LWR Cross Section Libraries for ORIGEN-ARP in SCALE 5.1

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INTRODUCTION

Modern fuel assembly designs for light water reactors (LWR) are characterized, as compared to previous designs, by higher fuel enrichments and burnups, and increased heterogeneity of the assembly configuration. An accurate treatment of the neutron transport and depletion in these more complex assemblies requires the use of advanced computational tools capable of simulating multi-dimensional geometries. The SCALE (Standardized Computer Analyses for Licensing Evaluations) code system [1] addresses this need through its depletion module TRITON, which allows a depletion simulation of two- or three-dimensional assembly configurations. The ORIGEN-ARP module in SCALE is a faster alternative to TRITON for fuel depletion, decay and source term analyses. This module, by employing pre-generated cross section libraries obtained with TRITON, allows a very fast analysis at an accuracy level comparable to that of a direct TRITON simulation.

This paper describes the methodology employed with TRITON to generate cross section libraries for LWR assembly configurations to be used in ORIGEN-ARP depletion simulations, and shows limited validation results for some of the libraries. The purpose of this work was twofold: to update the set of ORIGEN-ARP cross section libraries for LWR fuel types distributed in the version 5.0 of SCALE, and to extend it to include a wider range of modern assembly designs that are currently used in the nuclear industry.

CODES AND METHODOLOGY

TRITON allows a 2-D depletion analysis through coupling of the 2-D arbitrary polygonal mesh S_N transport code NEWT with the point depletion code ORIGEN-S. Additional 3-D depletion capabilities using KENO V.a and KENO-VI Monte Carlo transport codes will be available with SCALE 5.1. Due to the fact that most of the heterogeneity of the configuration for the LWR assemblies considered here is in the radial direction, the properties on the axial dimension being relatively uniform, the 2-D version of TRITON was used.

The ORIGEN-ARP sequence in SCALE is built within the framework of a Windows graphical user interface, allowing a fast and accurate depletion and decay analysis while at the same time permitting the user to generate and control the files involved with a minimum of effort. ORIGEN-ARP includes the following modules: ORIGEN-S to perform the depletion calculation, ARP to obtain problem-dependent cross sections for ORIGEN-S by interpolating on a set of pre-generated cross sections for a particular fuel type, and OPUS/PlotOPUS to extract and visualize depletion and decay calculated results. For uranium-based fuel types ARP can interpolate, using up to a third-order Lagrange polynomial, on three parameters: burnup, coolant density and fuel enrichment.

Generating cross section libraries for ORIGEN-ARP involved two computational steps. First, a TRITON depletion calculation was performed for 25 burnup steps, for each individual assembly configuration and value of enrichment and coolant density considered. Each depletion calculation produced an ORIGEN-S library containing 25 sets of burnup-dependent cross sections. The first set of cross sections represents effectively fresh fuel. The remaining cross section sets correspond to 24 burnup values equidistantly distributed from 1.5 GWd/MTU to 70.5 GWd/MTU.

The second computational step consisted of using the ARPLIB utility to thin each library file in order to reduce the file size. The number of cross section sets was reduced from 25 to 11 by removing cross-section sets in the burnup range where the cross sections show only small variations with changes in burnup. The thinned ORIGEN- ARP library contains a set of 11 burnup-dependent cross sections at the following burnup values: 0, 1.5, 4.5, 7.5, 10.5, 13.5, 16.5, 31.5, 46.5, 58.5, and 70.5 GWd/MTU.

The flow of the TRITON simulations to obtain the ORIGEN-S library containing 25 sets of burnup dependent cross sections as mentioned above is illustrated in Fig. 1. As shown, starting from the SCALE multigroup transport library, problem dependent (resonance and temperature corrected) cross sections are prepared for the NEWT transport calculation. The self-shielded cross sections obtained with the cross section processors BONAMI and NITAWL are applied to the NEWT transport calculation of the whole fuel assembly. The flux solution from the transport analysis is used to collapse the SCALE multigroup cross sections to one group effective cross section format for use with ORIGEN-S. The ORIGEN-S cross sections updating is carried out by the COUPLE code. The isotopic data resulted from the depletion and decay analysis with ORIGEN-S is used to update at defined time intervals the nuclide composition applied to the assembly transport calculation. The flux spectrum is recalculated with NEWT and cross sections for ORIGEN-S updated again for the next burnup step.

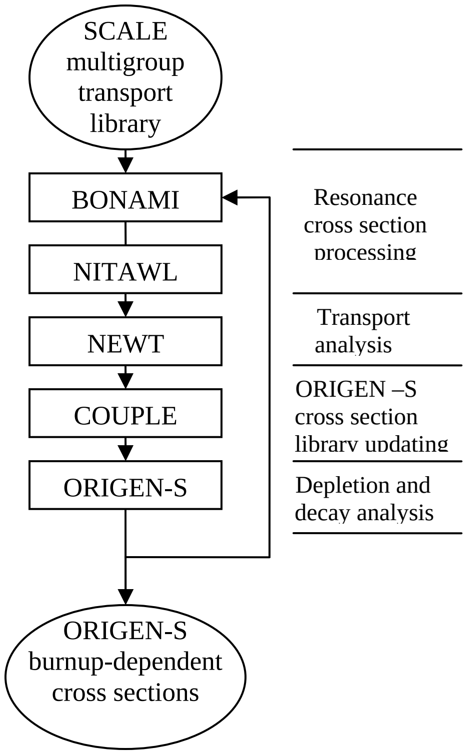


Fig.1 Computational flow of TRITON depletion

Table I. New LWR libraries for ORIGEN-ARP	
Reactor type	Assembly design description
PWR	Westinghouse CE 14x14 Westinghouse CE 16x16 Westinghouse 14x14 Siemens 14x14 Westinghouse 15x15 Westinghouse 17x17 Westinghouse 17x17 OFA*
BWR	GE 7x7 GE 8x8 ABB 8x8 GE 9x9 GE 10x10 ATRIUM-9 (9x9) ATRIUM-10 (10x10) SVEA-64 (8x8) SVEA-100 (10x10)
VVER	VVER-440 flat enrichment 1.6%, 2.4%, 3.6% VVER-440 profiled enrichment, average 3.82% VVER-440 profiled enrichment, average 4.25% VVER-440 profiled enrichment, average 4.38% VVER-1000

* OFA stands for Optimized Fuel Assembly

DESCRIPTION OF LIBRARIES

The LWR libraries previously released with SCALE 5.0 were created using the 1-D depletion sequence SAS2. The new cross section libraries were generated with TRITON for seven PWR, nine BWR, and five VVER assembly configurations, as listed in Table I. The range of the parameters for which the new libraries were generated was extended, as compared to the previous release, to include burnups up to 70.5 GWd/MTU and fuel enrichments up to 6 wt% ^{235}U.

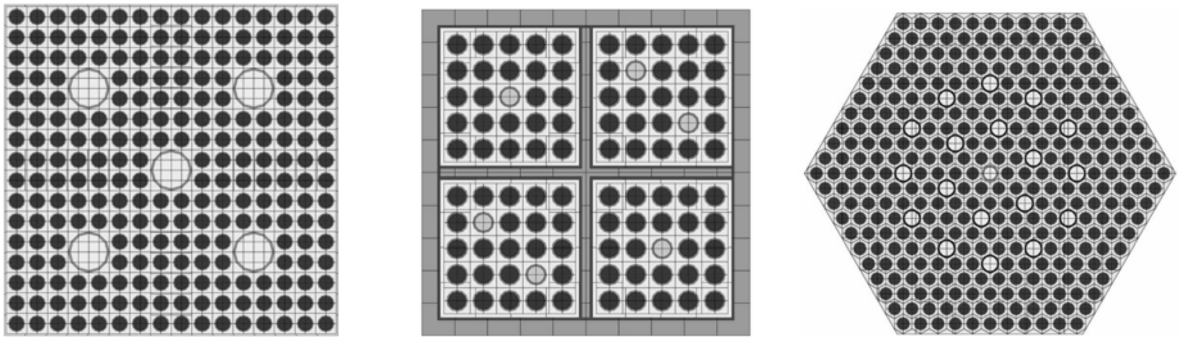
Unless otherwise noted in Table I, the new libraries were generated for six fuel enrichment values: 1.5, 2.0, 3.0, 4.0, 5.0, and 6.0 wt% ^{235}U. In the case of the BWR assembly designs, five values of coolant density were considered: 0.1, 0.3, 0.5, 0.7, and 0.9 g/cm^3, whereas for the PWR or VVER a core-average value was used for the moderator density. Three of the four VVER-440 configurations considered are characterized by a radial enrichment profile, and two of them contain burnable absorber rods.

An important aspect of the work presented here was collecting, from various sources, assembly data for each of the designs considered. As there are small variations in the parameters characterizing the assemblies of a specific design, these gathered data were analyzed in order to build a representative analysis model, typical for a large number of applications involving assemblies of that type. Most of the assembly information was taken from multiple sources, such as the 2004 World Nuclear Industry Handbook [2] and various technical reports issued by the US Nuclear Regulatory Commission (NRC) or Oak Ridge National Laboratory (ORNL). Typical values were used if data were not available. All PWR assemblies were modeled with no absorber rods/devices inserted into the guide or instrument tubes. The models used for TRITON simulations took advantage of the symmetry of the configuration, representing either a quarter or the full assembly geometry. The level of detail in the models is illustrated in Fig. 2 for three assembly designs, one for each reactor type: PWR (Westinghouse CE16x16), BWR (SVEA-100), and VVER (VVER-1000).

VERIFICATION AND VALIDATION

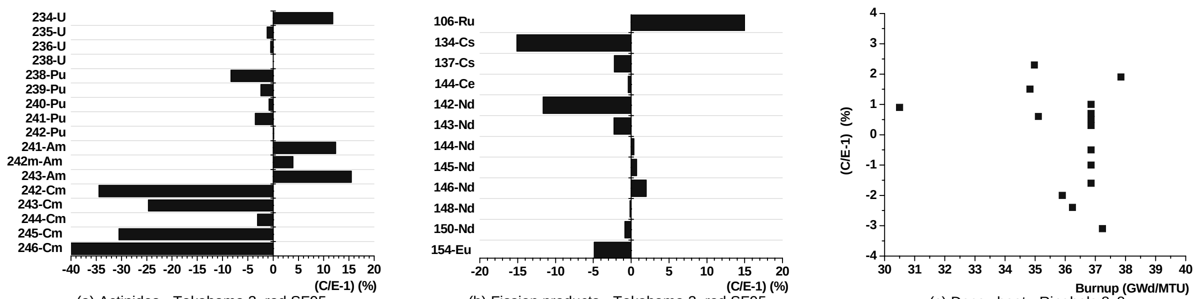
Verification and validation was carried out for most of the libraries, by comparison to measured values of isotope concentrations or residual decay heat for spent fuel assemblies. Based on comparison to measurements, it was assessed that the ORIGEN-ARP libraries provide results that are consistent with other computational methods. Validation results are illustrated in Fig. 3 for the PWR Westinghouse 17x17 and BWR ABB 8x8 libraries, respectively.

Validation of the PWR Westinghouse 17x17 libraries was performed using assay measurement data for



CE 16x16 SVEA-100 VVER-1000

Fig. 2. Selected assembly configurations



(a) Actinides - Takahama 3, rod SF95 (b) Fission products - Takahama 3, rod SF95 (c) Decay heat - Ringhals 8x8

Fig. 3. Validation results for W 17x17 and ABB 8x8 libraries for ORIGEN-ARP

Takahama 3 rod SF95 [3]; percent differences between calculation and experiment results are presented as averages over all five samples from rod SF95 in Fig. 3(a) for actinides and in Fig. 3(b) for fission products. Fig. 3(c) shows calculated-to-experimental ratios for residual decay heat measurements performed at the CLAB interim storage facility for spent fuel located in Sweden on fifteen 8x8 assemblies from the Ringhals-1 reactor [4].

In assessing the level of agreement between experiment and calculation for various applications the user needs be aware that these libraries were generated for typical assembly configurations and operating conditions; they characterize the assembly as a whole and might not be appropriate to use for every specific problem. Such a specific example could be isotopic analysis of fuel rods located in regions of the assembly where local effects could prevail and therefore assembly-averaged cross sections would not be appropriate to use.

CONCLUSION

LWR cross section libraries for ORIGEN-ARP have been generated using the 2-D depletion module TRITON of the SCALE code system for release in SCALE 5.1. Representative 2-D analysis models for TRITON simulations have been developed for a wide range of assembly designs, to include seven PWR, nine BWR and five VVER configurations. The newly generated ORIGEN-ARP libraries cover an increased burnup (up to 70.5 GWd/MTU) and fuel enrichment range (1.5 to 6 wt% ^{235}U); coolant density values from 0.1 to 0.9 g/cm^3 were considered for BWR, whereas for PWR and VVER core-average values were used for moderator density. Verification and validation studies of the libraries, performed by comparison to experimental data from isotopic assay and residual decay heat measurements for spent fuel, showed a good level of agreement between the measured data and ORIGEN-ARP results, comparable to that provided by other computational methods.

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