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ORIGEN-ARP, A FAST AND EASY-TO-USE SOURCE TERM GENERATION TOOL

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ORIGEN-ARP is a new SCALE analytical sequence for spent fuel characterization and source term generation that serves as a faster alternative to the SAS2H sequence by using the Automatic Rapid Processing (ARP) methodology for generating problem-dependent ORIGEN-S cross-section libraries. ORIGEN-ARP provides an easy-to-use menu-driven input processor. This new sequence is two orders of magnitude faster than SAS2H while conserving the rigor and accuracy of the SAS2H methodology. ORIGEN-ARP has been validated against pressurized water reactor (PWR) and boiling water reactor (BWR) spent fuel chemical assay data.

KEYWORDS: Source term generation, depletion, spent fuel, ORIGEN, SAS2, neutron spectra, gamma spectra, light-water reactor, SCALE

I. Introduction

The SAS2H sequence[1] of the SCALE code system[2] has been used worldwide for generation of source terms for spent nuclear fuel from light water and other types of reactors. The calculations, in general, consist of determining the isotopic compositions of the different materials present in the problem as a function of time, which subsequently enable the determination of the radiation source terms. In the SAS2H scheme, time-dependent material concentrations are obtained using the ORIGEN-S code[3] based on a point-depletion calculation that utilizes problem-dependent cross-section libraries generated by functional modules in the SAS2H sequence. ORIGEN-ARP is a new SCALE analytical sequence that serves as a faster alternative to the SAS2H sequence. ORIGEN-ARP uses the Automatic Rapid Processing (ARP) methodology for generating problem-dependent ORIGEN-S cross-section libraries by interpolating on previously generated SAS2H libraries. This new sequence is two orders of magnitude faster than SAS2H while conserving the rigor and accuracy of the SAS2H methodology.

II. Motivation for the Development of ORIGEN-ARP

The basic motivation for development of ORIGEN-ARP was to integrate the rigor and flexibility of the SAS2H sequence with the speed and ease-of-use provided by the ORIGEN2 program.[4] Although ORIGEN-S and ORIGEN2 both solve the same point depletion and decay equations in the same manner,[5] they were independently developed with different primary objectives. The primary objective of ORIGEN2 was a broad range of fuel cycle analyses with simple input specifications and a few select cross-section data libraries (e.g., two libraries for all PWRs). The changes in cross sections caused by reactor operating history and assembly design were deemed of minimum importance based on the broad nature of the fuel cycle studies at the heart of the ORIGEN2 development. Consequently, reliance on ORIGEN2 for results that are highly sensitive to cross-section variations has become a recurring problem. Conversely, ORIGEN-S was developed with less attention to user input simplification but a focus on providing a flexible and efficient interface with neutronic codes that would provide burnup-dependent cross sections based on assembly design information. This requirement for accurate assembly-specific cross sections was based on the use of SAS2H in spent fuel safety analysis where radiation sources, decay heats, and even specific isotopics were of primary importance. Although the SAS2H sequence provided input that was rather simple, some assembly material and design information was still required. In addition, the computing time for a depletion case using SAS2H was about two orders of magnitude greater than that for ORIGEN2 because of the time required by the neutronics codes to generate the burnup-dependent cross sections. Thus the computing efficiency and ease-of-use provided by ORIGEN2 together with its simple installation in comparison with the SCALE system made it a prime choice for many users who were willing to sacrifice the rigor provided by SAS2H.

To effectively address the user community needs for computational speed, ease of setup, and accuracy for a wide range of reactor conditions and assembly designs, the ORIGEN-ARP methodology was developed. ARP accurately produces ORIGEN-S libraries at any enrichment, burnup, and moderator density for a specific fuel assembly design. In addition, the ORIGEN-ARP system provides a user-friendly input menu program ORIGNARP for rapid setup and execution of specific reactor history scenarios.

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III. Overview of ORIGEN-ARP Sequence

ORIGEN-ARP consists of the ORIGNARP PC input processor and the ARP and ORIGEN-S functional modules in SCALE. ORIGNARP is an MS-DOS menu-driven program that creates an input file for ARP and ORIGEN-S, based on user responses and input. ORIGNARP can automatically call the SCALE driver to immediately execute ARP and ORIGEN-S on the PC, or the ARP/ORIGEN-S input file can be transferred to another computer, such as a Unix workstation, for execution.

ARP employs an interpolation algorithm on burnup, enrichment, and, optionally, moderator density to rapidly generate problem-dependent ORIGEN-S cross-section libraries from specially pregenerated SAS2H/ORIGEN-S multi-burnup libraries. The ARP program creates an ORIGEN-S cross-section library for each cycle based on the user-specified burnup history. It interpolates over basic cross-section libraries pregenerated by SAS2H and processed by the ARPLIB utility. The ARP basic cross-section libraries distributed in SCALE were generated at enrichments of 1.5, 2.0, 3.0, 4.0, and 5.0 wt % of ^{235}U and ten burnup steps from 0 to 60 GWd/MTU. Libraries were generated for fuel assembly designs 8 × 8 (General Electric BWR), 14 × 14 (ABB Combustion Engineering PWR), 15 × 15 (Westinghouse PWR), and 17 × 17 (Westinghouse PWR).

IV. ORIGNARP PC Input Processor

The purpose of the ORIGNARP PC input processor is to provide a user-friendly interface program that would be easy to learn and useful for most source term applications. ORIGNARP is specifically designed to assist an ORIGEN-S user in preparing an input file for execution of fuel depletion and/or decay cases within the ORIGEN-ARP analytical sequence. The ORIGNARP program is written in Microsoft BASIC 7.1 and runs on an MS-DOS or Windows PC. ORIGNARP generates a SCALE input file that may be used to execute ARP and ORIGEN-S on a PC or Unix workstation.

ORIGNARP features a pull-down menu system similar to the type used in many PC software products. The menu system organizes the major command categories as menu titles and pull-down commands and may be used with either a keyboard or a mouse. When an option is selected from the menu system, a data entry screen or series of screens is displayed. The input processor includes several different input screens. As an illustration, a black and white representation of one of these color screens is shown in Figure 1. Each field on a screen has a help message associated with it that may be displayed by pressing a help key. The message gives a brief description of the input parameter and occasionally refers to a section in the SCALE manual for more detailed information. This feature minimizes the amount of time that might be used searching through the documentation when setting up an ORIGEN-S input file. Some fields have a multiple-choice menu associated with them. These menus minimize the possibility of input errors by providing a complete list of valid choices for given parameters. Depending on input options selected, the program protects other fields that are not needed for those options. ORIGNARP performs extensive error checking for each input screen and displays appropriate warning and error message boxes when applicable.

V. ORIGEN-ARP Methodology Description

The main feature of the ORIGEN-ARP methodology is that problem-dependent ORIGEN-S cross-section libraries can be obtained by interpolation. As is well known, the success of an interpolation procedure depends on the choice of independent variables pertinent to the problem under consideration and consequently on the selection of a suitable interpolation scheme that provides results within the accepted error margin. To implement the methodology, cross-section changes versus several parameters were computed, and it was found that enrichment, burnup and water density were the independent variables best suited for interpolation. Therefore, cross-section libraries as a function of enrichment, burnup, and optionally, water density are created using the SAS2H sequence of the SCALE system. In particular, the water density effects impact BWR systems because the in-core boiling in these systems leads to an axial variation in the water density and significant cross-section changes as a function of the water density are observed. These pregenerated cross sections serve as the basic libraries from which the interpolation is performed.

The interpolation on the burnup variable is carried out with a scheme developed by Greene[6] for interpolation in Bondarenko factor tables. It states that for a function f(x) with known values at $x_1, x_2, \ldots x_n$ a value $f(x_q)$ can be interpolated according to

$$f(x_q) = f(x_i) + \frac{x_q^p - x_i^p}{x_{i+1}^p - x_i^p}\left(f(x_{i+1}) - f(x_i)\right), \quad (1)$$

where p is a function of x and is allowed to vary linearly as

$$p(x_q) = p(x_i) + \frac{x_q - x_i}{x_{i+1} - x_i}\left(p(x_{i+1}) - p(x_i)\right). \quad (2)$$

It is clear that for a constant p equal to 1, this scheme reduces to the familiar linear interpolation method. In general, however, the p values are determined from the known set $\{x_i, f(x_i)\}$ according to Eq. (2) in such a way that the function f(x) is reproduced within the desired accuracy. The value

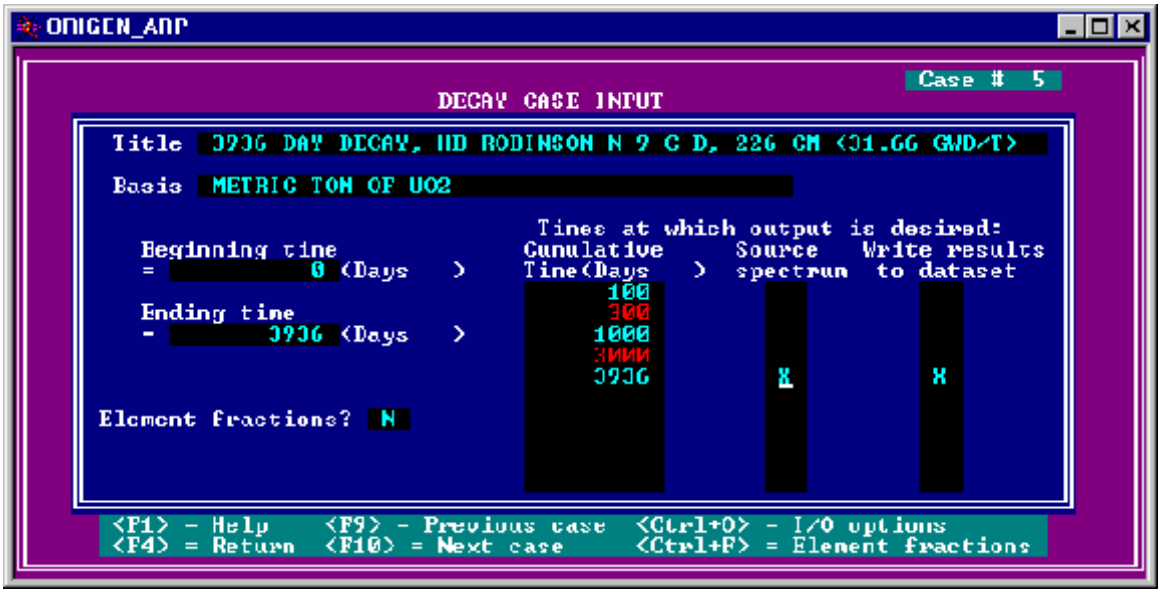

Figure 1. ORIGEN-ARP decay case history screen.

$p(x_i)$ is determined by solving equation (1) where $x_q = x_i$ using the known values of $f(x_{i-1})$, $f(x_i)$, $f(x_{i+1})$,

$$f(x_i) = f(x_{i-1}) + \frac{x_i^p - x_{i-1}^p}{x_{i+1}^p - x_{i-1}^p}\left(f(x_{i+1}) - f(x_{i-1})\right), \quad (3)$$

where $p = p(x_i)$. All values except p in equation (3) are known. The value of p is solved using an iterative technique.

Note that the change of the effective absorption cross sections with enrichment has been found to approach a linear shape in a log-linear scale. Therefore, log-linear interpolation is conducted for the cross section as a function of enrichment. Similar to enrichment, the effective absorption cross section varies linearly in a log-linear scale with the water density, and a log-linear interpolation is utilized.

VI. ARP Basic Cross-Section Libraries

The ARP program creates multiple ORIGEN-S cross-section libraries by interpolating over basic cross-section libraries pregenerated by SAS2H and processed by the ARPLIB utility. Various utility programs have been developed to automate the procedure so that users can create ARP basic cross-section libraries for other fuel assembly designs. The generation of the ARP basic libraries is performed only once for each fuel assembly type.

The following procedure was used to generate the libraries distributed with SCALE and is recommended for users who generate their own libraries. For each enrichment and water density combination, a SAS2H calculation is performed with 21 cycles and 1 library per cycle. The cross-section libraries created in this step must contain fresh-fuel cross sections for the first cycle. From studies performed with PWR and BWR assemblies, it is recommended that a specific power of 40 MW/MTU and a total irradiation period of 1500 days be applied for a total burnup of 60,000 MWd/MTU. To obtain the 21 burnup-dependent cross-section libraries, one initial burnup step of 1×10^{-15} days used to represent fresh fuel and 20 burnup steps of 3000 MWd/MTU are used. With the exception of the first library in the zero-burnup position, the remaining 20 libraries correspond to a burnup position at the midpoint of each burnup step.

To perform these SAS2H calculations for each enrichment/water density combination, a single SAS2H input file is constructed with generic flags substituted for the parameters that vary from case-to-case (i.e., enrichment and water density). This single SAS2H input file can be processed through the PRISM utility to generate specific SAS2H input files for each enrichment/density combination to automate production of the libraries. After the SAS2H calculations are performed, the 21-burnup SAS2H/ORIGEN-S libraries are reduced to 10-burnup ARP basic cross-section libraries using the ARPLIB utility. The ORIGEN-S burnup-dependent cross-section data can be listed with the XSECLIST utility.

VII. Validation of the ORIGEN-ARP Methodology

To evaluate the ORIGEN-ARP methodology, calculated PWR and BWR spent fuel nuclide concentrations were compared with those obtained from direct SAS2H calculations and existing measured values.[7] Fuel assemblies from three PWRs were used, namely, Calvert Cliffs (14 × 14), Obrigheim (14 × 14), and H. B. Robinson (15 × 15). A detailed description of these reactor assemblies, including significant design characteristics and operating conditions, can be found in Ref. 8. Similar calculations were performed for assemblies from three BWRs, Gundremmingen (6 × 6), JPDR (6 × 6), and

Cooper (7 × 7). A complete description of these reactor assemblies is given in Ref. 9.

The calculations in this work were performed using both ORIGEN-ARP and SAS2H with the SCALE 44GROUPNDF5 library, a 44-group library based primarily on ENDF/B-V data. For each reactor assembly, basic ARP cross-section libraries were created with the SAS2H sequence at enrichments 1.5, 2.0, 3.0, 4.0, and 5.0 wt % of ^{235}U. The burnup range in these libraries spans from 0 to 60 GWd/MTU.

Sample comparisons of the measured and computed fuel compositions for the 14 × 14 Calvert Cliffs assembly are shown in Table 1. Note that the calculated fuel nuclide concentrations with the cross-section data generated with the ARP methodology are in good agreement with the SAS2H results. In fact, the results of calculations performed with ORIGEN-ARP are expected to be as good as that of SAS2H, because the basic cross-section libraries for ARP are created within the SAS2H scheme.

Table 1. Measured and computed irradiated fuel composition[a] for 14 × 14 Calvert Cliffs assembly with 44.34-GWd/MTU burnup

Nuclide	Measured	ARP	Difference[b] %	SAS2H	Difference[b] %
^{234}U	0.12	0.1213	1.1	0.1217	1.4
^{235}U	3.54	3.148	-11.1	3.231	-8.7
^{236}U	3.69	3.764	2.0	3.759	1.9
^{238}U	824.9	824.0	-0.1	823.8	-0.1
^{238}Pu	0.269	0.2529	-6.0	0.2555	-5.0
^{239}Pu	4.357	4.329	-0.6	4.292	-1.5
^{240}Pu	2.543	2.484	-2.3	2.444	-3.9
^{241}Pu	1.02	0.997	-2.3	0.9959	-2.4
^{242}Pu	0.84	0.8751	4.2	0.8741	4.1
^{237}Np	0.468	0.5	6.9	0.5015	7.2
^{133}Cs	1.24	1.286	3.7	1.282	3.4
^{134}Cs	0.03	0.0244	-18.6	0.0244	-18.6
^{135}Cs	0.43	0.4328	0.6	0.4372	1.7
^{137}Cs	1.25	1.268	1.4	1.265	1.2
^{143}Nd	0.763	0.763	0.0	0.7667	0.5
^{144}Nd	1.643	1.657	0.9	1.647	0.2
^{145}Nd	0.74	0.7414	0.2	0.7396	-0.1
^{146}Nd	0.83	0.8429	1.6	0.8404	1.3
^{148}Nd	0.428	0.430	0.5	0.4291	0.3
^{150}Nd	0.208	0.217	4.5	0.2168	4.2

[a]In units of milligram per gram of UO_2.

[b]Percentage difference = (computed ! measured)/ measured × 100.0.

The axial variation in the water density in BWR systems leads to changes in the effective group cross sections. Although in PWR systems the axial change in the cross sections is not a major effect, these effects play an important role in BWR systems. In a SAS2H calculation the axial water-density is entered explicitly in the generation of ORIGEN-S cross-section libraries.

Axial water densities were required in a recent ORNL depletion calculation validation study[9] on the use of SAS2H in BWR analysis. Note that the SAS2H values presented in this section are from preliminary calculations performed for the validation study in Ref. 9. The ARP libraries generated here are consistent with these calculations.

To account for the BWR water density effects in the ARP scheme, SAS2H cross section libraries were generated at the water densities of 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, and 0.9 g/cm^3. The cross section at any water density is obtained by a log-linear interpolation on these pregenerated SAS2H libraries. These libraries were generated for this validation because the BWR library distributed with SCALE does not have water density interpolation data. Future versions of SCALE will include BWR libraries with water density data.

The ORIGEN-ARP calculated fuel nuclide concentrations agree very well with the SAS2H results. For BWR systems, an interpolation on the water density is required in addition to the burnup and enrichment. The sample results for two different water densities in the Cooper BWR shown in Tables 2 and 3 demonstrate the adequacy of the log-linear interpolation on the water density.

Table 2. Measured and computed irradiated fuel composition[a] for 7 × 7 Cooper assembly with 31.04-GWd/MTU burnup and 0.6124 g/cm^3 water density

Nuclide	Measured	ARP	Difference[b] %	SAS2H	Difference[b] %
^{234}U	0.1540	0.1472	-4.4	0.1466	-4.8
^{235}U	6.280	5.713	-9.0	5.746	-8.5
^{236}U	3.480	3.395	-2.4	3.387	-2.7
^{238}U	845.5	837.3	-1.0	837.4	-1.0
^{238}Pu	0.1389	0.1201	-13.5	0.1213	-11.4
^{239}Pu	3.668	3.486	-5.0	3.503	-4.5
^{240}Pu	2.082	1.969	-5.4	1.907	-8.4
^{241}Pu	0.6139	0.5688	-7.4	0.5771	-6.0
^{242}Pu	0.3823	0.3776	-1.2	0.3809	-0.4
^{137}Cs	0.06850	0.07086	3.4	0.07101	3.7

[a]Units of milligram per gram of UO_2.

[b]Percentage difference = (computed ! measured)/ measured × 100.0.

VIII. CONCLUSIONS

ORIGEN-ARP is a new SCALE analytical sequence that serves as a faster and easier-to-use alternative to SAS2H for spent fuel characterization and source term generation. It combines the rigor and accuracy of SAS2H with the speed and ease-of-use found in ORIGEN2. ORIGEN-ARP includes an easy-to-use menu-driven PC input processor and the ARP rapid interpolation scheme for problem-dependent cross sections for ORIGEN-S. ARP and

Table 3. Measured and computed irradiated fuel composition[a] for 7 × 7 Cooper BWR assembly with 30.07-GWd/MTU burnup and 0.4705 g/cm^3 water density

Nuclide	Measured	ARP	Difference[b] %	SAS2H	Difference[b] %
^{234}U	0.1350	0.1414	4.7	0.1410	4.5
^{235}U	5.340	5.556	4.0	5.525	3.5
^{236}U	3.530	3.452	-2.2	3.455	-2.2
^{238}U	834.6	834.8	0.0	834.8	0.0
^{238}Pu	0.1743	0.1563	-10.3	0.1549	-11.2
^{239}Pu	3.579	3.922	9.6	3.891	8.7
^{240}Pu	2.216	2.071	-6.5	2.068	-6.7
^{241}Pu	0.6390	0.6832	6.9	0.6673	4.4
^{242}Pu	0.4407	0.4473	1.5	0.4414	0.2
^{137}Cs	0.07480	0.07549	0.9	0.07557	1.0

[a]Units of milligram per gram of UO_2.

[b]Percentage difference = (computed ! measured)/ measured × 100.0.

ORIGEN-S can be executed on a PC or a Unix workstation.

To evaluate the ORIGEN-ARP methodology for PWR and BWR assembly depletion, calculated spent fuel nuclide concentrations for several PWR and BWR reactors were compared with those obtained from direct SAS2H calculations and existing measured values.

The ORIGEN-ARP method is two orders of magnitude faster that the SAS2H sequence for generating ORIGEN-S cross-section libraries. The results shown in this work indicate the accuracy and efficiency of the ORIGEN-ARP methodology. In fact, the results of calculations performed with ORIGEN-ARP are as good as those obtained with SAS2H, since the basic libraries for ARP are created within the SAS2H scheme. The primary limitations of the methodology lie in the boundaries of the available libraries, i.e., the fuel assembly designs and enrichment and water density ranges. Other possible limitations could be the accuracy of the interpolation or variations in the actual power/downtime histories. Based on the validation results, it appears the impact of these possible limitations is negligible.

IX. REFERENCES

1. O. W. Hermann and C. V. Parks, "SAS2H: A Coupled One-Dimensional Depletion and Shielding Analysis Module," Vol. I, Sect. S2 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 5 (ORNL/NUREG/CSD-2R5), Vols. I, II, and III, March 1997. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.

2. *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 5 (ORNL/NUREG/CSD-2R5), Vols. I, II, and III, March 1997. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.

3. O. W. Hermann and R. M. Westfall, "ORIGEN-S: SCALE System Module to Calculate Fuel Depletion, Actinide Transmutation, Fission Product Buildup and Decay, and Associated Radiation Source Terms," Vol. II, Sect. F7 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*," NUREG/CR-0200, Rev. 5 (ORNL/NUREG/CSD-2R5), March 1997. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.

4. A. G. Croff, *A User's Manual for the ORIGEN2 Computer Code*, ORNL/TM-7175, Union Carbide Corporation, Oak Ridge National Laboratory, July 1980. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-371.

5. C. V. Parks, "Overview of ORIGEN2 and ORIGEN-S: Capabilities and Limitations," in Proc. of the Third International Conference on High Level Radioactive Waste Management, Las Vegas, NV, April 12–16, 1992, Vol. 1, pp. 57–64.

6. N. M. Greene, "A Method for Interpolating in Bondarenko Factor Tables and Other Functions," *Symposium on ENDF/B Benchmark Analysis*, EPRI NP-2855, Electric Power Research Institute, February 1983.

7. L. C. Leal, O. W. Hermann, S. M. Bowman, and C. V. Parks, Automatic Rapid Process for the Generation of Problem-Dependent SAS2H/ORIGEN-S Cross-Section Libraries, *Nucl. Technol.* **127,** 1–23, July 1999.

8. O. W. Hermann, S. M. Bowman, M. C. Brady, and C. V. Parks, *Validation of the SCALE System for PWR Spent Fuel Isotopic Composition Analysis*, ORNL/TM-12667, Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory, March 1995.

9. O. W. Hermann and M. D. DeHart, *Validation of SCALE (SAS2H) Isotopic Predictions for BWR Spent Fuel*, ORNL/TM-13315, Lockheed Martin Energy Research Corp., Oak Ridge National Laboratory, 1998.