer	1010	11.45	11.56
32	2.02	0.76	outer	1413	11.24	15.89
36	2.09	0.46	outer	1233	14.14	17.43
1	1.80	0.45	outer	1684	10.36	17.45
39	2.09	0.76	outer	1233	14.83	18.28
26	2.00	0.76	outer	1281	16.69	21.38
19	1.80	0.72	outer	1591	13.77	21.91
6	1.80	0.76	outer	1685	13.42	22.62
18	1.80	0.72	outer	1462	15.95	23.31
31	2.02	0.76	outer	1413	16.61	23.47

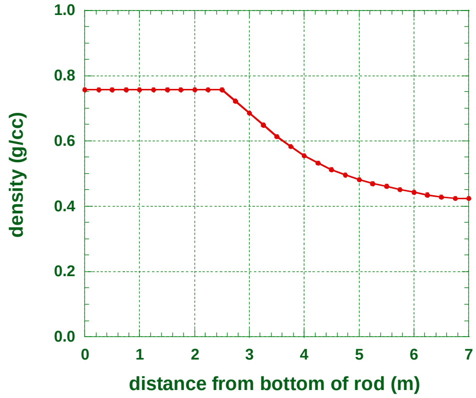

Fig. 2. Profile used to determine effective coolant densities for the assay samples.

For most of the samples, the Khlopin Institute reported concentration values for ^{237}Np; ^{137}Cs; and isotopes of uranium, plutonium, americium, curium, and neodymium. The measurements reported by the Khlopin Institute were for the end-of-irradiation date. Some concentration values were not reported for some of the samples, but in most cases, nuclides with significant concentrations were reported. The figures that follow (Figs. 3–9) show concentration values versus burnup for some of the more important species. Measured values are identified separately from values determined by simulation. For some nuclides, concentration values depend significantly on the initial enrichment, and in such cases, we indicate separate trend lines versus burnup for samples with different initial enrichments. Fuel-rod-averaged burnup estimates were supplied along with the sample data. The individual sample burnup values used in the simulations were determined by matching the concentration of ^{148}Nd in each case. Dates for the beginning and the end of irradiation were also reported for these samples, but no indication of any downtime was given. Because fuel loading can be done when the RBMK is at power, no downtime was assumed.

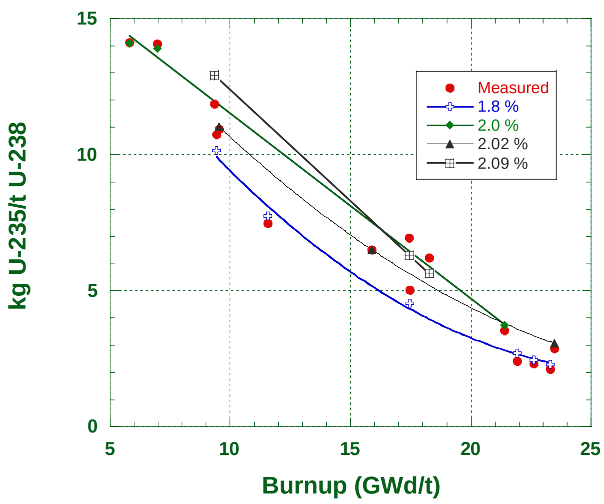

Fig. 3. Concentration of ^{235}U versus burnup. Individual trend lines are shown for groups of samples with different initial enrichments.

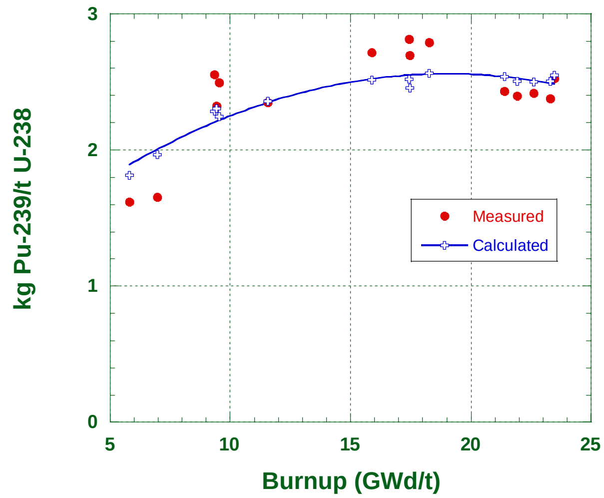

Fig. 4. Concentration of ^{239}Pu versus burnup. Only one trend line is shown for the calculated values, which are not separated according to enrichment.

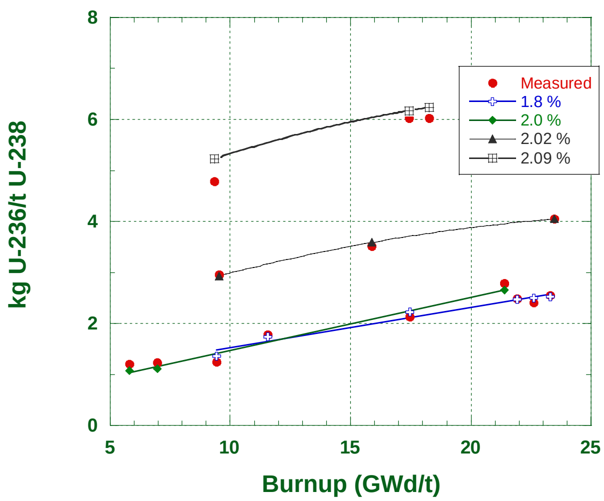

Fig. 5. Concentration of ^{236}U versus burnup. The simulations reproduce the measured values quite well. The simulated values are separated according to initial enrichment. The 2.02 and 2.09 wt% fuel was obtained from recycled uranium, and it therefore contained some ^{236}U at the beginning of irradiation.

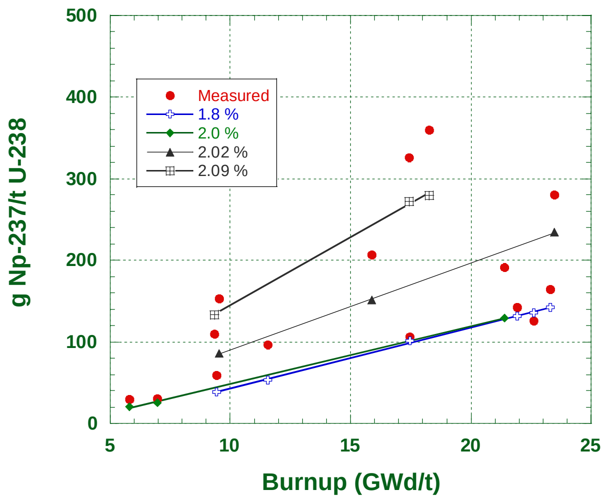

Fig. 6. Concentration of ^{237}Np versus burnup. The simulations produce the observed trends, but there is some scatter in the measurements. Samples with different initial enrichments are separately identified, and one can see the effect of the ^{236}U in the 2.02 and 2.09 wt% samples.

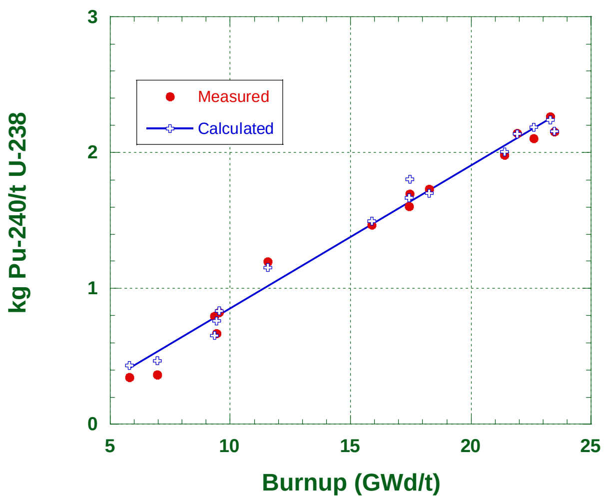

Fig. 7. Concentration of ^{240}Pu versus burnup. One trend line is shown for the simulated values as there does not appear to be a large effect from the enrichment. There is good agreement between measured and simulated values.

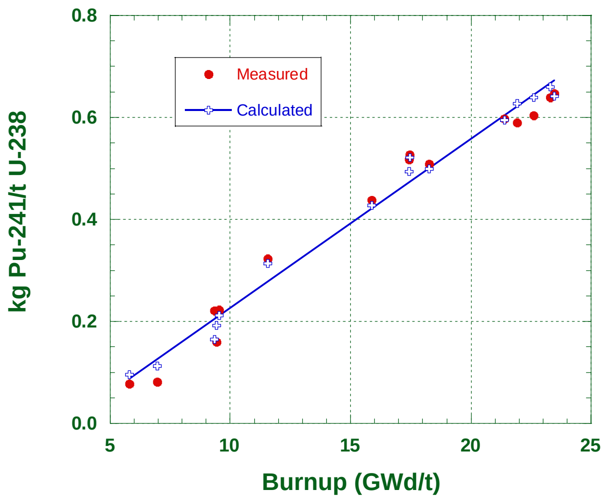

Fig. 8. Concentration of ^{241}Pu versus burnup. One trend line is shown for the simulated values as there does not appear to be a large effect from the enrichment. There is good agreement between measured and simulated values and the pattern of agreement is very similar to that for ^{240}Pu.

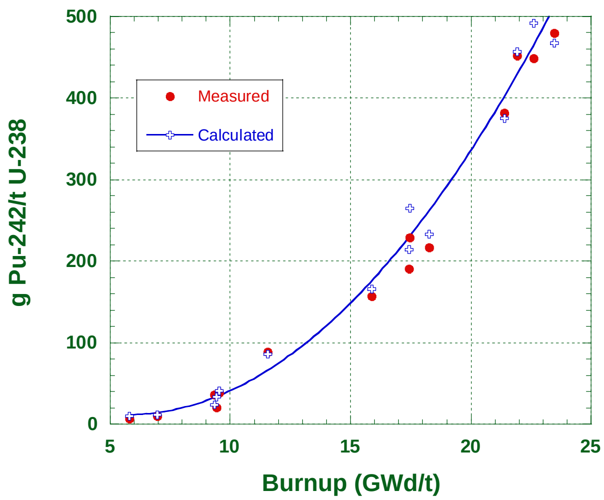

Fig. 9. Concentration of ^{242}Pu versus burnup. One trend line is shown for the simulated values as there does not appear to be a large effect from the enrichment.

The results for uranium, neptunium, and plutonium isotopes show good reproduction of the measured values. This is indicative of the reliability of cross-section libraries produced with these TRITON models of RBMK-1000 configurations and burnup conditions. The following four figures (10–13) show comparisons between measured and simulated concentration values for ^{244}Cm (each one of the four figures refers separately to one of the four initial enrichments).

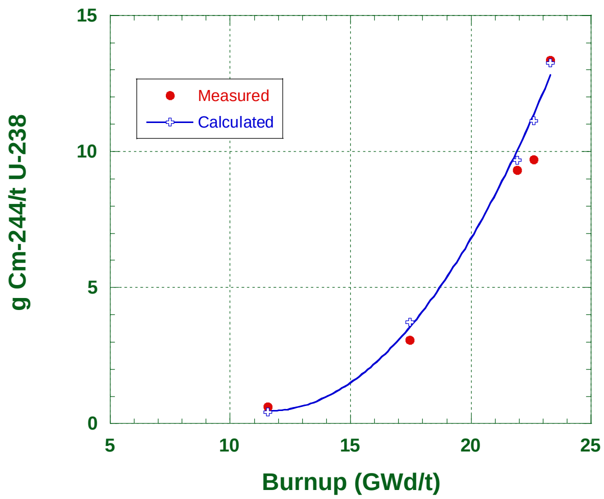

Fig. 10. Concentration of ^{244}Cm versus burnup for the samples with initial enrichment of 1.8 wt%.

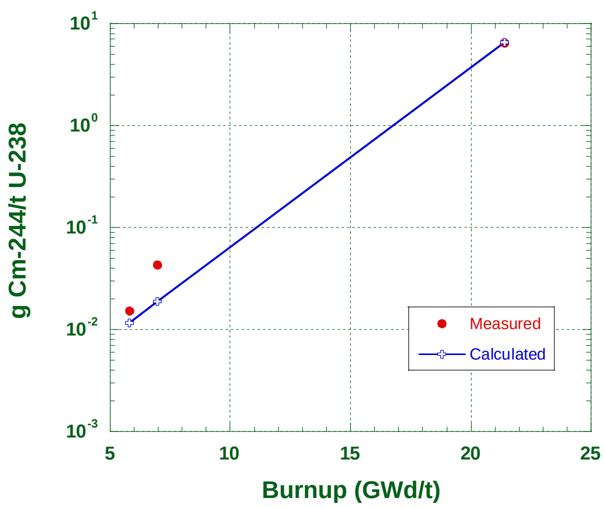

Fig. 11. Concentration of ^{244}Cm versus burnup for the samples with initial enrichment of 2.0 wt%. Because of the low concentrations for the two low-burnup samples, the ordinate scale is logarithmic.

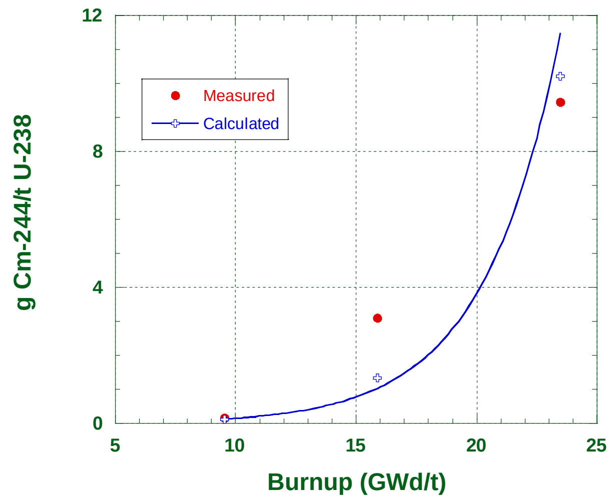

Fig. 12. Concentration of ^{244}Cm versus burnup for samples with initial enrichment of 2.02 wt%.

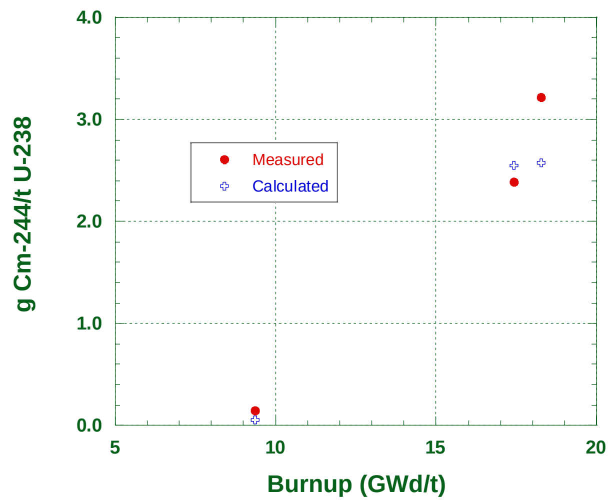

Fig. 13. Concentration of ^{244}Cm versus burnup for samples with initial enrichment of 2.09 wt%.

The simulation of ^{244}Cm concentration is one of the more rigorous tests of actinide concentration predictability. Figs. 10, 11, 12, and 13 refer, in order, to the samples with initial enrichments of 1.8, 2.0, 2.02, and 2.09 wt%. Presenting the four groups of samples separately allows for more clarity than is possible with all ^{244}Cm results on one plot.

The predictions for the ^{244}Cm concentrations are generally reasonable. It was found that the estimated ^{244}Cm concentration is quite sensitive to coolant density, and as explained, estimates of coolant density are poor towards the top of the fuel pins.

A summary of the numerical values both measured and calculated for the 15 spent-fuel samples is contained in Table 3. Concentration values are reported as grams per gram of ^{238}U, and the ratios for the calculated to measured comparisons are also shown.

Table 3. Measured and calculated results for 15 study samples
(values are grams per gram of ^{238}U)

	Sample 1 measured	Sample 1 calculated	calculated/ measured	Sample 6 measured	Sample 6 calculated	calculated/ measured	Sample 9 measured	Sample 9 calculated	calculated/ measured
^{234}U	9.136E-05	1.158E-04	1.27	8.681E-05	1.027E-04	1.18	1.057E-04	1.318E-04	1.25
^{235}U	5.016E-03	4.533E-03	0.90	2.305E-03	2.467E-03	1.07	7.469E-03	7.736E-03	1.04
^{236}U	2.134E-03	2.232E-03	1.05	2.408E-03	2.497E-03	1.04	1.785E-03	1.739E-03	0.97
^{237}Np	1.062E-04	1.017E-04	0.96	1.261E-04	1.359E-04	1.08	9.644E-05	5.352E-05	0.55
^{238}Pu	3.011E-05	3.055E-05	1.01	4.950E-05	5.156E-05	1.04	1.313E-05	9.097E-06	0.69
^{239}Pu	2.696E-03	2.456E-03	0.91	2.416E-03	2.498E-03	1.03	2.349E-03	2.356E-03	1.00
^{240}Pu	1.695E-03	1.803E-03	1.06	2.103E-03	2.186E-03	1.04	1.195E-03	1.151E-03	0.96
^{241}Pu	5.269E-04	5.218E-04	0.99	6.036E-04	6.394E-04	1.06	3.232E-04	3.137E-04	0.97
^{242}Pu	2.289E-04	2.646E-04	1.16	4.485E-04	4.918E-04	1.10	8.833E-05	8.643E-05	0.98
^{241}Am									
^{242m}Am				4.237E-07	4.211E-07	0.99	1.231E-07	1.642E-07	1.33
^{243}Am	1.547E-05	2.679E-05	1.73	4.826E-05	6.048E-05	1.25	4.822E-06	5.344E-06	1.11
^{242}Cm	6.702E-06	5.655E-06	0.84	9.870E-06	8.730E-06	0.88	1.231E-06	1.736E-06	1.41
^{244}Cm	3.073E-06	3.733E-06	1.21	9.715E-06	1.112E-05	1.14	6.156E-07	4.331E-07	0.70
^{137}Cs	5.867E-04	6.736E-04	1.15	8.464E-04	8.722E-04	1.03			
^{142}Nd	1.189E-05	9.526E-06	0.80	2.851E-05	1.755E-05	0.62	5.442E-06	3.726E-06	0.68
^{143}Nd	4.469E-04	4.341E-04	0.97	4.515E-04	4.747E-04	1.05	3.355E-04	3.394E-04	1.01
^{144}Nd	7.422E-04	6.320E-04	0.85	1.027E-03	9.203E-04	0.90	4.802E-04	3.350E-04	0.70
^{145}Nd	3.962E-04	3.969E-04	1.00	4.784E-04	4.909E-04	1.03	2.760E-04	2.786E-04	1.01
^{146}Nd	3.677E-04	3.717E-04	1.01	4.814E-04	4.898E-04	1.02	2.411E-04	2.429E-04	1.01
^{148}Nd	2.035E-04	2.038E-04	1.00	2.604E-04	2.633E-04	1.01	1.365E-04	1.361E-04	1.00
^{150}Nd	9.539E-05	9.728E-05	1.02	1.261E-04	1.292E-04	1.02	6.180E-05	6.225E-05	1.01

Table 3 (continued)

	Sample 11 measured	Sample 11 calculated	calculated/ measured	Sample 18 measured	Sample 18 calculated	calculated/ measured	Sample 19 measured	Sample 19 calculated	calculated/ measured
^{234}U	1.167E-04	1.401E-04	1.20	9.008E-05	1.007E-04	1.12	9.098E-05	1.045E-04	1.15
^{235}U	1.073E-02	1.015E-02	0.95	2.102E-03	2.296E-03	1.09	2.409E-03	2.698E-03	1.12
^{236}U	1.247E-03	1.362E-03	1.09	2.557E-03	2.520E-03	0.99	2.481E-03	2.468E-03	0.99
^{237}Np	5.940E-05	3.849E-05	0.65	1.646E-04	1.427E-04	0.87	1.427E-04	1.314E-04	0.92
^{238}Pu	5.407E-06	5.137E-06	0.95	5.871E-05	4.977E-05	0.85	5.635E-05	4.783E-05	0.85
^{239}Pu	2.322E-03	2.302E-03	0.99	2.374E-03	2.504E-03	1.05	2.396E-03	2.502E-03	1.04
^{240}Pu	6.656E-04	7.624E-04	1.15	2.264E-03	2.240E-03	0.99	2.141E-03	2.139E-03	1.00
^{241}Pu	1.598E-04	1.930E-04	1.21	6.388E-04	6.600E-04	1.03	5.893E-04	6.271E-04	1.06
^{242}Pu	2.048E-05	3.357E-05	1.64	5.291E-04	5.309E-04	1.00	4.518E-04	4.567E-04	1.01
^{241}Am									
^{242m}Am									
^{243}Am	9.626E-07	1.615E-06	1.68	5.260E-05	6.807E-05	1.29	5.087E-05	5.471E-05	1.08
^{242}Cm				1.149E-05	8.903E-06	0.77	1.034E-05	8.194E-06	0.79
^{244}Cm				1.336E-05	1.325E-05	0.99	9.305E-06	9.691E-06	1.04
^{137}Cs	2.960E-04	3.262E-04	1.10	8.936E-04	9.054E-04	1.01	8.499E-04	8.475E-04	1.00
^{142}Nd	1.328E-05	1.931E-06	0.15	4.555E-05	1.860E-05	0.41	6.511E-05	1.620E-05	0.25
^{143}Nd	2.739E-04	2.686E-04	0.98	4.517E-04	4.797E-04	1.06	4.422E-04	4.727E-04	1.07
^{144}Nd	3.318E-04	2.519E-04	0.76	1.085E-03	9.345E-04	0.86	1.010E-03	8.759E-04	0.87
^{145}Nd	2.060E-04	2.072E-04	1.01	4.914E-04	5.023E-04	1.02	4.637E-04	4.787E-04	1.03
^{146}Nd	1.772E-04	1.751E-04	0.99	5.029E-04	5.061E-04	1.01	4.769E-04	4.733E-04	0.99
^{148}Nd	9.933E-05	9.877E-05	0.99	2.702E-04	2.714E-04	1.00	2.543E-04	2.552E-04	1.00
^{150}Nd	4.564E-05	4.439E-05	0.97	1.332E-04	1.337E-04	1.00	1.273E-04	1.247E-04	0.98

Table 3 (continued)

	Sample 20 measured	Sample 20 calculated	calculated/ measured	Sample 25 measured	Sample 25 calculated	calculated/ measured	Sample 26 measured	Sample 26 calculated	calculated/ measured
^{234}U	1.506E-04	1.536E-04	1.02	1.496E-04	1.525E-04	1.02	1.117E-04	1.135E-04	1.02
^{235}U	1.410E-02	1.408E-02	1.00	1.405E-02	1.389E-02	0.99	3.527E-03	3.722E-03	1.06
^{236}U	1.213E-03	1.073E-03	0.88	1.229E-03	1.113E-03	0.91	2.792E-03	2.655E-03	0.95
^{237}Np	2.970E-05	2.044E-05	0.69	3.073E-05	2.590E-05	0.84	1.913E-04	1.295E-04	0.68
^{238}Pu	1.465E-06	1.458E-06	1.00	2.049E-06	1.950E-06	0.95	4.611E-05	3.805E-05	0.83
^{239}Pu	1.615E-03	1.813E-03	1.12	1.653E-03	1.964E-03	1.19	2.429E-03	2.538E-03	1.05
^{240}Pu	3.441E-04	4.347E-04	1.26	3.637E-04	4.676E-04	1.29	1.982E-03	2.005E-03	1.01
^{241}Pu	7.681E-05	9.599E-05	1.25	8.195E-05	1.129E-04	1.38	5.976E-04	5.947E-04	1.00
^{242}Pu	7.067E-06	9.946E-06	1.41	1.024E-05	1.213E-05	1.18	3.815E-04	3.750E-04	0.98
^{241}Am									
^{242m}Am							3.515E-07	3.224E-07	0.92
^{243}Am	5.121E-07	2.975E-07	0.58	1.844E-06	4.255E-07	0.23	3.763E-05	4.120E-05	1.09
^{242}Cm	1.966E-07	9.719E-08	0.49	2.247E-07	1.201E-07	0.53	6.545E-06	6.682E-06	1.02
^{244}Cm	1.536E-08	1.168E-08	0.76	4.302E-08	1.875E-08	0.44	6.452E-06	6.553E-06	1.02
^{137}Cs	2.376E-04	2.360E-04	0.99	2.448E-04	2.483E-04	1.01	8.457E-04	8.387E-04	0.99
^{142}Nd	3.941E-06	6.603E-07	0.17	5.528E-06	7.412E-07	0.13	2.387E-05	1.411E-05	0.59
^{143}Nd	2.054E-04	2.077E-04	1.01	2.119E-04	2.169E-04	1.02	4.663E-04	4.974E-04	1.07
^{144}Nd	2.107E-04	1.086E-04	0.52	2.149E-04	1.143E-04	0.53	9.391E-04	8.182E-04	0.87
^{145}Nd	1.479E-04	1.494E-04	1.01	1.534E-04	1.565E-04	1.02	4.625E-04	4.803E-04	1.04
^{146}Nd	1.219E-04	1.223E-04	1.00	1.269E-04	1.289E-04	1.02	4.518E-04	4.636E-04	1.03
^{148}Nd	6.964E-05	6.948E-05	1.00	7.273E-05	7.326E-05	1.01	2.471E-04	2.509E-04	1.02
^{150}Nd	3.010E-05	3.004E-05	1.00	3.148E-05	3.194E-05	1.01	1.165E-04	1.200E-04	1.03

Table 3 (continued)

	Sample 28 measured	Sample 28 calculated	calculated/ measured	Sample 31 measured	Sample 31 calculated	calculated/ measured	Sample 32 measured	Sample 32 calculated	calculated/ measured
^{234}U	1.890E-04	1.468E-04	0.78	1.432E-04	1.110E-04	0.77	1.683E-04	1.309E-04	0.78
^{235}U	1.093E-02	1.102E-02	1.01	2.888E-03	3.065E-03	1.06	6.489E-03	6.501E-03	1.00
^{236}U	2.959E-03	2.934E-03	0.99	4.058E-03	4.047E-03	1.00	3.515E-03	3.590E-03	1.02
^{237}Np	1.530E-04	8.636E-05	0.56	2.802E-04	2.347E-04	0.84	2.065E-04	1.512E-04	0.73
^{238}Pu	1.530E-05	1.239E-05	0.81	9.319E-05	7.587E-05	0.81	4.048E-05	3.373E-05	0.83
^{239}Pu	2.494E-03	2.243E-03	0.90	2.523E-03	2.547E-03	1.01	2.716E-03	2.515E-03	0.93
^{240}Pu	8.257E-04	8.368E-04	1.01	2.152E-03	2.158E-03	1.00	1.466E-03	1.494E-03	1.02
^{241}Pu	2.218E-04	2.123E-04	0.96	6.476E-04	6.421E-04	0.99	4.379E-04	4.270E-04	0.98
^{242}Pu	3.903E-05	4.073E-05	1.04	4.795E-04	4.672E-04	0.97	1.570E-04	1.661E-04	1.06
^{241}Am									
^{242m}Am									
^{243}Am	5.135E-07	1.981E-06	3.86	5.500E-05	5.675E-05	1.03			
^{242}Cm	1.284E-06	1.008E-06	0.79	8.925E-06	8.152E-06	0.91	2.582E-06	3.517E-06	1.36
^{244}Cm	1.541E-07	1.215E-07	0.79	9.444E-06	1.022E-05	1.08	3.098E-06	1.340E-06	0.43
^{137}Cs	3.810E-04	3.747E-04	0.98	9.423E-04	9.177E-04	0.97	6.000E-04	6.230E-04	1.04
^{142}Nd							2.957E-05	7.157E-06	0.24
^{143}Nd							4.142E-04	4.400E-04	1.06
^{144}Nd							6.691E-04	5.773E-04	0.86
^{145}Nd							3.575E-04	3.773E-04	1.06
^{146}Nd							3.304E-04	3.401E-04	1.03
^{148}Nd							1.838E-04	1.876E-04	1.02
^{150}Nd							9.542E-05	8.675E-05	0.91

Table 3 (continued)

	Sample 36 measured	Sample 36 calculated	calculated/ measured	Sample 39 measured	Sample 39 calculated	calculated/ measured	Sample 41 measured	Sample 41 calculated	calculated/ measured
^{234}U	2.271E-04	1.319E-04	0.58	2.221E-04	1.304E-04	0.59	2.465E-04	1.559E-04	0.63
^{235}U	6.927E-03	6.297E-03	0.91	6.206E-03	5.646E-03	0.91	1.186E-02	1.291E-02	1.09
^{236}U	6.024E-03	6.174E-03	1.02	6.019E-03	6.239E-03	1.04	4.786E-03	5.234E-03	1.09
^{237}Np	3.256E-04	2.721E-04	0.84	3.591E-04	2.790E-04	0.78	1.093E-04	1.335E-04	1.22
^{238}Pu	7.735E-05	6.879E-05	0.89	8.531E-05	6.884E-05	0.81	2.352E-05	1.610E-05	0.68
^{239}Pu	2.812E-03	2.520E-03	0.90	2.790E-03	2.562E-03	0.92	2.555E-03	2.281E-03	0.89
^{240}Pu	1.601E-03	1.668E-03	1.04	1.730E-03	1.700E-03	0.98	7.932E-04	6.542E-04	0.82
^{241}Pu	5.174E-04	4.943E-04	0.96	5.085E-04	5.000E-04	0.98	2.207E-04	1.646E-04	0.75
^{242}Pu	1.908E-04	2.139E-04	1.12	2.169E-04	2.328E-04	1.07	3.610E-05	2.400E-05	0.66
^{241}Am		0.000E+00							
^{242m}Am									
^{243}Am	1.348E-05	2.006E-05	1.49	1.297E-05	2.090E-05	1.61	4.126E-07	1.046E-06	2.54
^{242}Cm	4.562E-06	4.360E-06	0.96	5.396E-06	4.499E-06	0.83	1.238E-06	5.830E-07	0.47
^{244}Cm	2.385E-06	2.546E-06	1.07	3.217E-06	2.576E-06	0.80	1.444E-07	5.527E-08	0.38
^{137}Cs	6.667E-04	6.896E-04	1.03	7.202E-04	7.233E-04	1.00	3.744E-04	3.245E-04	0.87
^{142}Nd	2.571E-05	8.440E-06	0.33	1.867E-05	9.531E-06	0.51	8.445E-05	1.660E-06	0.02
^{143}Nd	4.681E-04	4.638E-04	0.99	4.791E-04	4.813E-04	1.00	2.676E-04	2.742E-04	1.02
^{144}Nd	7.046E-04	5.843E-04	0.83	7.626E-04	6.683E-04	0.88	3.220E-04	2.374E-04	0.74
^{145}Nd	3.975E-04	4.096E-04	1.03	4.174E-04	4.285E-04	1.03	2.000E-04	2.079E-04	1.04
^{146}Nd	3.706E-04	3.762E-04	1.02	3.914E-04	3.954E-04	1.01	1.818E-04	1.739E-04	0.96
^{148}Nd	2.043E-04	2.065E-04	1.01	2.148E-04	2.164E-04	1.01	9.799E-05	9.793E-05	1.00
^{150}Nd	9.647E-05	9.630E-05	1.00	1.002E-04	1.010E-04	1.01	4.772E-05	4.327E-05	0.91

4. RBMK ORIGEN-ARP CROSS-SECTION LIBRARIES

The comparison of results for the 15 nuclide assay samples indicates that the TRITON/NEWT model for the RBMK is valid. Using this model, libraries were developed to cover ranges of enrichment, burnup, and coolant density. The TRITON/NEWT model simulated an assembly as illustrated in Fig. 1. The unit cell length (assembly pitch) is 25 cm. The grid arrangement was chosen such that it is finer in the region closer to the assembly. An assembly contains three types of cladding: the fuel-pin cladding, the cladding in the central carrying rod and the cladding that surrounds the assembly. They are all predominantly zirconium and they are separately represented in the TRITON model, although the differences are probably of negligible neutronic importance.

The fuel mixtures in the inner and outer rods are treated as separate materials in the TRITON/NEWT model—they are separately identified in Fig. 1. Although the ORIGEN-ARP libraries developed here are representative of burnup conditions averaged over all the fuel in an assembly, the model allows one to create separate libraries for the inner and outer rods. However, the effective burnup values for the inner fuel, the outer fuel, and the assembly as a whole will all be slightly different. So, if libraries that refer to different parts of the fuel are prepared in one set of TRITON runs, different effective burnup values will be required depending on which set of libraries is being used. Note that in the comparison studies above, the simulations for the individual samples were carried out specifically for the location of the individual sample (i.e., whether the sample was from an inner or an outer rod).

The libraries were prepared to cover a range of coolant densities. The effective density should be chosen by the user. As regards enrichment, libraries were developed by specifying ^{235}U at the quoted enrichment and the remainder of the fuel was assumed to be ^{238}U. Initially there will likely be some ^{234}U and ^{236}U in the fuel, but because of uncertainty as to the likely amounts and the variability of those amounts, none of either was included in the fresh fuel.

Appendix A gives a typical TRITON RBMK input. The model uses ENDF/B-V cross-sections and is based on the parameters in Table 1. Resonance self-shielding was treated using the NITAWL module. As explained, the TRITON model is based on the configuration shown in Fig. 1; however, because of the symmetry of the configuration, one need only specify one quarter of what is shown in Fig. 1.

The ORIGEN-ARP libraries were prepared to cover the following ranges of parameters.

Enrichment: 1.8 wt%, 2.0 wt%, and 2.2 wt%.

Burnup: Up to 25,000 MWd/t. Each library file has a fresh-fuel library followed by ten libraries covering burnups that increase by 2500 MWd/t (we refer to these as the 10-step libraries).

Coolant density: 0.15 to 0.80 g/cc. The libraries were prepared for coolant-density values of 0.15, 0.28, 0.41, 0.54, 0.67, and 0.80 g/cc.

In the burnup simulations used to develop the libraries, the reactor power level was assumed to be 16 MW/t.

The libraries were named as follows.

rb10E1.8D0.15.lib
rb10E1.8D0.28.lib

rb10E1.8D0.41.lib
rb10E1.8D0.54.lib
rb10E1.8D0.67.lib
rb10E1.8D0.80.lib
rb10E2.0D0.15.lib
rb10E2.0D0.28.lib
rb10E2.0D0.41.lib
rb10E2.0D0.54.lib
rb10E2.0D0.67.lib
rb10E2.0D0.80.lib
rb10E2.2D0.15.lib
rb10E2.2D0.28.lib
rb10E2.2D0.41.lib
rb10E2.2D0.54.lib
rb10E2.2D0.67.lib
rb10E2.2D0.80.lib

This amounts to 18 files covering three enrichments and six values of coolant density. Thus the file rb10E1.8D0.15.lib, for instance, refers to an RBMK library containing 10 burnup steps, for an enrichment of 1.8 wt%, and for a coolant density of 0.15 g/cc. A set of libraries with 20 burnup steps was also developed during the course of this work and hence the need to identify these libraries as having 10 steps.

The following is the arpdata.txt file needed when executing ORIGEN-ARP with the ten-step libraries (it can be part of a larger arpdata.txt file).

```
!rb10
3 6 11
1.8 2.0 2.2
0.15 0.28 0.41 0.54 0.67 0.80
'rb10E1.8D0.15.lib'
'rb10E1.8D0.28.lib'
'rb10E1.8D0.41.lib'
'rb10E1.8D0.54.lib'
'rb10E1.8D0.67.lib'
'rb10E1.8D0.80.lib'
'rb10E2.0D0.15.lib'
'rb10E2.0D0.28.lib'
'rb10E2.0D0.41.lib'
'rb10E2.0D0.54.lib'
'rb10E2.0D0.67.lib'
'rb10E2.0D0.80.lib'
'rb10E2.2D0.15.lib'
'rb10E2.2D0.28.lib'
'rb10E2.2D0.41.lib'
'rb10E2.2D0.54.lib'
'rb10E2.2D0.67.lib'
'rb10E2.2D0.80.lib'
0.0   2500  5000  7500  10000
    12500 15000 17500  20000
    22500 25000
```

For the 20-step libraries, the string “rb10” should be replaced with “rb20,” and in the arpdata.txt file there will be 21 burnup entries (0.0 plus 20 evenly-spaced steps to 20000).

5. VERIFICATION OF THE ORIGEN-ARP RBMK LIBRARIES

After the libraries had been prepared, verification checks were carried out. The purpose of these checks was to verify that the libraries reproduced the concentration values that would be predicted by a SCALE code such as TRITON for the same burnup conditions. In contrast, the comparison checks described earlier ensure that the TRITON code used for library preparation allows for a valid modeling of burnup conditions in the RBMK. In effect, this second group of checks is being carried out to ensure that all steps in the library preparation process have been implemented correctly.

Four cases were chosen with different values of enrichment and burnup. The enrichment refers to the ^{235}U content, and for all of these four test cases the fuel was composed of just ^{235}U and ^{238}U (some of the assay samples also contained ^{236}U). All cases were for a coolant density of 0.5 g/cc. The four cases are as follows:

1. 1.8% enrichment and 6 GWd/t burnup,
2. 1.9 % enrichment and 12 GWd/t burnup,
3. 2.1 % enrichment and 18 GWd/t burnup, and
4. 2.2 % enrichment and 24 GWd/t burnup.

For each of the four cases, ORIGEN-ARP and TRITON calculations were executed and comparisons are presented between the ARP and TRITON predictions for a number of actinides. We first show the comparisons using ten-step libraries. These results are shown in Fig. 14. Figure 14 shows the ARP/TRITON ratios for cases 1 and 2 (the low burnup and enrichment cases) and separately for cases 3 and 4 (medium to high burnup and enrichment).

The comparisons in Fig. 14 show that by using the ARP libraries we reproduce the predictions of a TRITON calculation, although not with great accuracy in the case of the higher actinides. For the higher actinides and for the americium and curium isotopes in particular, the ARP predictions are consistently higher than are the TRITON values. In doing the comparisons, both TRITON and ARP calculations were run such that the burnup steps were about 2500 MWd/t using one library per step.

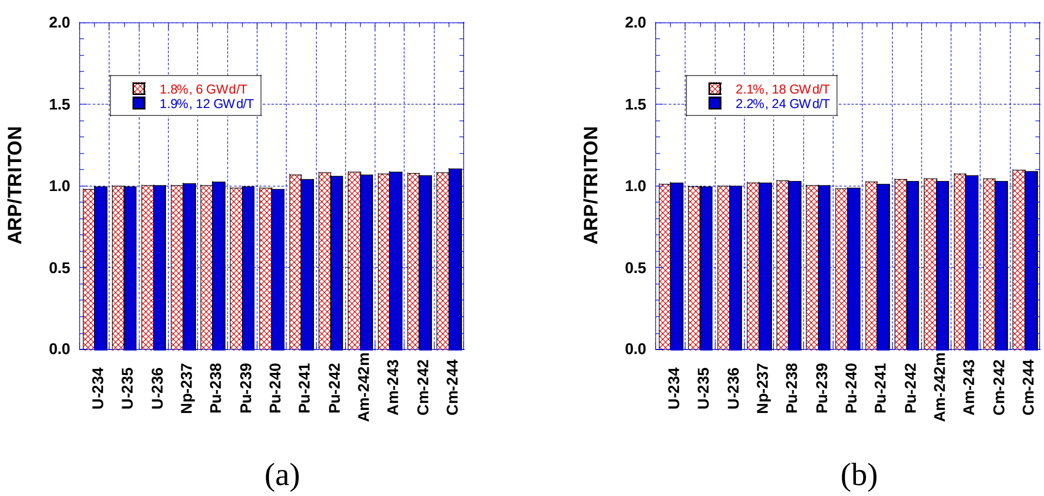

Fig. 14. ARP to TRITON comparisons of actinide concentrations. Fig. 14(a) shows results for cases 1 and 2; Fig. 14(b), results for cases 3 and 4.

For three of the actinides, ^{235}U, ^{239}Pu, and ^{244}Cm, we show ARP and TRITON results plotted as a function of burnup for the four cases. These plots are shown in Figs. 15, 16, and 17. The results are displayed as concentration versus burnup, but enrichment is also varying from case to case. The ^{244}Cm results show the higher concentrations predicted by ARP relative to a full TRITON calculation.

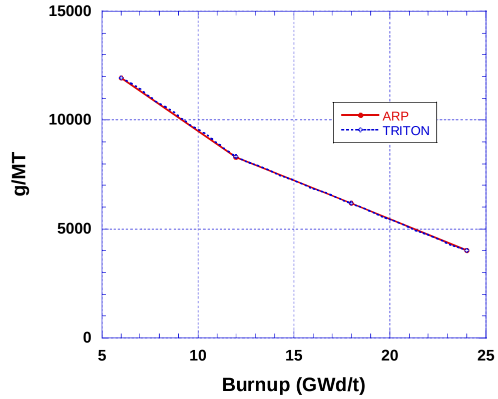

Fig. 15. ARP and TRITON concentrations for ^{235}U versus burnup.

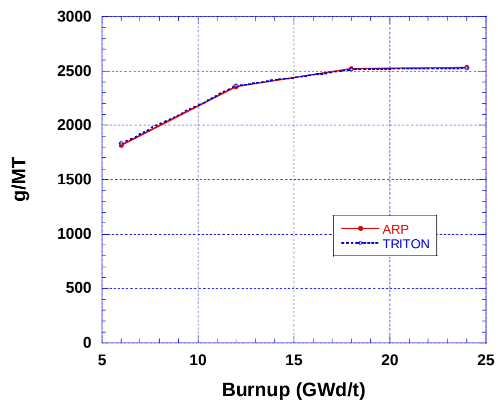

Fig. 16. ARP and TRITON concentrations for ^{239}Pu versus burnup.

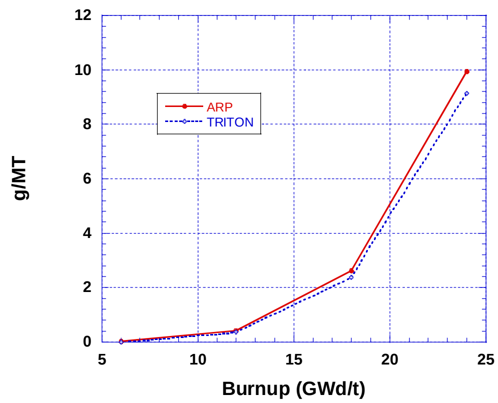

Fig. 17. ARP and TRITON concentrations for ^{244}Cm versus burnup.

The ARP/TRITON comparisons that we have shown so far are for a coolant density of 0.5 g/cc, using ten-step burnup libraries. Repeating the comparisons with a coolant density of 0.2 g/cc showed essentially the same level of agreement. However, using the 20-step ARP libraries, one sees much better agreement between ARP and TRITON for the higher actinides. Results using the 20-step libraries (coolant density of 0.5 g/cc) are shown in Fig. 18. As in the case of the ten-step libraries, these tests were conducted using burnup steps of about 2500 MWd/T.

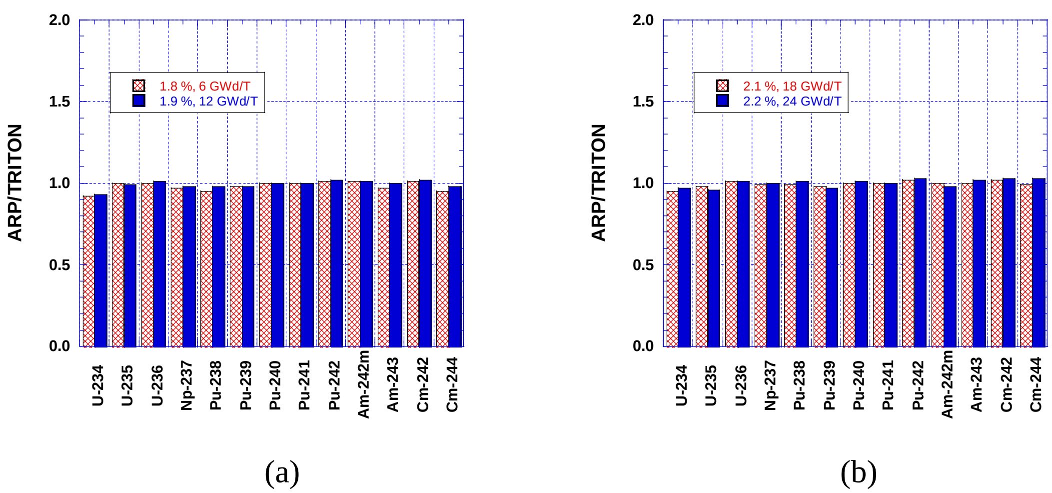

Fig. 18. ARP to TRITON comparisons of actinide concentrations. Fig. 18(a) shows results for cases 1 and 2; Fig. 18(b), results for cases 3 and 4.

Comparing Fig. 18 with Fig. 14, one sees the improved agreement for the americium and curium isotopes. We may therefore conclude that the 20-step libraries are more accurate in reproducing the TRITON results, and this is as might be expected. However, given the overall accuracy with which burnup simulations can predict higher actinide concentrations, the ten-step ARP libraries are probably quite adequate for most purposes.

6. SUMMARY

A TRITON/NEWT reactor-analysis model was developed for an RBMK-1000 system. The model simulates burnup in a representative assembly of the reactor. The representative assembly includes the fuel pins, the coolant water, the assembly hardware, and the associated graphite moderator. Predicted spent-fuel nuclide concentrations using this model compared favorably with laboratory measurements. Using the TRITON model, both 10-step and 20-step burnup libraries were developed and used with ORIGEN-ARP. These libraries were subjected to verification checks in comparisons with full TRITON calculations. The 20-step burnup libraries, as might be expected, are somewhat better in reproducing the full TRITON calculations than are the 10-step ones. However, both sets of libraries are adequate for predicting spent-fuel nuclide concentrations for most practical applications.

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APPENDIX A. SAMPLE TRITON INPUT FOR RBMK-1000

APPENDIX A. SAMPLE TRITON INPUT FOR RBMK-1000

```
=t-depl parm=nitawl
 RBMK-1000
' TRITON model of RBMK-1000; 44-group ENDF/B-V library.
44groupndf
'
' -------------------------------------------------------------------
' TRITON model of RBMK-1000; 44-group ENDF/B-V library.
'
'  enrichment:                    2.0 wt% U235
'  fuel density:                  9.393 g/cc
'  coolant density:               0.54 g/cc
'  moderator (graphite) density:  1.65 g/cc
'  fuel temperature:              1005 K
'  clad temperature:              560 K
'  coolant temperature:           560 K
'  graphite temperature:          873 K
'  specific power:                16 MW/T
'
'  fuel density determined from total fuel mass in the 18 rods and
'  assuming this fills volume to inside of clad over fuel length
'
' -------------------------------------------------------------------
read comp
' material no. 1 refers to the outside ring of fuel rods
'
 uo2 1 den=9.393 1 1005 92235 2.0 92238 98.0 end
' add other important nuclides that may be needed
' -------------------------------------------------------------------
'  Three types of clad. Clad and coolant all have same temperature.
'  ----------------------------------
' fuel clad  (Zr + 1%Nb + 0.03%Hf); repeat once.
 arbm-clad 6.45 3 0 0 0 40000 98.97 41093 1.0 72000 0.03  2 1 560 end
 arbm-clad 6.45 3 0 0 0 40000 98.97 41093 1.0 72000 0.03 12 1 560 end
'  ----------------------------------
' tube clad  (Zr + 2.5%Nb + 0.03%Hf)
 arbm-clad 6.45 3 0 0 0 40000 97.47 41093 2.5 72000 0.03 22 1 560 end
'  ----------------------------------
' assembly clad  (Zr + 2.5%Nb)
 arbm-clad 6.45 2 0 0 0 40000 97.50 41093 2.5            32 1 560 end
'  ----------------------------------
' coolant and part moderator (boiling H2O); repeat once
 h2o  3  den=0.54 1                                           560 end
 h2o 13  den=0.54 1                                           560 end
'  ----------------------------------
' central tube material  (normally, air or solid rod)
 n-14 23  den=0.00125  1                                      560 end
'  ----------------------------------
' graphite moderator
 c   5  den=1.65 1                                            873 end
'  ----------------------------------
' material no. 6 refers to the inside ring of fuel rods
' (this is the same as material no. 1)
'
 uo2 6 den=9.393 1 1005 92235 2.0 92238 98.0 end
' add other important nuclides that may be needed
```

```
'  ------------------------------------
end comp
' ---------------------------------------------------------------
read celldata
 latticecell triangpitch pitch=1.77  3 fuelr=0.5975 1 cladr=0.68  2 end
 latticecell triangpitch pitch=1.77 13 fuelr=0.5975 6 cladr=0.68 12 end
end celldata
' ---------------------------------------------------------------
'
 read depletion
  1 6
 end depletion
'
'  Burnup is 25,000 MWd/T in 20 steps.  First burnup step is used
'  to produce a fresh-fuel ("zero-burnup") library, if needed.
'
 read burndata
  power=16.00  burn=1.0e-10 down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
  power=16.00  burn=78.125  down=0  end
 end burndata
'
read model
 RBMK physical model consists of one graphite block and one assembly.
read parm
  drawit=no  run=yes
end parm
'
read materials
 1 3 'outer-ring fuel'    end
 2 1 'fuel clad'          end
22 1 'tube clad'          end
32 1 'assembly clad'      end
 3 3 'boiling water'      end
23 3 'central-tube air'   end
 5 3 'graphite moderator' end
 6 3 'inner-ring fuel'    end
end materials
'
```

```
read geom
' outer fuel rod
unit 1
 cylinder 10 0.5975 sides=40
 cylinder 20 0.68   sides=40
 media 1 1 10
 media 2 1 20 -10
 boundary  20 4 4
'
' inner fuel rod
unit 6
 cylinder 10 0.5975 sides=40
 cylinder 20 0.68   sides=40
 media 6 1 10
 media 2 1 20 -10
 boundary  20 4 4
'
' top half, inner fuel rod
unit 16
 cylinder 10 0.5975 chord +y=0.0 sides=40
 cylinder 20 0.68   chord +y=0.0 sides=40
 media 6 1 10
 media 2 1 20 -10
 boundary  20 2 2
'
' central tube
unit 2
 cylinder 10 0.625  chord +x=0.0 chord +y=0.0 sides=40
 cylinder 20 0.75   chord +x=0.0 chord +y=0.0 sides=40
 media 23 1 10
 media 22 1 20 -10
 boundary  20 2 2
'
' assembly
unit 5
 cylinder 10 4.0  chord +x=0.0 chord +y=0.0 sides=40
 cylinder 20 4.4  chord +x=0.0 chord +y=0.0 sides=40
 media 3 1 10
 media 32 1 20 -10
' insert central tube
 hole 2
'  --------------------------------------
' insert outer ring of fuel rods
'  --------------------------------------
 hole 1  origin x= 2.995  y= 0.803
 hole 1  origin y= 2.995  x= 0.803
'  --------------------------------------
 hole 1  origin y= 2.193  x= 2.193
'  --------------------------------------
' insert inner ring of fuel rods
'  --------------------------------------
 hole 6  origin x= 0.803  y= 1.39
 hole 16 origin y= 0.0    x= 1.6050
'  --------------------------------------
 boundary  20 12 12
'
 unit 50
```

```
'
' this unit is the immediate surrounds of the assembly
'
 cuboid 30  6 0 6 0
 hole 5
 media 5 1 30
 boundary 30  6  6
'
' now, an intermediate part of the graphite block
'
 unit 60
 cuboid 30  10 0 10 0
 hole 50
 media 5 1 30
 boundary 30  6  6
'
' this is the unit for the total RBMK model
' (one graphite unit cell)
'
 global unit 70
 cuboid 30    12.5 0 12.5 0
 hole 60
 media 5 1 30
 boundary 30  5  5
'
end geom
 read bounds
 all=white
 end bounds
end model
end
```

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