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MOX Cross-Section Libraries for ORIGEN-ARP

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CONTENTS

CONTENTS (continued)

LIST OF FIGURES

LIST OF FIGURES (continued)

LIST OF TABLES

ACRONYMS AND ABBREVIATIONS

ARIANE   Actinides Research In A Nuclear Element
APOLLO   Reactor Physics Cell Code (France)
ARP   Automatic Rapid Processing
BNFL   British Nuclear Fuels
BWR   Boiling-water reactor
C/E   Calculated-to-experimental
DG-TREN   Directorate-General for Energy and Transport
DOE   U.S. Department of Energy
EURATOM   European Atomic Energy Community
HELIOS   Commercial lattice physics code by Studsvik Scandpower, Inc.
HM   Heavy metal
IAEA   International Atomic Energy Agency
LEU   Low-enriched uranium
LWR   Light-water reactor
MALIBU   Radiochemical analysis of MOX and UOX LWR fuels Irradiated to high
             Burnup
MOX   Mixed oxide
NNSA   National Nuclear Security Administration
OECD   Organization for Economic Cooperation and Development
ORIGEN-S   Oak Ridge Isotope Generation Code (of SCALE)
ORNL   Oak Ridge National Laboratory
PSI   Paul Scherre Institute
Pu-U   Plutonium-uranium
PWR   Pressurized-water reactor
RG   Reactor-grade
SAS2H   Shielding Analysis Sequence (of SCALE)
SCALE   Standardized Computer Analyses for Licensing Evaluation
SCK-CEN   Studiecentrum voor Kernenergie-Centre d'étude du l'Energie Nucléaire
TRU   Transuranic
WG   Weapons-grade

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ABSTRACT

The use of mixed-oxide (MOX) fuel in commercial nuclear power reactors operated in Europe has expanded rapidly over the past decade. The predicted characteristics of MOX fuel such as the nuclide inventories, thermal power from decay heat, and radiation sources are required for design and safety evaluations, and can provide valuable information for non-destructive safeguards verification activities. This report describes the development of computational methods and cross-section libraries suitable for the analysis of irradiated MOX fuel with the widely-used and recognized ORIGEN-ARP isotope generation and depletion code of the SCALE (Standardized Computer Analyses for Licensing Evaluation) code system. The MOX libraries are designed to be used with the Automatic Rapid Processing (ARP) module of SCALE that interpolates appropriate values of the cross sections from a database of parameterized cross-section libraries to create a problem-dependent library for the burnup analysis. The methods in ORIGEN-ARP, originally designed for uranium-based fuels only, have been significantly upgraded to handle the larger number of interpolation parameters associated with MOX fuels. The new methods have been incorporated in a new version of the ARP code that can generate libraries for low-enriched uranium (LEU) and MOX fuel types. The MOX data libraries and interpolation algorithms in ORIGEN-ARP have been verified using a database of declared isotopic concentrations for 1042 European MOX fuel assemblies. The methods and data are validated using a numerical MOX fuel benchmark established by the Organization for Economic Cooperation and Development (OECD) Working Group on burnup credit and nuclide assay measurements for irradiated MOX fuel performed as part of the Belgonucleaire ARIANE International Program.

ACKNOWLEDGEMENTS

1 INTRODUCTION

The use of mixed-oxide (MOX) fuel in commercial nuclear power reactors operated in Europe has expanded rapidly over the past decade. In Europe, the countries of France, Germany, Belgium, and Switzerland currently operate reactors that routinely utilize MOX fuel. Nuclear power utilities in Sweden and Japan are also preparing to use MOX fuel in nuclear power plants in the near future. MOX fuel contains mixed plutonium-uranium (Pu-U) oxide. The plutonium in commercial MOX fuel is separated from reprocessed reactor-irradiated low-enriched uranium (LEU) fuel (e.g., UO_2) and is referred to as reactor-grade (RG) MOX. The uranium in MOX fuel is typically derived from either natural or depleted uranium. The Pu oxide mass typically ranges from 2 to 10 wt % of the MOX fuel mass, depending on the fissile content of the Pu, to obtain the target fissile content for the MOX assembly. Reactor-based disposition of weapons-grade (WG) Pu in MOX fuel (WG MOX) is also being considered as one option to reduce the weapons Pu stockpile. The Pu in WG MOX typically contains a much higher percentage of the fissile isotope ^{239}Pu (>90 wt %) compared to RG MOX. However, large-scale utilization of WG MOX has not been initiated to date.

The ability to accurately predict the radiological properties of fresh and irradiated MOX fuel is an important requirement for the design and safety analysis of fuel handling operations, transportation, and storage facilities. The nuclide compositions of the discharged fuel are needed to determine the decay heat power, the neutron and gamma-ray source terms, and inventories for the analysis of releases under accident conditions. Computational methods to predict the neutron and gamma radiation fields on the basis of declared fuel records and operating history also represent a potentially important tool for safeguards inspectors to verify declared safeguarded materials by comparing measurements (e.g., using ion Fork detector instruments) against predicted radiation levels.

The computing methods needed to predict the wide range of radiological properties for design and safeguards applications requires that large numbers of actinides and fission products can be tracked simultaneously. For these types of calculations, the ORIGEN class of codes are internationally recognized and used because of their ability to rapidly calculate nuclide compositions for more than 1600 actinides, fission products, and activation products, and calculate their associated characteristics and radiation source levels. The ORIGEN codes are already widely used for the analysis of light-water-reactor LEU fuel types. However, their extension to MOX fuel is limited by the lack of appropriate cross-section libraries that can be used for the burnup analysis. Because of the much greater variability in initial MOX fuel compositions, compared to LEU fuel, the development of ORIGEN libraries for MOX fuel has not been widely pursued because of the large number of different libraries that would be needed to cover the wide range of potential MOX fuel compositions.

To address the need for MOX fuel analysis capability, MOX fuel libraries and cross-section processing methods have been developed and integrated into the ORIGEN-ARP sequence of the SCALE (Standardized Computer Analyses for Licensing Evaluation) code system. SCALE is developed and maintained by the Oak Ridge National Laboratory (ORNL). The ORIGEN-ARP sequence uses the Automatic Rapid Processing (ARP) module to prepare problem-dependent cross-sections for the SCALE version of the ORIGEN code, called ORIGEN-S code. The ARP module employs an interpolation strategy to reduce the number of libraries required to described

the wide range of potential MOX fuel compositions, and significantly reduces computing times and data storage requirements.

1.1 BACKGROUND

The work described in this report was funded by the U.S. Department of Energy, National Nuclear Security Administration (DOE/NNSA) under the International Safeguards program. This program supports the International Atomic Energy Agency (IAEA) and other agencies with responsibilities to detect clandestine nuclear activities and safeguard declared nuclear material. The IAEA has the task of providing continuing assurance to the international community that States having entered into safeguards agreements with the IAEA are meeting their obligations. Within the European Community, the European Atomic Energy Community (EURATOM) operates a regional safeguards inspectorate through the EURATOM Directorate General Energy and Transport (DG-TREN) of the European Community. This project was undertaken in cooperation with EURATOM DG-TREN.

Three EURATOM member countries, Belgium, Germany, and France, currently operate light water reactor (LWR) nuclear reactors that routinely utilize MOX fuel, and the number of nuclear plants being licensed for MOX use is steadily increasing each year. In many of the reactors operating with MOX fuel, a mix of LEU and MOX assemblies are used concurrently within the core. The physical designs of LEU and MOX assemblies are nearly identical. This presents a challenge for non-destructive safeguards materials verification, because low-burnup MOX fuel has many properties that are similar to those of high burnup LEU fuel.

Predictive computer codes that can estimate the expected properties of these fuel types provide a potentially important tool to enhance the ability of safeguards inspectors to verify declared fuel records. Such codes can be used to predict the radiation fields and spectral signatures based on the declared fuel type and reactor irradiation history. The computed results can be compared to actual measurements on the discharged assemblies to confirm declarations, and potentially identify discrepancies in declarations or diversion of safeguards materials.

1.2 OBJECTIVES

This report describes the development of an RG MOX burnup analysis capability using the ORIGEN-ARP sequence. The objectives of this work are to develop new methodologies required for MOX fuels and demonstrate their application and accuracy for pressurized-water reactor (PWR) MOX and boiling-water reactor (BWR) MOX fuel assemblies. However, the MOX data libraries developed under this project do not extend to WG MOX fuel. Although the MOX methods and cross-section libraries described in this work were developed primarily for safeguards applications using MOX fuel parameters and reactor design data compiled for European reactors, the methods and data are expected to be sufficiently general to be applicable to a broad class of RG MOX fuel designs. The potential range of applications extends beyond just safeguards, since the ORIGEN-ARP code is a multipurpose depletion analysis sequence that can be used to predict a wide range of spent fuel properties, and is well suited for analyzes for a wide range of fuel design and safety analysis applications.

The methods described in this report are currently being implemented for use in a PC Windows graphical user interface developed for ORIGEN-ARP that will automatically prepare code input for a burnup and decay analysis, execute the required codes, and perform post-analysis processing to provide output for the specific types of information required by inspectors. This Windows program will provide a tool for RG MOX fuel analysis that is easy to use, extremely fast, and accurate.

The remainder of this report is divided into the following sections: Sect. 2 provides a general review and summary of MOX fuel properties; Sect. 3 describes the new computational methods developed to create MOX cross-section libraries using the ARP interpolation approach, and presents the results of methods testing; Sect. 4 gives the detailed design specifications for the different MOX fuel assemblies considered in this report; Sect. 5 discusses the methods and procedures used to generate the different MOX fuel libraries; and Sect. 6 presents preliminary validation results of the MOX methods and libraries using selected benchmarks.

2   MOX FUEL DESCRIPTION

This section provides an overview of the MOX fuel properties important to the development of cross-section libraries. Although the properties presented here were obtained using information and declared inventory records for European MOX fuel, it is expected that the properties will be similar to other countries and reactors that operate with RG MOX fuel. The description of MOX fuel presented in this section does not extend to MOX manufactured using weapons-grade plutonium.

The analysis of MOX fuel cross sections requires consideration of many more fuel parameters compared to conventional LEU fuel. For LEU fuel in a given fuel assembly configuration, the cross sections can be accurately described in terms of the initial uranium enrichment, burnup, and water moderator density. However, for MOX fuel, a larger number of potential parameters must be considered, such as:

- Total plutonium content;

- Plutonium vector (the initial distribution of the isotopes ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, and ^{242}Pu);

- Uranium vector (e.g., typically depleted or natural uranium);

- Americium-241 content;

- Burnup; and

- Moderator density.

A change in any of these parameters will influence the value of the effective cross sections used in the burnup analysis. The large number of potential MOX parameters necessitates careful consideration of the sensitivity of these variables on the cross sections to determine the variables that have the most important effect on the cross sections, and the variables with low importance that can be eliminated without significantly affecting the accuracy of the calculations. Before such an evaluation can be performed, the range of these parameters for MOX fuel must be established.

The ranges considered in the development of the methods and data for this work were determined using data from a previous study involving MOX fuel in Europe,[1] and from fuel composition data compiled using declared records for 1042 MOX fuel assemblies supplied by EURATOM. The assemblies in the database represent a diverse set of designs, covering all designs currently being used in Europe: 14×14, 15×15, 16×16, 17×17, and 18×18 PWR assembly designs, and 8×8, 9×9, and 10×10 BWR assembly designs. The database contained data for 666 PWR MOX assemblies and 376 BWR MOX assemblies. The range of parameters describing the initial compositions of the MOX fuel is summarized in Table 1.

Table 1. Composition ranges for European RG MOX fuel

Parameter	Minimum	Maximum
wt % ^{238}Pu / Pu	0.88	2.40
wt % ^{239}Pu / Pu	53.8	68.2
wt % ^{240}Pu / Pu	22.3	27.3
wt % ^{241}Pu / Pu	5.38	9.66
wt % ^{242}Pu / Pu	2.85	7.59
wt % ^{241}Am / Pu	0.71	2.59
wt % Pu / HM[a]	4.0	9.1
wt % ^{235}U / U	0.24	1.18[b]
wt % $^{239+241}$Pu / Pu	65.4	73.9
wt % fissile Pu + ^{235}U/HM	3.65	5.25

[a] HM = Heavy metal (U + Pu).

[b] Maximum value for PWR MOX assemblies only was 0.72 wt % ^{235}U / U.

The plutonium vector is the distribution of the Pu isotopic concentrations (from ^{238}Pu to ^{242}Pu) and generally sums to 100%. The Pu vector is dependent primarily on the source of the separated plutonium. For RG Pu, the vector is determined to a large extent by the initial enrichment and burnup of the reprocessed uranium fuels. The total storage time of the fuel also influences the vector because ^{241}Pu decays to ^{241}Am with a half-life of approximately 14.4 years. The reduction in ^{241}Pu (and buildup of ^{241}Am) causes the relative fraction of the other Pu isotopes ^{238}Pu, ^{239}Pu, ^{240}Pu, and ^{242}Pu to increase. For example, a decay time of 8 years will result in a reduction of about 35% of the ^{241}Pu inventory, and consequently up to about a 3 wt % increase in the relative isotopic concentrations of the other plutonium isotopes. The Pu vector is not influenced by the time of separation, but only the total time from discharge of the uranium fuel to loading of the MOX fuel in the reactor. However, the time from Pu separation to loading of the MOX fuel in the reactor determines the amount of ^{241}Am in the fuel, since the only source of ^{241}Am in the fabricated MOX fuel is from the decay of ^{241}Pu. Therefore, the time periods important to the fresh MOX fuel compositions are the total time from discharge of the uranium fuel (used to manufacture the MOX) to the loading date of the MOX fuel (effect on the Pu vector), and the time from reprocessing to the loading date (effect on the ^{241}Am content). The storage time of reprocessed Pu is constrained to limit the amount of ^{241}Am to 3 wt % or less to minimize the radiation dose to operators.

The residence times of the spent fuel prior to reprocessing based on data from the U.K. for years from 2000–2002 average 13 years for PWR fuel and 16 years for BWR fuel. In France, the figure is somewhat lower, with an average length of storage before processing of 8 years for

PWR fuel and 6 years for BWR fuel. The average storage time prior to reprocessing at the La Hague plant in France during 2001 was eight years,[2] but with wide variation, dependent on the UO_2 burnup. The storage time is correlated to the spent fuel burnup, with high burnup assemblies typically requiring longer storage time before reprocessing. The average time between reprocessing and MOX fabrication to the reference loading date of the fuel in the reactor was determined directly from the MOX fuel database using the reported ^{241}Am concentrations. Because ^{241}Am is formed from the decay of ^{241}Pu after reprocessing, the time since reprocessing can be determined directly from the ratio of these two nuclides. An evaluation of the declared Pu + Am compositions indicates that the average time between reprocessing and loading was 3.4 years with a standard deviation of ±0.8 years. The minimum and maximum times derived from the database are 1.2 and 6.3 years, respectively.

The majority of MOX fuel rods use either depleted or natural uranium. The values listed in the table represent assembly-averaged compositions. Unlike PWR MOX fuel assemblies that use only MOX fuel rods, BWR MOX fuel assemblies use a combination of MOX and low-enriched UO_2 fuel rods within the same assembly (described in Sect. 4). The maximum average ^{235}U enrichment values reflect the combined use of depleted uranium (in the MOX fuel rods) and low enriched UO_2 fuel rods in the BWR MOX assemblies.

The parameter values in Table 1 were used as a basis to establish the nominal range of validity for the computational methods. In general, the methods and data extend beyond these limits to permit analysis of MOX fuel compositions that may be encountered in the future. However, the principal testing and validation were performed for fuel parameters within these limits.

3   METHODS DEVELOPMENT

The computational methods developed for MOX fuel were based on the existing ORIGEN-ARP sequence[3] of the SCALE code system. This sequence uses the ARP module of SCALE to prepare problem-dependent cross sections for use by the ORIGEN-S isotope generation and decay code.[4] ORIGEN-S is a powerful and flexible computer code for performing isotopic generation and depletion calculations within SCALE for a wide range of spent fuel applications. ORIGEN-S computes time-dependent concentrations and source terms for 1700 nuclides that are simultaneously generated or depleted through neutronic transmutation, fission, and radioactive decay processes. ORIGEN-S also calculates gamma radiation sources using an extensive database that include line-energy photon yields for decay gamma rays and X-rays, prompt and equilibrium spontaneous fission gamma rays, gamma rays accompanying (alpha,n) reactions, and bremsstrahlung radiation created by beta particles slowing down in the medium.[5] Neutron sources are calculated from spontaneous fission, (alpha,n) reactions for any general medium, and delayed neutrons.[6] ORIGEN-S is therefore well suited to accurately characterize the radiation sources for LEU or MOX fuel.

3.1 ARP METHODOLOGY

The ARP methodology adopted for the MOX analysis work generates a problem-dependent cross-section library for use by the ORIGEN-S code from a parameterized database of pre-generated libraries created for a given fuel assembly configuration. If cross sections are calculated for discrete parameter values, such as initial enrichment, moderator density, etc., it is possible to determine cross sections at intermediate values by interpolation. For example, the variation of enrichment in commercial uranium fuel is typically described using enrichment values of 1.5, 2.0, 3.0, 4.0, and 5.0 wt % ^{235}U. A separate cross-section library is generated for each fuel parameter at each discrete parameter value. Cross sections for any intermediate parameter value can then be obtained by interpolating the cross sections generated at the tabulated values. The procedure produces a matrix of libraries that cover the fuel parameters and ranges required for the intended application.

The ARP code functions as a library pre-processor for the ORIGEN-S code. ARP reads the parameterized libraries and interpolates cross sections to produce a single library that contains appropriate cross sections for the particular conditions specified by the user. Interpolating on pre-generated libraries dramatically reduces the computation times compared to conventional reactor physics methods that must perform transport analysis calculations to derive the problem- and time-dependent reaction rates.

Several cross-section interpolation schemes are available within ARP: linear-linear, logarithmic-logarithmic, and logarithmic-linear interpolation. Interpolation of cross sections vs. burnup variable is performed using a unique power-fitting algorithm, originally developed to interpolate resonance self-shielded cross sections.[7] The scheme has been demonstrated to be robust for fitting functions of varying and unknown complexity.

The ARP methods currently implemented in SCALE for uranium fuel types allow a maximum of three interpolation parameters: enrichment, burnup, and (optionally) moderator density. Separate libraries have been developed for the different fuel assembly design types (classes). For PWR

assemblies, libraries are typically generated using a single, average moderator density, and therefore these libraries use only two parameters, enrichment and burnup, to characterize the fuel cross-section variation for a given assembly design. Since the burnup-dependent cross-section sets are contained within the same physical library, the current methods require relatively few libraries, about five, to cover the range of enrichments in typical commercial PWR fuels. For BWRs that typically have eight variable water moderator densities, the methods typically require 40 separate libraries.

3.2 MOX FUEL PARAMETERS

Development of an interpolation strategy for MOX fuel libraries requires the consideration of more parameters than is necessary for LEU. The parameters that were considered for MOX fuels in this study include:

1. Reactor type and assembly design;

2. Total plutonium content;

3. Plutonium vector (the distribution of the plutonium isotopes ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, and ^{242}Pu);

4. Uranium vector (e.g., typically depleted or natural uranium);

5. Americium-241 content (generated by decay of ^{241}Pu after reprocessing);

6. Burnup; and

7. Moderator density.

The reactor type and fuel assembly design is an important consideration in developing MOX cross-section libraries. There are a wide range of assembly designs in use. Assembly design (and reactor type) was not considered as an interpolation parameter. To address the variability of the different designs, separate MOX libraries were developed for each distinct assembly design.

Some of the parameters, such as the plutonium content and burnup, will have a large effect on the value of the cross sections. Other parameters, such as the uranium vector and ^{241}Am content, are expected to have a much smaller effect since the variability of these parameters for MOX fuel is typically small and the effect on the neutronic environment is thus small. Considering only the parameters associated with plutonium (e.g., Pu content, and the vector for the five Pu isotopes) yields a total of six potential interpolation parameters. If every parameter is represented by just three tabulated cross-section points over the range of each parameter (each point requires a unique cross-section library), a total of 3^6 (=729) separate cross-section libraries would be required. This does not include consideration of the other potential interpolation parameters, such as the uranium vector or moderator density, which would require considerably more libraries. Clearly, the large number of potential parameters for MOX fuel necessitates a more pragmatic solution to avoid having to generate large numbers of libraries with excessive

data storage requirements. To minimize the number of parameters and libraries, it is necessary to evaluate the different parameters and identify those parameters that have a large effect on the cross sections, and those that do not have a significant effect (and therefore may not warrant separate libraries). Parameters that are not considered variable (i.e., low-importance parameters) are typically set to their average values.

The remainder of this section describes each of the parameters considered in the development of MOX cross-section libraries, the variability of the cross sections for each parameter, and the verification and testing of the methods that were performed.

3.2.1 Plutonium Content

The total Pu content in MOX fuel varies according to the amount of fissile ^{239}Pu and ^{241}Pu in the plutonium and the required total fissile loading for the assembly. The range of plutonium content in MOX fuel currently used in Europe varies from about 4 to 9 wt % Pu in total heavy metal (see Table 1). Cross-section libraries were developed in this work to cover a range from 4 to 10 wt % Pu to cover potential future MOX fuel that may utilize higher Pu contents to compensate for the trend towards plutonium from higher burnup fuel (with smaller quantities of fissile Pu).

The effective absorption cross-section variation of the major uranium and plutonium isotopes in typical MOX fuel with changing total Pu content is illustrated in Fig. 1. The effective cross section is defined here as the flux-weighted one-group microscopic cross section normalized to the thermal flux below 0.5 eV. The cross sections for most actinides exhibit a relatively low sensitivity to the Pu loading over the range of interest. The cross section for ^{238}U shows the largest sensitivity, increasing from about 150 barns at 4 wt % Pu/HM^a to 300 barns at 10 wt % Pu/HM. Notably, the variation for all major actinides is uniform over the range, and is very nearly linear for many nuclides. The cross-section variations for several transuranic (TRU) nuclides are illustrated in Fig. 2. The TRU nuclides were selected on the basis that they are the principal transmutation chain for the production of ^{244}Cm, the dominant spontaneous fission neutron source nuclide in spent fuel. The variation for the fission products ^{133}Cs and ^{153}Eu are also shown in Fig. 2. These fission products are the precursor nuclides to the important gamma-ray sources ^{134}Cs and ^{154}Eu, which are thus highly influenced by the value of their precursor cross sections. These nuclides differ from many other fission products that are produced predominantly by direct fission yield and exhibit less sensitivity to the value of the cross sections. Again, the variations in the cross sections are observed to be smooth over the range of interest. The cross sections for ^{243}Am and ^{153}Eu exhibit the largest relative changes with respect to Pu content.

In all cases, the variation of the cross sections is seen to be smooth and well behaved over the region. The importance of this behavior to the library development is that the cross sections may be accurately interpolated over the range of Pu content values using a relatively broad cross-section grid.

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^{a} HM = Heavy metal (total U + Pu).
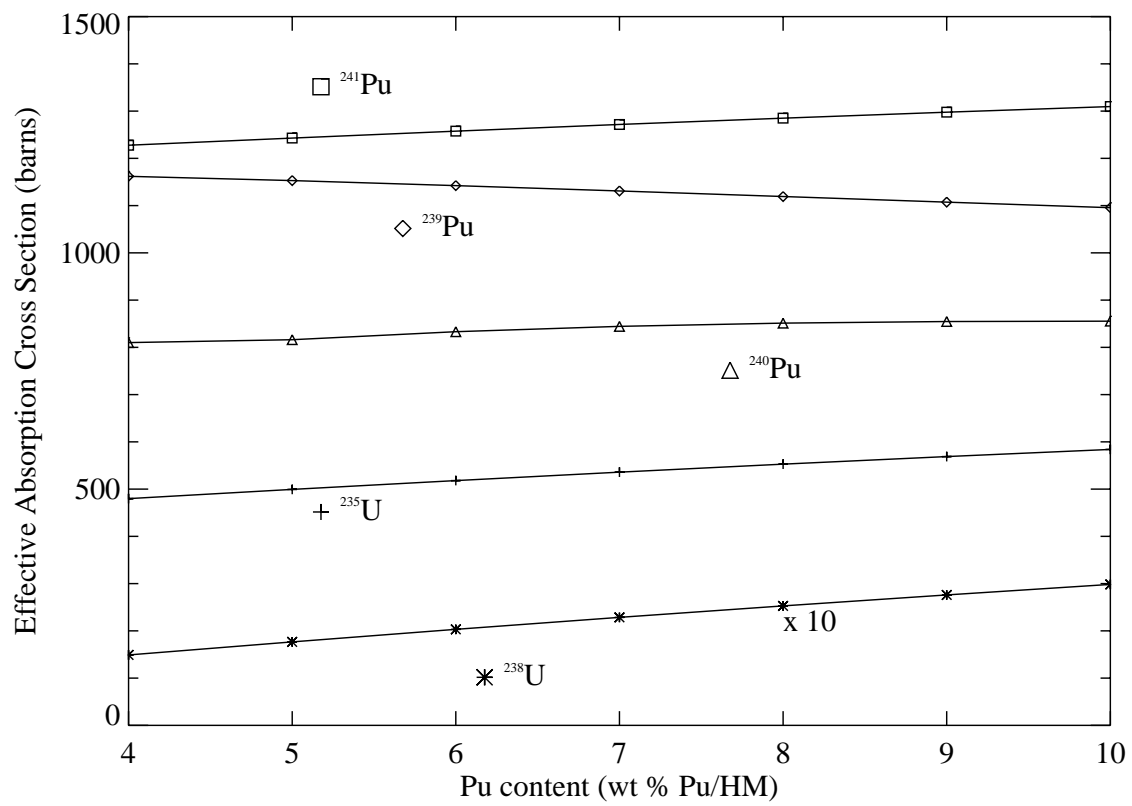
Fig. 1. Uranium and plutonium absorption cross sections vs. plutonium content.

12
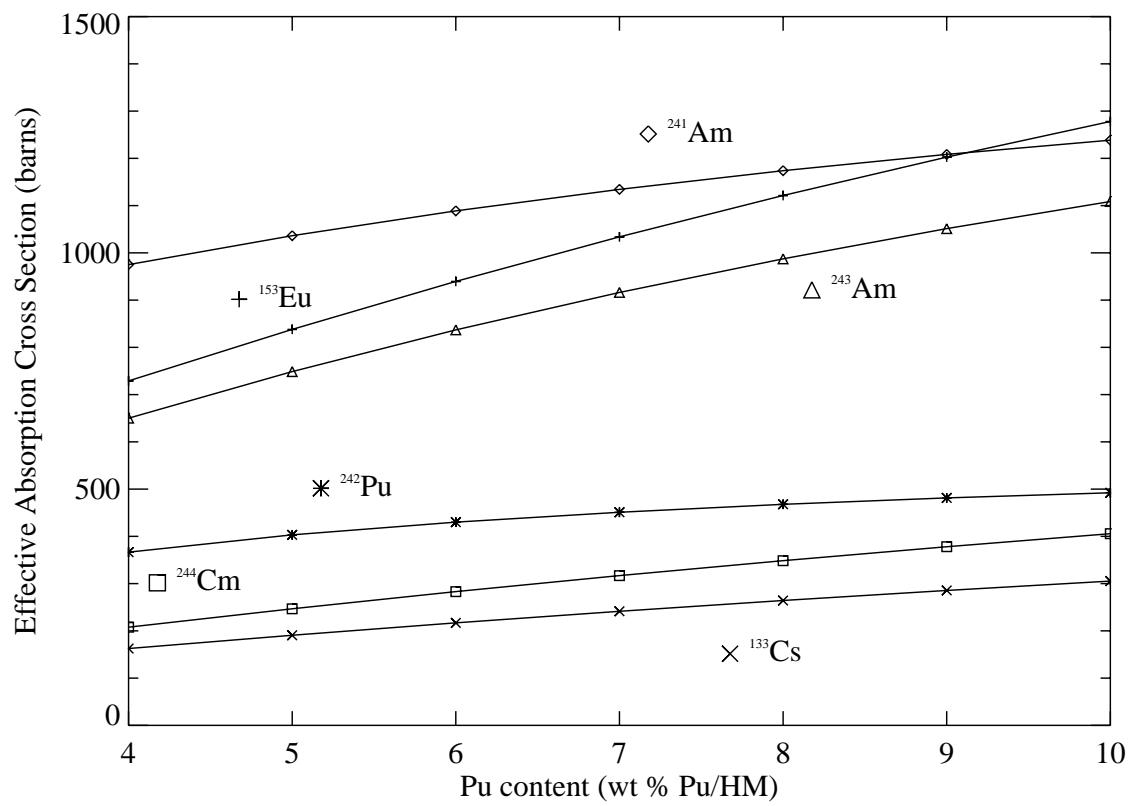
Fig. 2. TRU and fission product absorption cross sections vs. plutonium content.

3.2.2 Plutonium Isotopic Vector

The distribution of the Pu isotopic vector represents the most complex parameter in developing MOX cross-section libraries using an interpolation strategy. The Pu vector is made up of five individual isotopes (^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, and ^{242}Pu), which represent potentially five different interpolation parameters. Parameterization of the Pu vector is complicated by the fact that each isotope in the vector is dependent on the other isotopes. Increasing or decreasing the amount of one isotope requires a corresponding decrease or increase in the other Pu isotopes, since the sum of the Pu vector is 100%. This dependency necessitates that the Pu vector be considered as a group, and that the variation in the vector used to tabulate the cross sections over the range be done in a way that preserves the variation observed in actual MOX fuels.

Although, individually, the Pu isotopic concentrations in MOX fuel vary over a relatively wide range, the concentrations are highly correlated to one another. The vector correlation is a result of the relationships defined by the transmutation cross sections that govern the Pu production chain. The correlation limits the Pu isotopic vector combinations that can physically be obtained. The high degree of correlation in the Pu isotopic fractions is illustrated in a scatter-plot matrix in Fig. 3 using declared fuel data compiled for 1042 MOX fuel assemblies from Europe. The concentration (wt %) of each Pu isotope is plotted as a function of all other isotopes for each of the 1042 assemblies. The correlation coefficients (c_{ij}) for any pair of Pu isotopes, which represent the degree to which the data are interrelated, are listed in Table 2.

Table 2. Correlation coefficients (c_{ij}) for the plutonium isotopic vector

Pu isotope	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu
^{238}Pu	1.0000				
^{239}Pu	0.9113	1.0000			
^{240}Pu	0.6956	0.9017	1.0000		
^{241}Pu	0.7511	0.8048	0.5414	1.0000	
^{242}Pu	0.9519	0.9763	0.8574	0.7241	1.0000
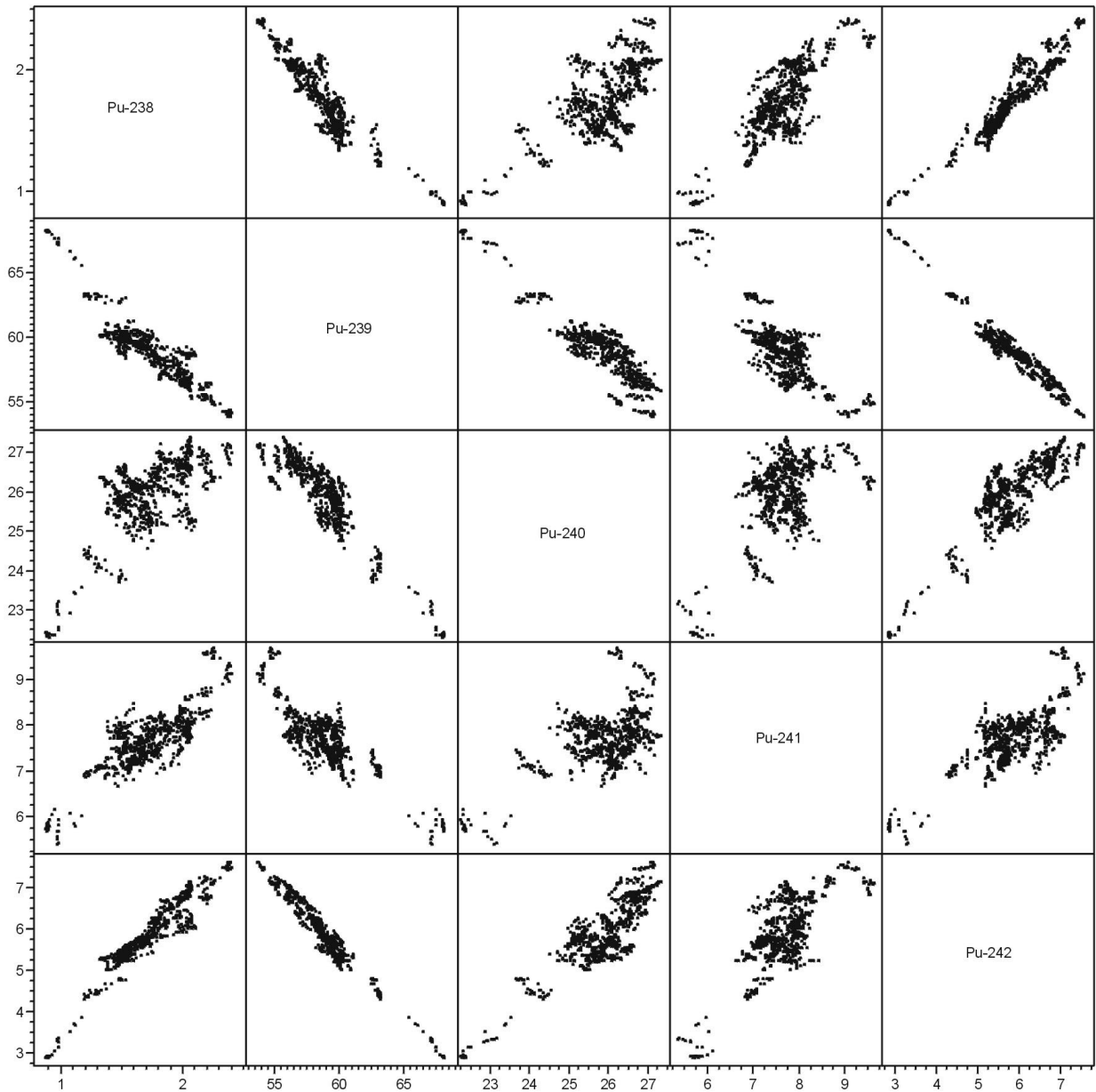
Fig. 3. Scatter-plot matrix of Pu isotopic vectors from 1042 MOX assemblies. Axis units are wt % of each Pu isotope relative to the total Pu mass.

A review of the correlation coefficients indicates that ^{239}Pu has the highest degree of overall correlation to the concentrations of the other isotopes in the Pu vector, with all coefficients $c_{ij} = 0.9$ or greater, with the exception of ^{241}Pu ($c_{ij} = 0.80$). Therefore, given the concentration of ^{239}Pu the concentrations of all other Pu isotopes can be estimated to a high degree of accuracy. As uranium burnup increases, the ^{239}Pu isotopic fraction decreases while the ^{238}Pu, ^{240}Pu, ^{241}Pu, and ^{242}Pu fractions all increase with burnup. The larger variability (smaller correlation coefficient) observed for ^{241}Pu is attributed to its relatively short half life of 14.4 years that makes it particularly sensitive to variations in the storage and decay time.

The factors that influence the variability in the Pu vector include the burnup of the discharged uranium fuel elements from which the Pu is separated, the fuel assembly design (e.g., 17×17, 14×14, 15×15), fuel-to-moderator ratio, use of burnable poison rods, control rod use, soluble moderator boron levels, reactor type (e.g., PWR, BWR, MAGNOX, AGR, etc.), and storage time. The impact of the total storage time on the Pu vector was briefly discussed previously in Sect. 2. Because the total cooling time of the spent fuel will depend on the burnup, and will vary by country and nuclear power plant, there is no single value for storage time that will be representative of all MOX fuel.

The interpolation strategy implemented for the Pu vector exploits the correlation in the different isotopes in the vector to determine appropriate cross-section values used in the depletion analysis. Several interpolation approaches were studied. These methods are discussed in the following sections.

3.2.2.1   Single-parameter approach

The relatively high correlation of ^{239}Pu to all other Pu isotopes was used as a basis for a single-parameter interpolation strategy, whereby cross sections for all isotopes in the vector were determined on the basis of the ^{239}Pu concentration only. This effectively reduces the five isotopic parameters (one for each Pu isotope) representing five "degrees of freedom," to a single parameter. A limitation of this procedure is that the Pu vector is only represented accurately for vectors that are typical of RG MOX fuel.

The weight percentage of ^{238}Pu, ^{240}Pu, ^{241}Pu, and ^{242}Pu as a function of the ^{239}Pu are shown in Fig. 4 based on the MOX data for the 1042 assemblies. The data were fit using a least-squares regression analysis to a second-order polynomial (quadratic) equation of the form:

$$v_i = a_i x^2 + b_i x + c_i ,$$

where x is the ^{239}Pu concentration in relative wt %, and v_i are the vector concentrations for all other Pu isotopes (i). The coefficients obtained from the regression analysis are listed below.

i	a	b	c
^{238}Pu	4.5678E-03	−6.6370E-01	2.4941E+01
^{240}Pu	−1.1329E-02	1.0271E+00	4.7929E+00
^{241}Pu	1.8630E-03	−4.2787E-01	2.6355E+01
^{242}Pu	4.8985E-03	−9.3553E-01	4.3911E+01
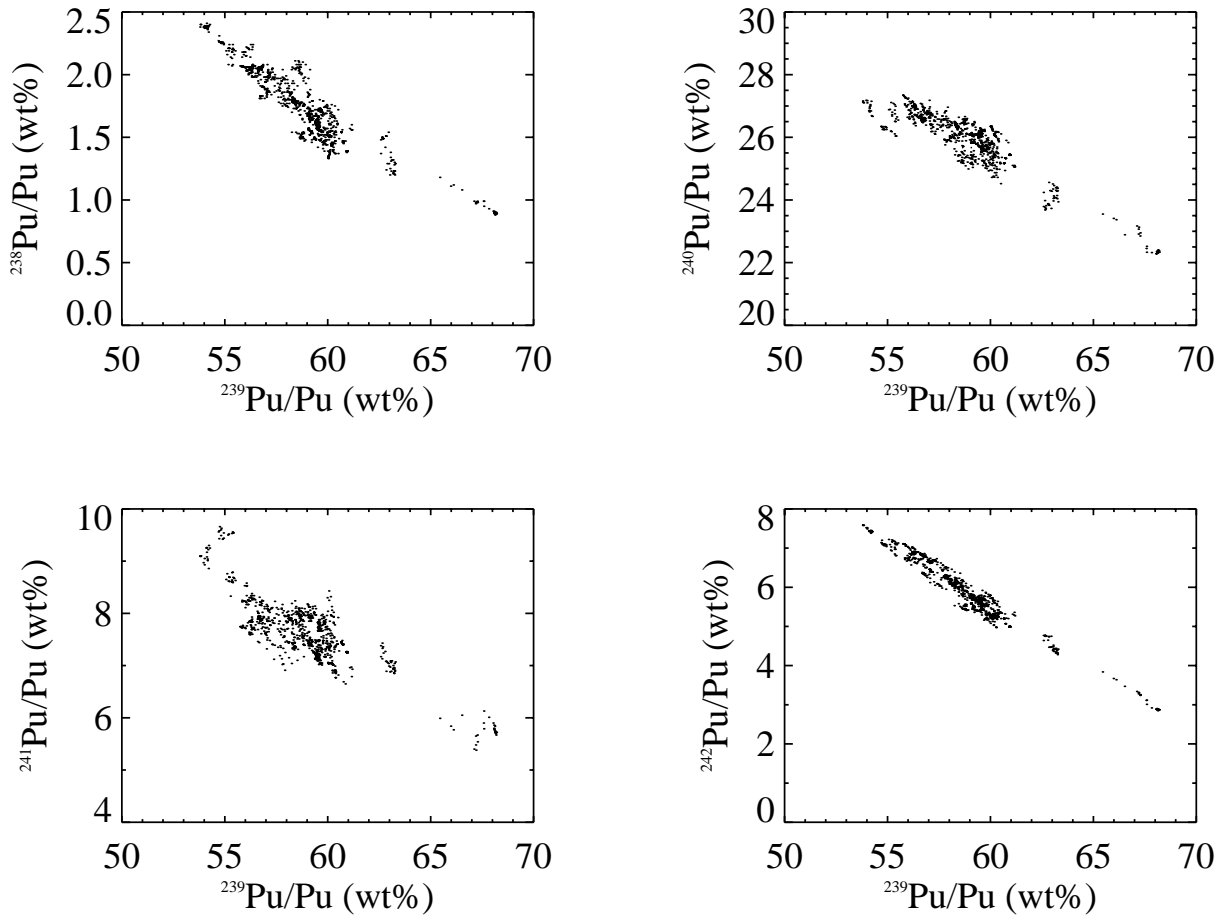
Fig. 4. Relative plutonium isotopic concentrations vs. ^{239}Pu/Pu concentration for declared MOX data.

The polynomial equations reproduce the values of the isotopic vector in the database with relative standard errors of 6.1% (^{238}Pu), 1.3% (^{240}Pu), 4.3% (^{241}Pu), and 2.8% (^{242}Pu). That is, given only the relative ^{239}Pu content, the concentration of all other Pu isotopes are generally predicted to within several percent of the actual values. The residuals (differences between the actual and predicted vectors), expressed as the relative standard error (percent difference), are illustrated in Fig. 5. The sum of the vector components using the interpolated vector data are required to sum to 100%. The results using the MOX data sets were within 0.001% of the required total for all sets indicating that the fit procedure produces reliable vector results.

3.2.2.2   Two-parameter approach

In an attempt to decrease the deviations in the single-parameter interpolation (^{239}Pu), a two-parameter approach was investigated. The variability observed in the ^{239}Pu approach is attributed to the fact that only fuel burnup is considered. Variations in the relative concentrations of other isotopes to ^{239}Pu are influenced by many factors (discussed in Sect. 3.2.2) which can not be accounted for with only one parameter. By interpolating with two vector components, instead of only one, greater accuracy may be achieved. The remaining Pu isotopes that exhibit the largest correlation coefficients are ^{238}Pu and ^{242}Pu. Intuitively, these isotopes are likely candidates since they are strongly influenced by the neutron flux spectrum in the fuel (i.e., the cross sections), and thus will be sensitive to the assembly designs and reactor types. An evaluation of these isotopes indicated both had favorable characteristics; however the response surface of ^{239}Pu and ^{238}Pu provided the best overall fit results.

The variation of the ^{240}Pu, ^{241}Pu, and ^{242}Pu were each determined as a function of ^{238}Pu and ^{239}Pu using a surface response regression analysis of second-order having the form:

$$v_i = a_i x_8 + b_i x_9 + (x_8 - \varepsilon_1)^2 c_i + (x_9 - \varepsilon_2)^2 d_i + (x_8 - \varepsilon_1)(x_9 - \varepsilon_2) e_i + f_i ,$$

where x_8 is the ^{238}Pu concentration, x_9 is the ^{239}Pu concentration (both in units of relative wt %), v_i are the concentrations for all other dependent isotopes (i) in the vector, ε_1 and ε_2 are independent variable offsets, and variables a_i, b_i, c_i, d_i, e_i, and f_i are coefficients for each isotope i, derived from the fit. The fit coefficients are listed below.

i	^{240}Pu	^{241}Pu	^{242}Pu
a	64.8180	17.6426	17.5408
b	−2.20373	0.12082	1.08276
c	−0.59528	−0.17501	−0.22973
d	−1.36949	3.82216	−2.45304
e	−0.10985	0.49296	−0.38331
f	0.00089	0.01338	−0.01429
ε_1	58.9217	58.9217	58.9217
ε_2	1.71672	1.71672	1.71672
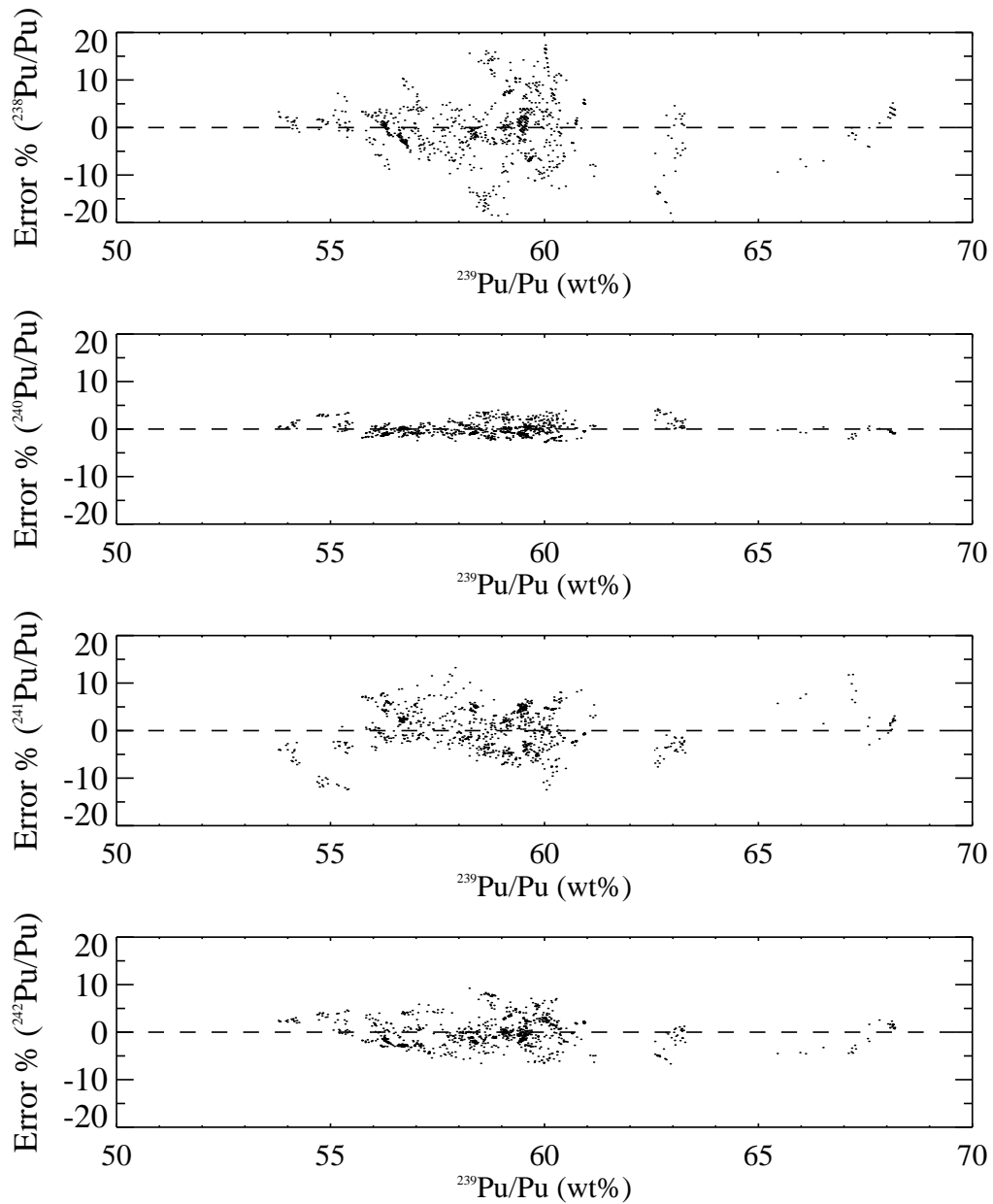
Fig. 5. Relative standard error in the Pu vector concentrations obtained using single-parameter (^{239}Pu) interpolation for the 1042 assemblies in the MOX vector database.

The two-vector interpolation approach reproduced the values of the dependent isotopic vector components with relative standard errors of 1.0% (^{240}Pu), 4.2% (^{241}Pu), and 1.8% (^{242}Pu). These errors are somewhat smaller compared to the single vector approach described in the previous section. Again, the larger variability in ^{241}Pu is attributed to the effect of different MOX fuel storage times.

For the analysis of European MOX fuel, the single-parameter approach using only the relative ^{239}Pu content to derive cross sections for the other isotopics in the vector was deemed to be of sufficient accuracy. This approach minimizes the number of cross-section libraries that must be generated and stored for the analysis. The accuracy of the single-parameter approach is validated in benchmarks described in Sect. 6. For analysis of MOX fuel vectors that are atypical of those used in deriving the fit coefficients, the ability to use a second vector interpolation parameter (^{238}Pu) has been retained in ARP and may be used in the future. All subsequent analyses described in this report were performed using the single-parameter approach.

It is important to emphasize here that the interpolation procedure is used only to obtain the cross sections used in the MOX burnup calculation. Although the cross sections for the analysis are derived using a plutonium vector derived from the least squares analysis of the MOX data, the actual Pu vector is always used to define the actual compositions input to the ORIGEN-S code. As shown in the previous section, the fit procedure reproduces the actual Pu vector to within several percent on average, for each vector isotope. The impact of the vector approximations on the Pu cross-section values, rather than just the concentrations, is evaluated later in Sect. 3.

3.2.3 Americium-241 Content

Americium-241 exists in unirradiated MOX fuel as a result of β^- decay of ^{241}Pu after the plutonium is separated from the irradiated uranium fuel. The ^{241}Pu decays with a half life of 14.4 years. Consequently, the amount of ^{241}Am increases rapidly within several years of reprocessing, and can cause a significant radiation hazard from the neutron and gamma rays associated with the decay of ^{241}Am. The dose rate increases about a factor of two every 120 days of storage for the first several years caused by ^{241}Am in-growth at a rate of 0.48% of the ^{241}Pu concentration per year.[8] Therefore, there is considerable incentive to limit the amount of storage time of reprocessed plutonium or fabricated MOX fuel prior to reactor loading.

The ^{241}Am content in MOX fuel was studied to determine the typical range of variation, and the importance of the variation on the cross sections. A review of the composition database of MOX fuel assemblies indicates that the time from reprocessing to the reference reactor loading date, based on the declared ^{241}Pu and ^{241}Am concentrations, ranged from a minimum of 1.2 years to a maximum of 6.3 years, with an average of 3.4 ± 0.8 years. This result indicates that the majority of fuel has a relatively consistent storage time, e.g., 67% of the fuel is within $\pm 25\%$ of the average value. These values are consistent with other MOX data from independent accountancy declarations that give a time from reprocessing to the reference MOX fuel loading date of 1.5 to 4.4 years, with an average time (for the year 2001) of 2.5 years.

Based on this relatively low variability, and the small concentration of ^{241}Am typically present in MOX fuel (about 1% of the total Pu content), the MOX cross-section libraries were developed assuming a ^{241}Am concentration based on constant storage time after reprocessing of 3.4 years.

However, the actual concentration of ^{241}Am is used in the initial MOX fuel composition for a burnup analysis. To assess the effect of this library approximation on typical MOX calculations, the results from simulations that explicitly accounted for the ^{241}Am variation were compared to the results obtained using the approximations described. The results confirmed the relatively low sensitivity of the cross-section values to ^{241}Am content. Further quantitative evaluation of the methods and approximation are described later in Sect. 3.

3.2.4   Uranium Isotopic Vector

The uranium in MOX fuel rods is typically either depleted or natural uranium oxide. The range of the average ^{235}U/U concentrations in MOX fuel assemblies used in Europe is from 0.2 to 1.2 wt %. Enrichments of 0.24 wt % and 0.71 wt % are most common for PWR assemblies. Assembly-averaged enrichments greater than 0.71 wt % are attributed to the use of both low-enriched UO$_2$ fuel rods and MOX fuel rods in BWR MOX assembly designs.

The importance of the uranium vector in developing MOX fuel cross sections was evaluated by comparing the nuclide concentrations predicted with MOX libraries, created with a fixed nominal uranium enrichment, against more rigorous SCALE depletion calculations performed assuming variable uranium enrichments. The calculations performed assuming 0.71 wt % ^{235}U in the MOX fuel yielded a bias in the predicted concentrations of the major actinides (through ^{244}Cm) and important fission products that was typically less than 1% when compared to cross sections developed assuming a fixed enrichment of 0.24 wt %. The maximum bias observed in the predicted concentrations of any isotope was about 5% (for ^{245}Cm). The bias introduced by using a constant ^{235}U enrichment is considered acceptable for typical MOX analyses.

The libraries developed for PWR MOX in this project assumed a nominal fixed uranium enrichment of 0.24 wt % ^{235}U. For BWR MOX fuels, a higher average ^{235}U enrichment is appropriate. Although the user may specify any enrichment to define the actual initial fuel compositions used in the burnup calculation, the cross sections are developed for MOX fuel assuming the ^{235}U enrichment is invariant. In all cases studied, the net effect on the predicted nuclide concentrations was observed to be small. The effect of this approximation is evaluated later in Sect. 3.

3.2.5   Burnup

The variation of the major actinide cross sections as a function of burnup is illustrated in Fig. 6 for a composition representative of European MOX fuel. This example corresponds to a 17×17 MOX assembly with 6 wt-% plutonium and a typical first-recycle Pu isotopic vector. The cross sections plotted in the figure are the effective total absorption cross sections, normalized to the thermal flux. The figure shows that the cross sections exhibit a smooth variation with burnup over the range. The cross sections typically exhibit a small increase immediately after the start of irradiation, due to the spectral shift caused by the rapid buildup of short-lived fission products. The cross-section variation for selected fission products and minor actinides is shown in Fig. 7. These nuclides were selected because of their importance to the production of ^{244}Cm or their importance as neutron capture precursors to the radiological important fission products ^{134}Cs and

Fig. 6. Effective absorption cross-section variation with burnup for major uranium and plutonium isotopes in MOX fuel. The cross sections are normalized to thermal neutron flux.

Fig. 7. Effective absorption cross-section variation with burnup for minor actinides and selected fission products in MOX fuel. The cross sections are normalized to thermal neutron flux.

[154]Eu. Again, the variation in the cross sections for these nuclides is observed to be smooth over the burnup range.

The cross-section behavior is somewhat different than that observed in UO_2 fuel, particularly for [240]Pu, which exhibits a dramatic change with burnup in UO_2 fuel (see Ref. 1), decreasing from about 1700 barns for fresh fuel, to about 800 barns for a burnup of 50 GWd/t. This rapid decrease is not observed to the same extent in MOX fuel because MOX fuel contains a substantial quantity of plutonium initially, unlike UO_2 that contains no initial plutonium. Therefore the plutonium concentrations, and thus the cross sections, exhibit smaller changes in MOX fuel during irradiation. This behavior in the cross section allows MOX cross sections to be interpolated accurately from tabulated cross-section data using a relatively broad burnup grid compared to LEU fuel.

3.2.6 Moderator Density

The effect of moderator density on the cross sections is most pronounced in BWRs because of the large axial variation in the void fraction. The change in the moderator density (void fraction) alters the fuel-to-moderator ratio and shifts the neutron flux spectrum in the fuel. As the density decreases, the spectrum becomes less thermal (harder) resulting in increased plutonium production. This, in turn, alters the value of the effective cross sections.

A review of the axial variation in moderator temperature for a PWR indicates the density typically ranges from about 0.78 g/cm^3 at the bottom of the assembly, to a minimum of about 0.68 g/cm^3 at the top of the assembly, for a pressure of 158 kg/cm^2 (2250 psi). Although some reactors may operate outside of this range to some degree, the range is expected to be representative of the vast majority of PWRs. The average moderator temperature for the European MOX reactors, determined from reactor operating data,[9] is about 576 K. This temperature yields a mean moderator density of about 0.72 g/cm^3.

The axial moderator density variation means that the effective cross sections will also vary axially. Thus, compositions predicted using cross sections developed for the top of an assembly will be different than the compositions using cross sections at the bottom of the assembly, for the same burnup. The importance of simulating variable moderator density in the PWR MOX libraries, compared to using an average moderator density, was investigated.

The predicted concentrations for more than 50 nuclides important to a wide range of radiological properties calculated using a mean moderator density of 0.72 g/cm^3 were compared to the results calculated using limiting values of 0.68 and 0.78 g/cm^3. The results, for a cooling time of 5 years, show that the maximum relative deviation from the mean moderator density was 5% for any single nuclide. The average deviation was about 2%. The deviation observed for [244]Cm was 4%, and the deviations for [134]Cs and [154]Eu were 3% and 4%, respectively. The deviations in the total neutron and gamma-ray sources were 4% and <1%, respectively.

Based on these findings, variable moderator density was not implemented in the PWR MOX libraries. The MOX libraries were generated using the average axial moderator density representative of the different PWRs. If warranted, variable moderator density may be implemented for PWR fuels in the future.

Variable moderator density was implemented in the BWR MOX libraries because of the large axial variations experienced by the assembly. The effect of moderator density on the effective cross sections for MOX fuel is illustrated in Figs. 8 and 9. The cross sections exhibit a strong dependence on the moderator density over the range of 0.2 to 0.8 g/cm^3.
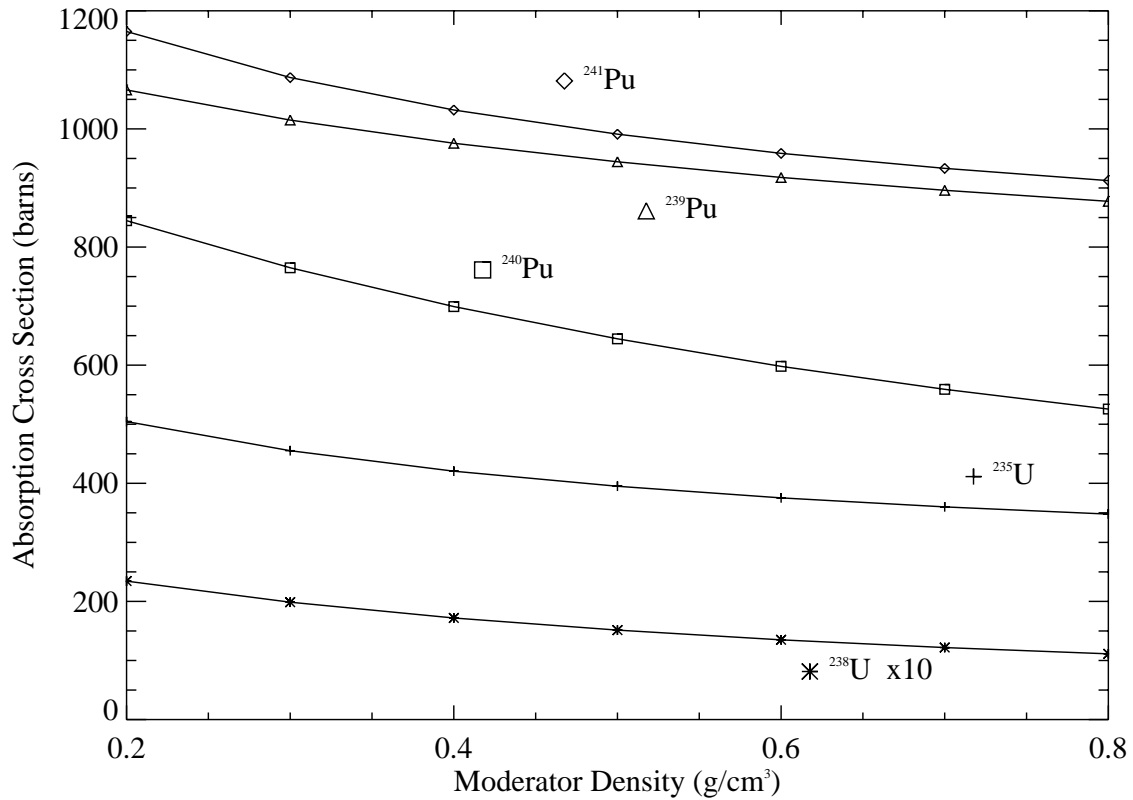
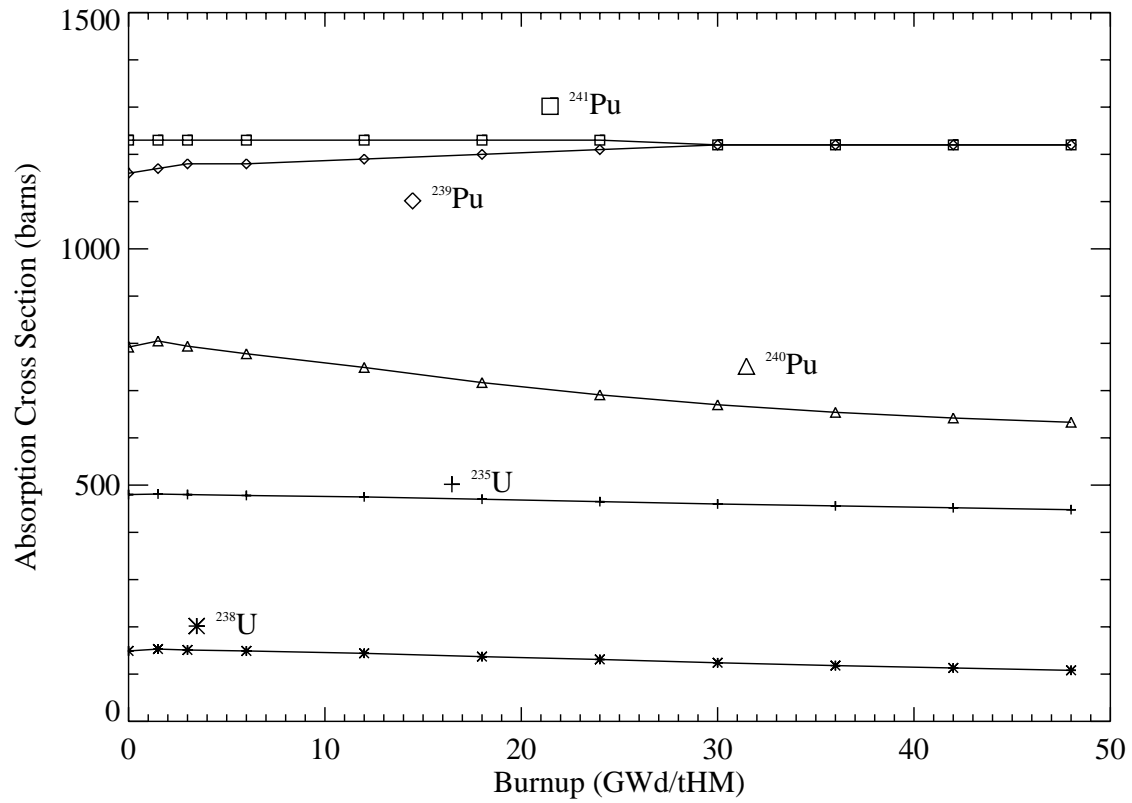**Fig. 8. Effective absorption cross-section variation with water moderator density for major uranium and plutonium isotopes in MOX fuel. The cross sections are normalized to thermal neutron flux.**

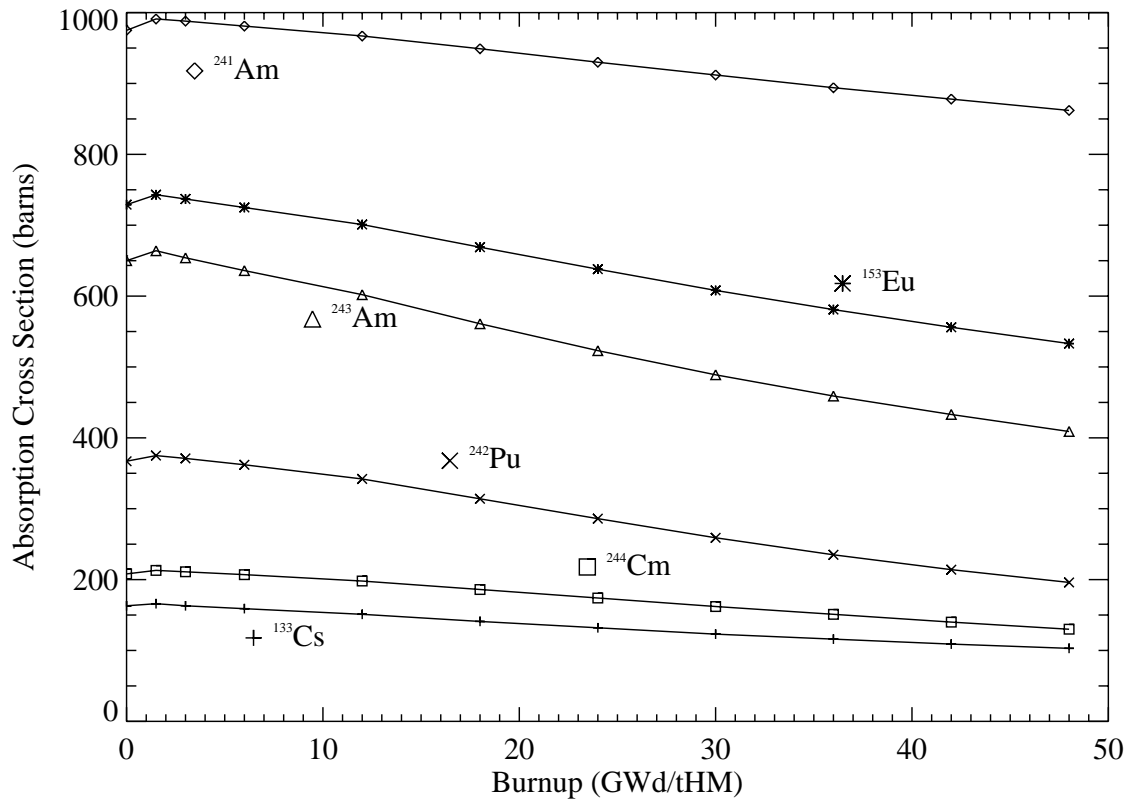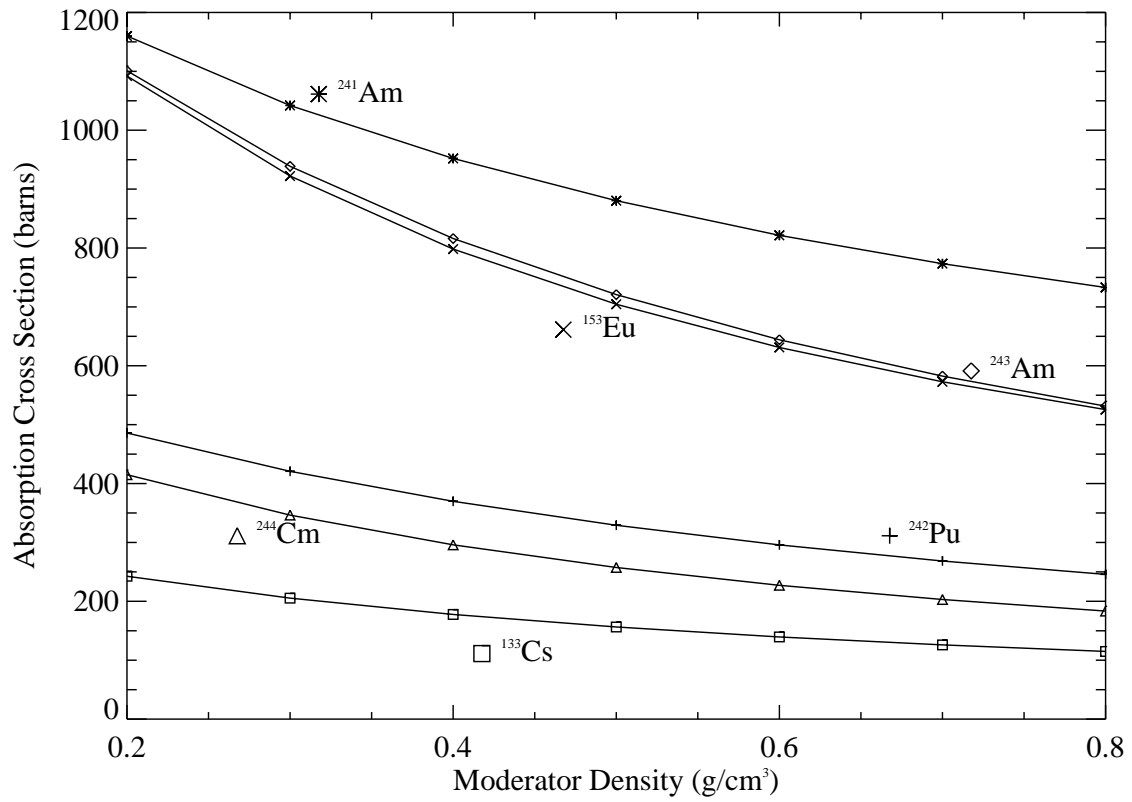**Fig. 9.** Effective absorption cross-section variation with water moderator density for minor actinides and selected fission products in MOX fuel. The cross sections are normalized to thermal neutron flux.

3.3 INTEGRAL METHODS VERIFICATION

Additional methods verification studies were performed to evaluate the accuracy of the interpolation methods described in the preceding sections for determining appropriate cross sections for MOX burnup calculations. Again, the database of declared compositions for 1042 MOX assemblies supplied from EURATOM were used for this purpose. The integral effect of the interpolation methods and assumptions used in developing MOX cross sections were evaluated for the following parameters:

- the Pu vector,

- Pu content,

- assumption of a constant uranium enrichment, and

- assumption of a constant storage time to derive the ^{241}Am concentration.

The interpolation methods developed for MOX fuel were applied to determine cross sections for the dominant uranium and plutonium isotopes, and selected minor actinides and fission products, for each of the 666 PWR assemblies in the database. The interpolated cross sections were then compared to those calculated using the SAS2H depletion analysis code of SCALE, using the actual declared concentrations for each of the Pu, U, and ^{241}Am isotopes. Because the SAS2H code was used to generate the basic MOX cross-section libraries used by the ARP code (as described in Sect. 5), any differences between the cross sections can be directly attributed to the interpolation methods and approximations.

The calculations were performed for a 17×17 PWR MOX assembly model. The results are summarized in Table 3 for each of the selected nuclides as the average relative deviation (bias) between the effective one-group cross-section values determined by interpolation, and the values calculated by SAS2H. Overall, the interpolation methods reproduce the more exact cross sections calculated by SAS2H to within 1% on average for all of the actinides studied. In all cases, the standard error of the interpolated cross sections was within about 1% of the SAS2H values.

Table 3. Relative standard error in the interpolated cross sections based on analysis of 666 PWR MOX assemblies

Nuclide	Cross-section relative error (%)
^{235}U	-0.4 ± 0.2
^{238}U	-1.0 ± 2.0
^{238}Pu	0.5 ± 0.1
^{239}Pu	-0.4 ± 0.2
^{240}Pu	-0.3 ± 1.3
^{241}Pu	-0.5 ± 0.2
^{242}Pu	-0.8 ± 2.0
^{241}Am	-0.3 ± 1.0
^{243}Am	-1.0 ± 1.8
^{244}Cm	-0.9 ± 1.9
^{133}Cs	-0.9 ± 1.8
^{153}Eu	-2.3 ± 0.8

4   MOX FUEL ASSEMBLY DESIGNS

MOX assemblies differ from LEU assemblies only in fuel material; the UO_2 is replaced by PuO_2-UO_2 mixed oxide. In general, the geometry, the dimensions, and the cladding material are identical for MOX and UO_2 assemblies. The MOX fuel material compositions, based on experience in Europe, were summarized previously in Sect. 2. This section summarizes the assembly design characteristics for the MOX fuel assemblies used in Europe, and the fuel design specifications and reactor operating conditions used to generate the MOX fuel cross-section libraries. The reactors currently operating with MOX fuel in Europe are listed in Table 4 with a description of the plant type and fuel assembly design. The majority of MOX fuel is currently irradiated in PWRs, with a smaller quantity used in BWRs. Although the U.K. reprocesses spent fuel for MOX fuel production at its Sellafield and THORP MOX plants, it does not currently use MOX fuel. The MOX assembly designs currently used in Europe include: 14×14, 15×15, 16×16, 17×17, and 18×18 PWR assembly designs, and 9×9 and 10×10 BWR assembly designs.

The basic fuel assembly design specifications (dimensions) for each assembly type are listed in Table 5. The values for the number of fuel rods, fuel rod pitch, fuel pellet outside diameter, and the cladding (rod) outside diameter were compiled from data in Refs. 9, 10 and 11. The table includes specifications for a MOX 8×8 BWR assembly, although this design is presently not in use. The assembly specifications listed in Table 5 were used to develop models to generate cross-section libraries for each of the respective MOX assembly designs. Where design specifications differed by fuel vendor for the same assembly type, the specifications that were considered most representative of the nuclear plants in Europe were selected.

When a burnup calculation is performed using ORIGEN-ARP, the user selects the cross-section library for the assembly type, assembly-averaged compositions, and the power history information. The details of the assembly design information are reflected in the values of the cross sections in the library used in a burnup analysis. Therefore, it is important that the design information and fuel configurations used in developing the libraries accurately represent the types of configurations to be analyzed. The reactor conditions and details of the assembly material specifications used in developing the MOX libraries for this project are described in more detail in Sect. 5.

4.1 PWR MOX ASSEMBLY DESIGNS

PWRs utilizing MOX assemblies typically operate with a mixed core of both MOX assemblies and UO_2 assemblies. The MOX assemblies typically contain only MOX rods. MOX fuel rods with different plutonium contents are used within the same assembly, called MOX zoning, in order to achieve a more balanced power distribution in the assembly. Three zones are typically used in the MOX assemblies, with the plutonium content of each rod being dependent on the position of the rod in the assembly. Low Pu content zones are located at the assembly periphery to compensate for power variations caused by a large thermal flux at the interface of the MOX and UO_2 assemblies. A typical fuel rod arrangement for a 17×17 MOX assembly is illustrated in Fig. 10.

Table 4. Nuclear reactors operating with MOX fuel in Europe

Country	Reactor	Type / MWe	Lattice
Belgium	Tihange 2	PWR 900	17×17
	Doel-3	PWR 900	17×17
France	St. Laurent B1	PWR 900	17×17
	St. Laurent B2	PWR 900	17×17
	Gravelines 1	PWR 900	17×17
	Gravelines 2	PWR 900	17×17
	Gravelines 3	PWR 900	17×17
	Gravelines 4	PWR 900	17×17
	Dampierre 1	PWR 900	17×17
	Dampierre 2	PWR 900	17×17
	Dampierre 3	PWR 900	17×17
	Dampierre 4	PWR 900	17×17
	Le Blayais 1	PWR 900	17×17
	Le Blayais 2	PWR 900	17×17
	Triscastin 1	PWR 900	17×17
	Triscastin 4	PWR 900	17×17
	Chinon B1	PWR 900	17×17
	Chinon B2	PWR 900	17×17
	Chinon B3	PWR 900	17×17
	Chinon B4	PWR 900	17×17
Germany	Brokdorf	PWR 1300	16×16
	Grafenrheinfeld	PWR 1300	16×16
	Grohnde	PWR 1300	16×16
	Gundremmingen B	BWR 1300	$9 \times 9 / 10 \times 10$
	Gundremmingen C	BWR 1300	$9 \times 9 / 10 \times 10$
	Isar 2	PWR 1440	18×18
	Neckarwestheim 2	PWR 840	18×18
	Obrigheim	PWR 350	14×14
	Philippsburg 2	PWR 1300	16×16
	Unterweser	PWR 1300	16×16
Switzerland	Beznau 1	PWR 350	14×14
	Beznau 2	PWR 350	14×14
	Goesgen	PWR 1020	15×15

Table 5. MOX fuel assembly design parameters

Reactor type	Lattice type	No. of MOX rods	No. of UO$_2$/Gd rods	Fuel pitch (cm)	Pellet diameter (mm)	Cladding diameter (mm)	Assembly pitch (cm)
	18×18	300	–	1.27	8.05	9.5	23.0
	17×17	264	–	1.26	8.19	9.5	21.5
PWR	16×16	236	–	1.43	9.11	10.75	23.0
	15×15	205	–	1.43	9.13	10.75	21.6
	14×14	179	–	1.41	9.29	10.72	19.8
	$10 \times 10 - 9$	81	10	1.30	8.7	10.05	15.2
BWR	$9 \times 9 - 9$	60	12	1.43	9.5	10.8	15.2
	$9 \times 9 - 1$	68	12	1.43	9.5	10.8	15.2
	$8 \times 8 - 2$	62	14	1.63	10.3	12.3	15.2

4.2 BWR MOX ASSEMBLY DESIGNS

The fuel configuration in BWR MOX assembly designs is considerable more complex and heterogeneous than PWR MOX designs. Unlike PWR MOX assemblies that use only MOX fuel rods, BWR MOX assemblies utilize both MOX and UO$_2$ fuel rods within the same assembly. The UO$_2$ rods typically contain Gd$_2$O$_3$ burnable poison (Gd rods) to achieve a more uniform power distribution in the assembly. The number of Gd rods deployed in an assembly can vary considerably depending on the lattice type (e.g., 8×8 vs. 10×10), the quantity of total Pu in the MOX, the Pu vector (fissile content), location of the assembly in the reactor core, and compatibility with adjacent fuel assemblies. In addition to variations in the number of Gd rods, the enrichment of the Gd poison and U in the rods are variable. BWR assemblies may use partial length fuel rods within an assembly that results in axial variations in the fuel rod arrangements (increased moderator near tops of assembly). In general, the Gd rods are located adjacent to a central water channel (box) and partial length rods. Further heterogeneity is introduced in BWRs by the use of absorbing control rods (cruciforms) for reactivity control.

Within Western Europe, there are only five countries operating BWRs: Sweden, Switzerland, Spain, Germany, and Finland. Of the EURATOM member countries, only Germany is currently operating BWRs with MOX at its Gundremmingen NPP, although MOX has been used previously at the Krümmel plant, and MOX has been approved for use in the Swedish Oskarshamn BWR NPP.
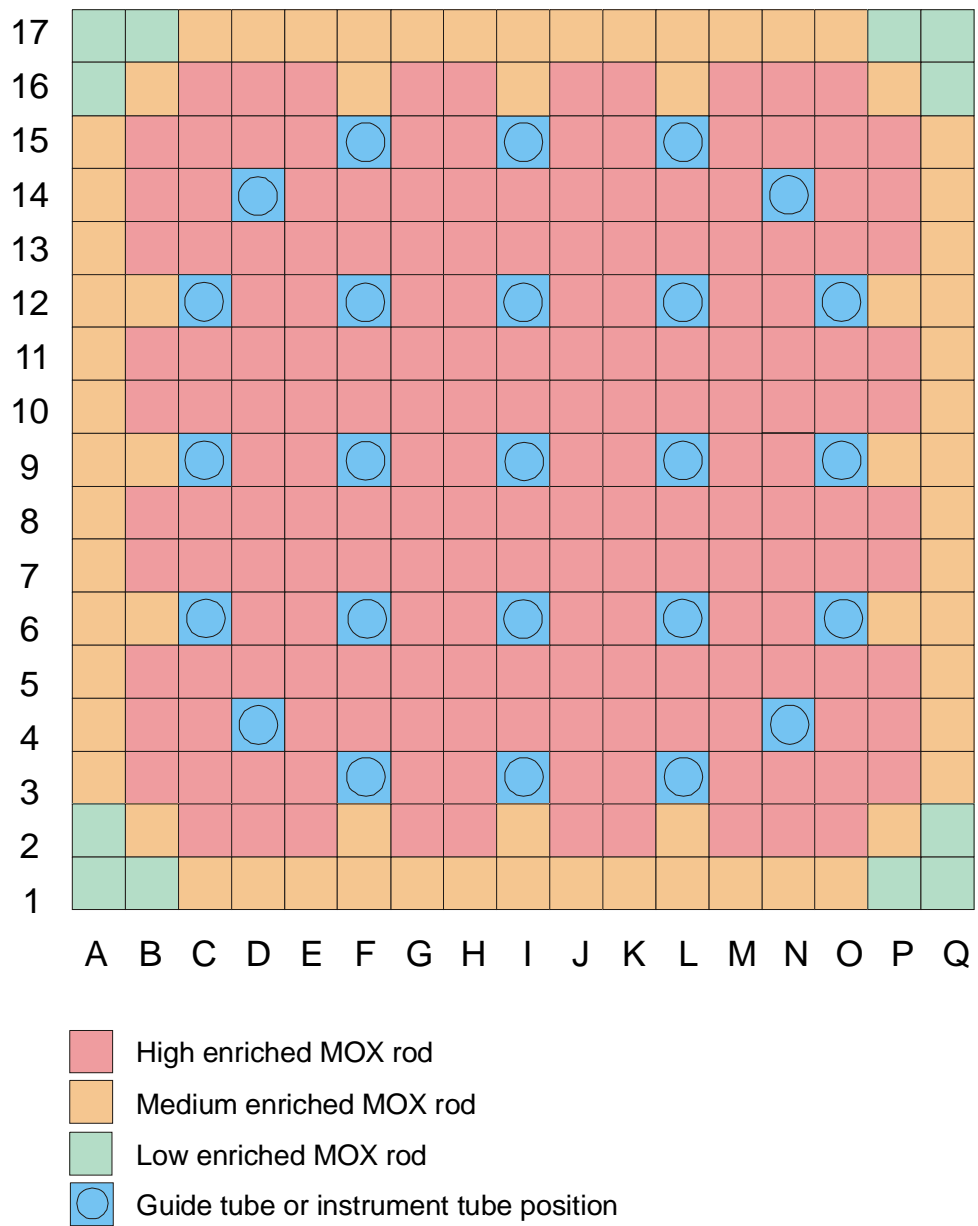
Fig. 10. Typical fuel rod arrangement of a zoned 17 × 17 PWR MOX fuel assembly.

The current trend in assembly design is towards the use of assemblies with more fuel rods that allow greater control of enrichment zoning to provide a more uniform power distribution. Currently the 10×10 design is used almost exclusively in Europe. The predominant 10×10 design used at the Gundremmingen NPP is the Siemens AG ATRIUM 10 assembly design. The ATRIUM 10 is characterized by a large (3×3) water channel, located near the center of the assembly. The assembly has a Zircaloy flow box located in the water channel that contains water with a higher density (non-boiling region) than the surrounding moderator. The assembly is surrounded by an outer Zircaloy flow channel. This assembly design is designated in this report as the $10 \times 10 - 9$ design (10×10 lattice with 9 non-fueled lattice positions). The number of non-fueled water sites does not include potential water sites associated with the use of partial length rods that would increase the amount of moderation in the assembly, usually near the top of the assembly.

There are several 9×9 MOX assembly designs in use: the ATRIUM 9 design (similar to ATRIUM 10, both with 9 central water sites), designated $9 \times 9 - 9$, and a design with a single, central, lattice water site, designated $9 \times 9 - 1$. Because the fuel-to-moderator ratio in these two 9×9 designs is significantly different, the fuel spectrum (and therefore the average fuel cross sections) is potentially very different. Therefore, ORIGEN-ARP cross-section libraries were generated for both of the 9×9 designs described.

Cross-section libraries were also developed for a MOX 8×8 assembly, although no such assemblies are currently in operation in Europe. This library may be useful for the assessment of older assemblies currently stored in pools. The specifications for the 8×8 assembly model were based on a BNFL design with two non-fueled lattice positions, designated $8 \times 8 - 2$.

The MOX BWR assembly specifications used in developing libraries for the 8×8, $9 \times 9 - 1$, $9 \times 9 - 9$, and $10 \times 10 - 9$ designs are listed in Table 5. The $9 \times 9 - 9$ and $9 \times 9 - 1$ assembly configurations are illustrated in Figs. 11 and 12, respectively. The Gd rod arrangement and the MOX zones can vary significantly, and these layouts are only given as examples. However, the MOX zoning pattern and the positions of the Gd rods are not factors in developing the MOX models that generate the cross-section libraries. Because the libraries were developed using a 1-D assembly model with SAS2H, and considered only a single assembly-averaged fuel composition (i.e., all zones are averaged), the models are only influenced by the total number of fuel rods, the total number of Gd rods, and number of non-fueled water locations in the assembly.

Fig. 11. Simplified fuel rod arrangement of a 9 × 9 – 9 BWR MOX fuel assembly.
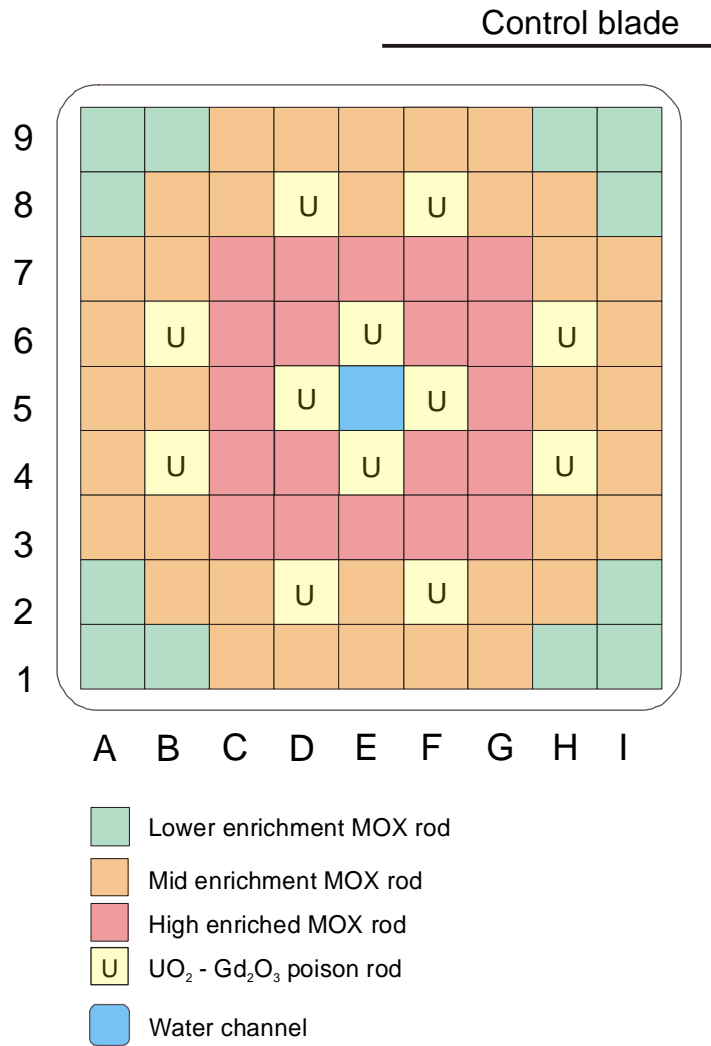
Fig. 12. Simplified fuel rod arrangement of a 9 × 9 − 1 BWR MOX fuel assembly.

5   GENERATION OF MOX LIBRARIES

Cross-section libraries were generated for each of the PWR MOX assembly designs described in Sect. 4, using the dimensions in Table 5. The reactor and assembly data were selected to be representative of each class of lattice design. The libraries were created for a wide range of initial MOX fuel 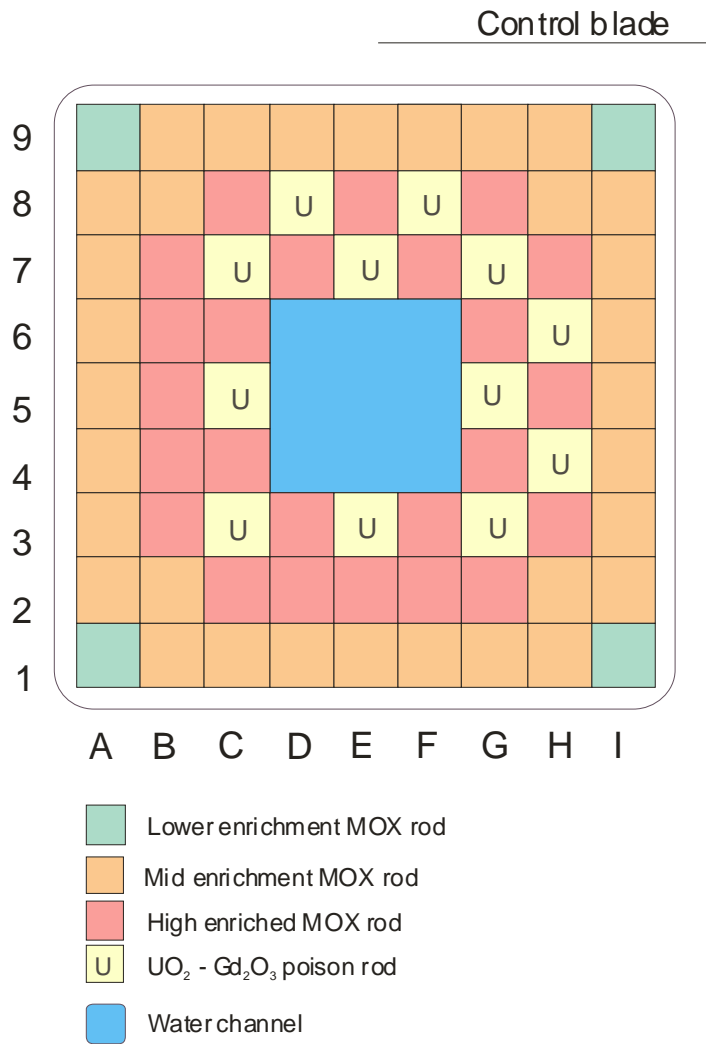compositions (Pu content and isotopic vectors) sufficient to cover the range for current and anticipated near-future needs. The MOX libraries were designed to be used with the ORIGEN-ARP sequence of SCALE. The ARP code interpolates tabulated cross sections from the basic MOX libraries to create an appropriate library for ORIGEN-S for the selected fuel design and MOX compositions specified by the user. This section describes the computation methods and data used in creating the basic cross-section libraries.

5.1   COMPUTATIONAL METHODS

The MOX cross-section libraries were created using the SAS2H depletion analysis sequence[12] of the SCALE code system. All calculations were run on a COMPAQ XP1000 Alpha Unix workstation using the development version of SCALE 5 at ORNL.

The SAS2H depletion analysis sequence comprises the established and well-known ORIGEN-S depletion and decay code for the burnup calculations, and the XSDRNPM one-dimensional (1-D) discrete ordinates (S_N) transport code for the fuel lattice simulation. Other SCALE codes are also used in the sequence to perform resonance cross-section self-shielding calculations for the burnup analysis.

Within the SCALE depletion sequence, problem-dependent cross sections are generated using specified fuel compositions, unit-cell geometry, and a 1-D model of the assembly. For an initial fuel composition, XSDRNPM performs a neutron transport analysis of the reactor fuel assembly to determine the neutron flux spectrum for the assembly model. The spectrum is used to weight the cross sections for the particular assembly geometry, reactor conditions, and specified burnup-dependent fuel composition. The cross sections derived from the transport analysis at each time step are used in an ORIGEN-S point-depletion computation that produces the burnup-dependent fuel composition to be used in the next transport calculation. This sequence is fully automated and repeated over the operating history of the reactor. The cross sections derived from XSDRNPM at each burnup interval during the depletion analysis are saved and can be used in subsequent ORIGEN-S analyses involving the same configuration and initial fuel compositions.

The library used in the XSDRNPM transport analysis of the fuel assembly model was the 238-group ENDF/B-V cross-section library, a general-purpose fine-group library that contains cross sections for all nuclides (more than 300) available in ENDF/B-V. The 238-group library also contains ENDF/B-VI cross sections for a few nuclides to correct deficiencies in the ENDF/B-V evaluations. The 238-energy-group cross sections are collapsed by the XSDRNPM code into the effective cross sections used in the ORIGEN-S burnup analysis.

A matrix of libraries was created using different combinations of the variable fuel parameters, covering the desired range of each MOX parameter. For each given parameter combination, a separate SAS2H problem was run to create the MOX library.

5.2 MOX LIBRARY DESCRIPTION

MOX cross-section libraries were generated using SAS2H for the PWR and BWR MOX assembly models described in Sect. 3. For each assembly, libraries were generated over the range of parameters described in Sect. 4. The variable parameters used in the development of the MOX libraries were:

1. Total plutonium content (wt % Pu / HM),
2. Plutonium vector (the distribution of the plutonium isotopes $^{238-242}$Pu),
3. Burnup (MWd/tHM), and
4. Moderator density (g/cm^3).

As described previously, the Pu vector was represented using only the ^{239}Pu concentration (although an option to perform vector interpolation using both ^{239}Pu and ^{238}Pu is retained). Also, variable moderator density was only implemented in the BWR MOX libraries. However, variable moderator density may be added to the PWR libraries in the future.

The uranium composition and ^{241}Am content in MOX were not considered to vary in the development of the cross-section libraries because of their relatively low variability and importance to the cross sections. Although the cross sections were developed assuming fixed nominal compositions for these nuclides, the actual concentrations are applied in the depletion analysis. In other words, while the actual values of the concentrations for these nuclides are always specified in the ORIGEN-ARP calculation, the *cross-section values* are based on the average concentrations.

The MOX libraries were generated for plutonium contents of 4, 7 and 10 wt % Pu in total Heavy Metal (HM), sufficient to cover the range of data in Table 1.

The Pu vectors used in generating the MOX libraries were calculated for initial ^{239}Pu concentrations of 50, 55, 60, 65, and 70 wt % in total Pu. Again, these values are sufficient to cover (and extended beyond) the range required for the analysis of European MOX fuel. The total storage time assumed for ^{241}Am content was 3.4 years, based on the average value calculated from the database.

The cross sections were generated for MOX fuel burnup intervals ranging up to 60 GWd/tHM, sufficient for the analysis of all existing MOX fuel, and fuel for the foreseeable future. The burnup-dependent cross sections are stored within a single MOX library, and each library is representative of a specific Pu content and Pu vector. Each set of burnup-dependent cross sections in a library are stored, and accessed, by position number in the library, with the first position corresponding to initial (unirradiated) MOX fuel compositions. The position and specific burnup values associated with each position in a library is listed in Table 6. The cross sections are tabulated at uniform intervals of 4800 MWd/tHM, with the exception of the first interval tabulated at 2400 MWd/tHM.

Table 6. Fourteen burnup-dependent MOX cross-section library positions

Position	Burnup (MWd/tHM)
1	0
2	2400
3	7200
4	12000
5	16800
6	21600
7	26400
8	31200
9	36000
10	40800
11	45600
12	50400
13	55200
14	60000

Water moderator density was represented at four points, 0.20, 0.4, 0.6 and 0.80 g/cm^3.

A total of five MOX libraries (for each assembly design) is needed to represent the Pu isotopic vector. The Pu content, represented at three tabulated points, increases the total number of libraries to 15. For the BWR MOX libraries with variable moderator density, the number of required libraries increases to 60.

Other general fuel and reactor operating parameters important to the development of the MOX libraries are listed in Table 7. These values are based on typical LWR fuel and reactor experience and were used in the development of all MOX libraries.

An example of the SAS2H input files used to generate the cross-section libraries for the PWR MOX 17×17 assembly design is listed in Table 8. A separate calculation was run to generate each of the 27 cross-section libraries for each assembly type. The models for each assembly design were identical except for the assembly information and dimensions as listed in Table 5. An input file for the BWR MOX 10×10 assembly design is listed in Table 9.

Table 7. Nominal fuel and reactor operating conditions used in creating MOX libraries

Parameter	PWR MOX value	BWR MOX value
Fuel density	10.4 g/cm^3	10.4 g/cm^3
Fuel temperature	900 K	843 K
^{235}U enrichment[a]	0.24 wt % in U total	0.74 wt % in U total
Cladding material	Zircaloy-2	Zircaloy-2
Cladding temperature	640 K	640 K
Moderator temperature	577 K	574 K
Moderator density	0.72 g/cm^3	0.2 to 0.8 g/cm^3
Average moderator boron	600 ppm	0 ppm
Nominal reactor power	30 MW/tHM[b]	30 MW/tHM

[a] Assembly average value.
[b] HM = Heavy Metal (U + Pu).

Table 8. Example of SAS2H input file used to generate 17×17 PWR MOX libraries

```
=sas2       parm='skipshipdata'
MOX fuel - 7 wt% Pu in 17x17 assembly, PWR 900
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'   mixtures of fuel-pin-unit-cell:
'
238group    latticecell
'  mox fuel description
 uo2   1 den=10.4 0.93  900 92234 0.001 92235 0.24 92238 99.759  end
 puo2 1 den=10.4 0.07  900 94238 1.3970 94239 58.080 94240 26.340
     94241 8.0900 94242 6.0930 end
 am-241 1 den=0.1319 0.07 900 end
'
zr-94  1 0 1-20 900   end
mo-94  1 0 1-20 900   end
nb-95  1 0 1-20 900   end
mo-95  1 0 1-20 900   end
tc-99  1 0 1-20 900   end
rh-103 1 0 1-20 900   end
rh-105 1 0 1-20 900   end
ru-106 1 0 1-20 900   end
sn-126 1 0 1-20 900   end
xe-131 1 0 1-20 900   end
cs-133 1 0 1-20 900   end
cs-134 1 0 1-20 900   end
cs-135 1 0 1-20 900   end
cs-137 1 0 1-20 900   end
pr-143 1 0 1-20 900   end
nd-143 1 0 1-20 900   end
ce-144 1 0 1-20 900   end
nd-144 1 0 1-20 900   end
nd-145 1 0 1-20 900   end
nd-146 1 0 1-20 900   end
nd-147 1 0 1-20 900   end
pm-147 1 0 1-20 900   end
sm-147 1 0 1-20 900   end
nd-148 1 0 1-20 900   end
pm-148 1 0 1-20 900   end
sm-148 1 0 1-20 900   end
pm-149 1 0 1-20 900   end
sm-149 1 0 1-20 900   end
nd-150 1 0 1-20 900   end
sm-150 1 0 1-20 900   end
sm-151 1 0 1-20 900   end
eu-151 1 0 1-20 900   end
sm-152 1 0 1-20 900   end
eu-153 1 0 1-20 900   end
eu-154 1 0 1-20 900   end
gd-154 1 0 1-20 900   end
eu-155 1 0 1-20 900   end
gd-155 1 0 1-20 900   end
gd-157 1 0 1-20 900   end
gd-158 1 0 1-20 900   end
gd-160 1 0 1-20 900   end
pu-236 1 0 1-20 900   end
pu-237 1 0 1-20 900   end
pu-243 1 0 1-20 900   end
pu-244 1 0 1-20 900   end
am-241 1 0 1-20 900   end
```

```
am-242m 1 0 1-20 900  end
am-243 1 0 1-20 900  end
cm-242 1 0 1-20 900  end
cm-243 1 0 1-20 900  end
cm-244 1 0 1-20 900  end
cm-245 1 0 1-20 900  end
cm-246 1 0 1-20 900  end
cm-247 1 0 1-20 900  end
cm-248 1 0 1-20 900  end
bk-249 1 0 1-20 900  end
cf-249 1 0 1-20 900  end
cf-250 1 0 1-20 900  end
cf-251 1 0 1-20 900  end
cf-252 1 0 1-20 900  end
'
zirc2  2 1      640 end
h2o  3 den=0.725  1  574 end
arbm-bormod  0.725 1 1 0 0 5000 100 3 600.e-6  574  end
'
'  600 ppm avg boron (wt) in moderator
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
end comp
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'      fuel-pin-cell geometry:
'
squarepitch   1.260  0.819 1 3 0.95 2  end
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'    assembly design parameters:
'
npin/assm=264 fuelnght=782.478  ncycles=14  nlib/cyc=1
printlevel=2 lightel=2  inplevel=1
numholes=24 numinst=1 ortube=0.612 srtube=0.572
asmpitch= 21.50 end
'
'    fuel cycle history data:
'
 power=30.   burn=1e-15  down=0  bfrac=1.  end
 power=30.   burn=160    down=0  bfrac=1.  end
 power=30.   burn=160    down=0  bfrac=1.  end
 power=30.   burn=160    down=0  bfrac=1.  end
 power=30.   burn=160    down=0  bfrac=1.  end
 power=30.   burn=160    down=0  bfrac=1.  end
 power=30.   burn=160    down=0  bfrac=1.  end
 power=30.   burn=160    down=0  bfrac=1.  end
 power=30.   burn=160    down=0  bfrac=1.  end
 power=30.   burn=160    down=0  bfrac=1.  end
 power=30.   burn=160    down=0  bfrac=1.  end
 power=30.   burn=160    down=0  bfrac=1.  end
 power=30.   burn=160    down=0  bfrac=1.  end
 power=30.   burn=160    down=0  bfrac=1.  end
'    light element mass (kg)
  o 134
  zr 221
'
end
```

Table 9. Example of SAS2H input file used to generate $9 \times 9 - 9$ BWR MOX libraries

```
=sas2        parm='skipshipdata'
mox 7wt% pu in 9x9 bwr asmby - Framatome ANP Atrium
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'   mixtures of fuel-pin-unit-cell:
'
238group    latticecell
'
'  mox fuel description
'
 uo2  1 den=10.4 0.93  843 92235 0.7417 92238 99.2583  end
 puo2 1 den=10.4 0.07  843 94238 1.6750 94239 60.122 94240 24.750
  94241 8.0590 94242 5.3940 end
 am-241 1 den=0.1330 0.07 843 end
 u-236    1 0 1-20 843 end
 am-241   1 0 1-20 843 end
 am-243   1 0 1-20 843 end
 am-242m  1 0 1-20 843 end
 np-237   1 0 1-20 843 end
 cm-242   1 0 1-20 843 end
 cm-244   1 0 1-20 843 end
 cm-245   1 0 1-20 843 end
 tc-99    1 0 1-20 843 end
 ag-109   1 0 1-20 843 end
 ru-101   1 0 1-20 843 end
 rh-103   1 0 1-20 843 end
 xe-131   1 0 1-20 843 end
 xe-135   1 0 1-20 843 end
 cs-133   1 0 1-20 843 end
 sm-151   1 0 1-20 843 end
 sm-152   1 0 1-20 843 end
 sm-149   1 0 1-20 843 end
 eu-153   1 0 1-20 843 end
 eu-154   1 0 1-20 843 end
 eu-155   1 0 1-20 843 end
 nd-143   1 0 1-20 843 end
 nd-145   1 0 1-20 843 end
 nd-147   1 0 1-20 843 end
 pm-147   1 0 1-20 843 end
 pm-148m  1 0 1-20 843 end
'
zirc2  2 1      640  end
' coolant water
h2o  3 den=0.45  1  574 end
' channel water
h2o  4 den=0.72  1  574 end
' gadolinium-uo2 rod
uo2  8   den=10.4 0.96  843 92235 0.7417 92238 99.2583  end
arbm-gd2o3 10.4  2 0 1 0 64000 2 8016 3 8 0.035 843 end
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
end comp
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'     fuel-pin-cell geometry:
'
squarepitch  1.445  0.950 1 3 1.100 2  end
'
```

```
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'    assembly design parameters:
'
npin/assm=72 fuelnght=2136.67 ncycles=14  nlib/cyc=1
printlevel=4 lightel=4  inplevel=2  numzones=7 end
'
 8 0.475 2 0.550 3 0.8153 500 1.997 3 2.090 2 2.199 4 2.476
'
'    fuel cycle history data:
'
'
 power=30.    burn=1e-15  down=0  bfrac=1.   end
 power=30.    burn=160    down=0  bfrac=1.   end
 power=30.    burn=160    down=0  bfrac=1.   end
 power=30.    burn=160    down=0  bfrac=1.   end
 power=30.    burn=160    down=0  bfrac=1.   end
 power=30.    burn=160    down=0  bfrac=1.   end
 power=30.    burn=160    down=0  bfrac=1.   end
 power=30.    burn=160    down=0  bfrac=1.   end
 power=30.    burn=160    down=0  bfrac=1.   end
 power=30.    burn=160    down=0  bfrac=1.   end
 power=30.    burn=160    down=0  bfrac=1.   end
 power=30.    burn=160    down=0  bfrac=1.   end
 power=30.    burn=160    down=0  bfrac=1.   end
 power=30.    burn=160    down=0  bfrac=1.   end
'
'    light element mass (kg)
  o 134
  zr 221
  nb  0.71
  sn  3.6
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
end
```

5.3 LIMITATIONS AND RESTRICTIONS

The MOX cross-section libraries created with the SAS2H depletion code of the SCALE code system, for use with the ORIGEN-ARP sequence, will produce results that are as accurate as the original SAS2H calculations, provided the interpolation by the ARP code is performed with sufficient accuracy. However, use of these cross-section libraries also imposes the limitations and restrictions of SAS2H on the ORIGEN-ARP calculations. The main restrictions associated with the libraries include:

1. The SAS2H assembly model is restricted to 1-D geometry. Simplifying assumptions are therefore required to represent non-symmetric assembly configurations such as complex enrichment UO_2 and MOX fuel rods patterns, burnup poison rods, water holes and water channels, and control rods.

2. Axial variations in the assembly compositions or design must be simulated using separate models for each axial segment, i.e., the models are assumed infinite in the axial direction.

3. The MOX assembly compositions must be represented with a single, average composition. Thus, different composition rods within an assembly must be averaged instead of simulating the burnup of the different regions of an assembly individually. The methods are therefore only appropriate to calculating assembly-averaged MOX characteristics.

4. The MOX cross sections are developed using a single-assembly lattice model. Only the assembly of interest is modeled, neglecting the potential effects due to adjacent assemblies (potentially different than MOX).

The use of more accurate two-dimensional (2-D) transport methods in SCALE 5, such as TRITON,[13] to simulate the complex BWR MOX assembly designs is currently being explored.

6   VALIDATION BENCHMARKS

The computational methods and cross-section libraries developed for MOX fuel types were validated using selected numerical (computational) benchmarks and available radiochemical assay experiments. The numerical benchmark was selected from a series of benchmarks developed for MOX fuels as part of an OECD Working Group on burnup credit. Experimental measurements of spent MOX fuel compositions were obtained from the ARIANE International Program coordinated by Begonucleaire, in Belgium. This program reported nuclide compositions in irradiated UO_2 and MOX fuel samples irradiated in both PWRs and BWRs.

Other potential sources of experimental data were also reviewed, including MOX samples irradiated and measured as part of the Saxton experimental program conducted in the U.S. in the 1960s and 1970s, and MOX assemblies irradiated in the San Onofre Unit 1 PWR from 1970–1974 in a joint U.S. government and industry program. However, the plutonium isotopic vectors of the Saxton and San Onofre MOX samples were well beyond the range of the typical reactor grade vectors considered in this work (see Table 1) and thus, these samples were not considered applicable for benchmarking.

6.1   OECD PHASE IV-B BENCHMARK

Cross-section data and methods testing was first performed using a computational benchmark developed by the OECD/NEANSC Criticality Working Party, Burnup Credit Working Group.[14] The Working Group developed the Phase IV-B benchmark to address the calculation of irradiated MOX fuel compositions. The benchmark includes a series of well-defined computational problems involving weapons-grade, and first-recycle RG MOX fuel. The configuration included (1) a simple MOX pin-cell problem, (2) a MOX-only assembly lattice, and (3) a MOX assembly surrounded by UO_2 fuel assemblies (supercell geometry). Computed results from the benchmarks have been submitted by a large number of organizations, using a wide range of nuclear data sources and computational methods. The participating countries and computational methods are listed in Table 10.

For the current study, the average of the calculated results from all submissions was used to verify the MOX methodology and libraries generated in this work. Although there are no "correct" results for numerical benchmarks since they are based on calculations only, they provide assurances that the methods perform adequately by demonstrating that the code can produce results that are within the range predicted by other more rigorous codes. In this study, testing was performed using the MOX assembly benchmark for the RG plutonium vector.

The MOX assembly geometry adopted for the benchmark was a 17×17 PWR fuel assembly with three enrichment zones. For the ORIGEN-ARP calculations, only a single fuel material may be specified. Therefore, the average assembly compositions were calculated using the zone-weighted average composition of the three enrichment zones. The results from ORIGEN-ARP were then compared to the assembly-averaged compositions from the various submissions.

The first-recycle MOX plutonium isotopic composition specified in the benchmark was 2.5/54.7/26.1/9.5/7.2 for the isotopes $^{238-242}$Pu. The plutonium content, averaged over all zones of the assembly, was 8.0 wt-% Pu/HM. The uranium composition assumed depleted uranium

with 0.25 wt % ^{235}U/U. The MOX assembly dimensions were similar to the dimensions for the 17×17 assembly (Table 5) used in this work. The irradiation history involved exposure for three reactor cycles of 16 GWd/tHM each, with a 30 day downtime between each cycle, achieving a final discharge burnup of 48 GWd/tHM. The nuclide compositions were compared for selected actinides and fission products after a cooling time of 5 years.

Table 10. Participants in the OECD Phase IV-B benchmark

Organization	Country	Computer code	Cross-section library
BNFL	United Kingdom	WIMS8A	JEF2.2
PSI	Switzerland	BOXER/ETOBOX	JEF 1/2
GRS	Germany	KENOREST-99	JEF2.2
CEA	France	APPOLO2/PEPIN2	JEF2.2
ORNL	United States	SCALE/SAS2D	ENDF/B-V
NUPEC	China	CASLIB	ENDF/B-IV
JAERI	Japan	MVP-BURN	JENDL-3.2
DTLR	United Kingdom	MONK8A	JEF2.2

The Phase IV-B MOX assembly results from the ORIGEN-ARP calculations are compared with those of other organizations (using independent codes and data) for selected actinides in Fig. 13 and fission products in Fig. 14. The ORIGEN-ARP results are presented as the percentage difference from the average of all of the benchmark participants for each nuclide. The standard deviation of the results from all participants is also shown, giving an indication of the variation between contributions from each organization. The ORIGEN-ARP results showing a deviation similar to the standard deviation from all participants indicates that the ORIGEN-ARP are in good agreement with the other calculated results.

Overall, the ORIGEN-ARP results are comparable to the results calculated using other more rigorous computational methods. The deviation for most nuclides is comparable or better than the standard deviation from all submitted calculations. This indicates that the ORIGEN-ARP results are in general very close to the average of the other calculations. A similar level of agreement is seen for the actinides and fission products. Notably, the predicted concentration of ^{244}Cm, a significant spontaneous fission neutron source in spent fuel, is predicted with a level of accuracy very similar to other codes. The total ORIGEN-ARP computing time required for the OECD benchmark problem was under 4 seconds.
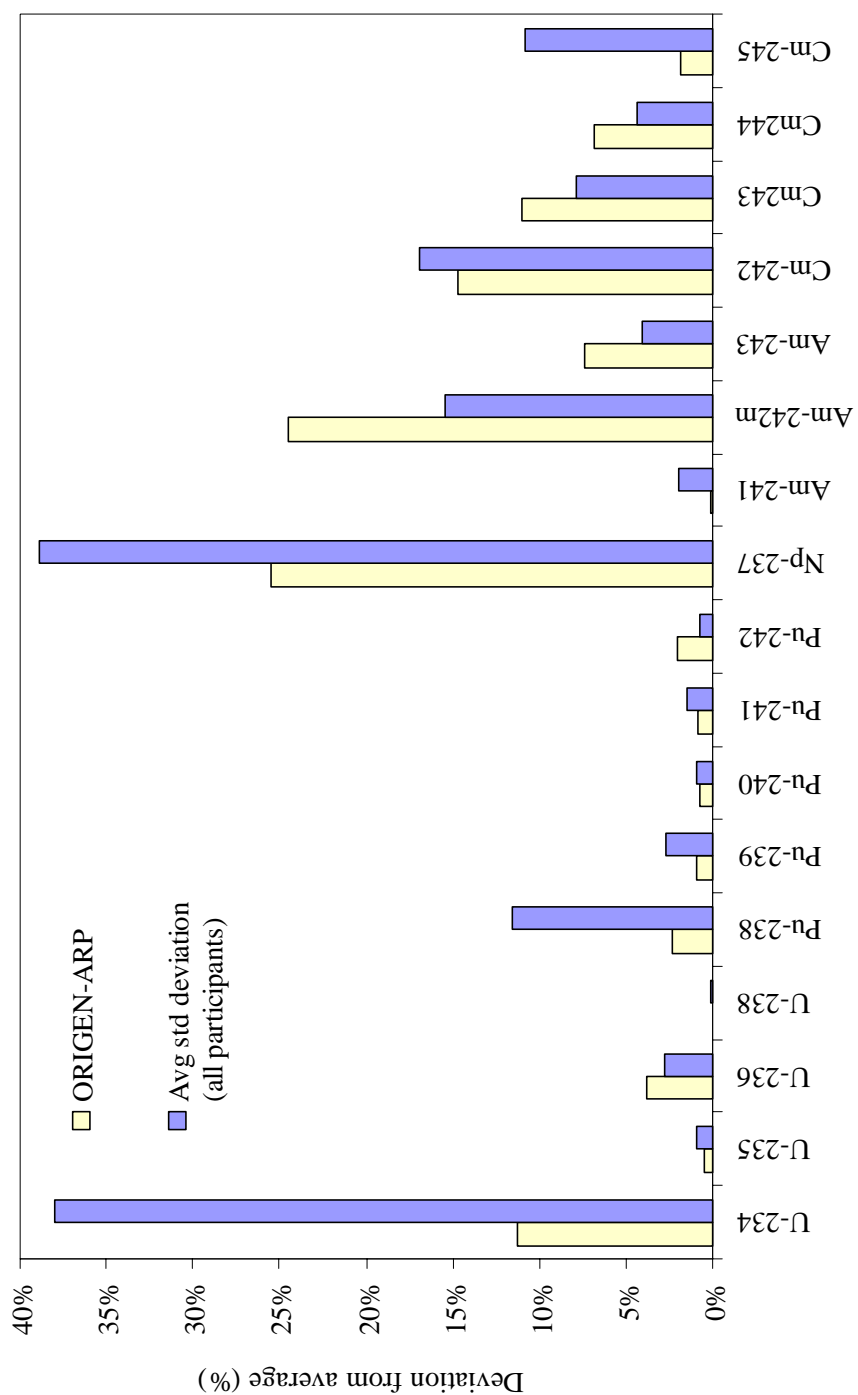
Fig. 13. Actinide results for the OECD Phase IV-B RG MOX assembly benchmark.
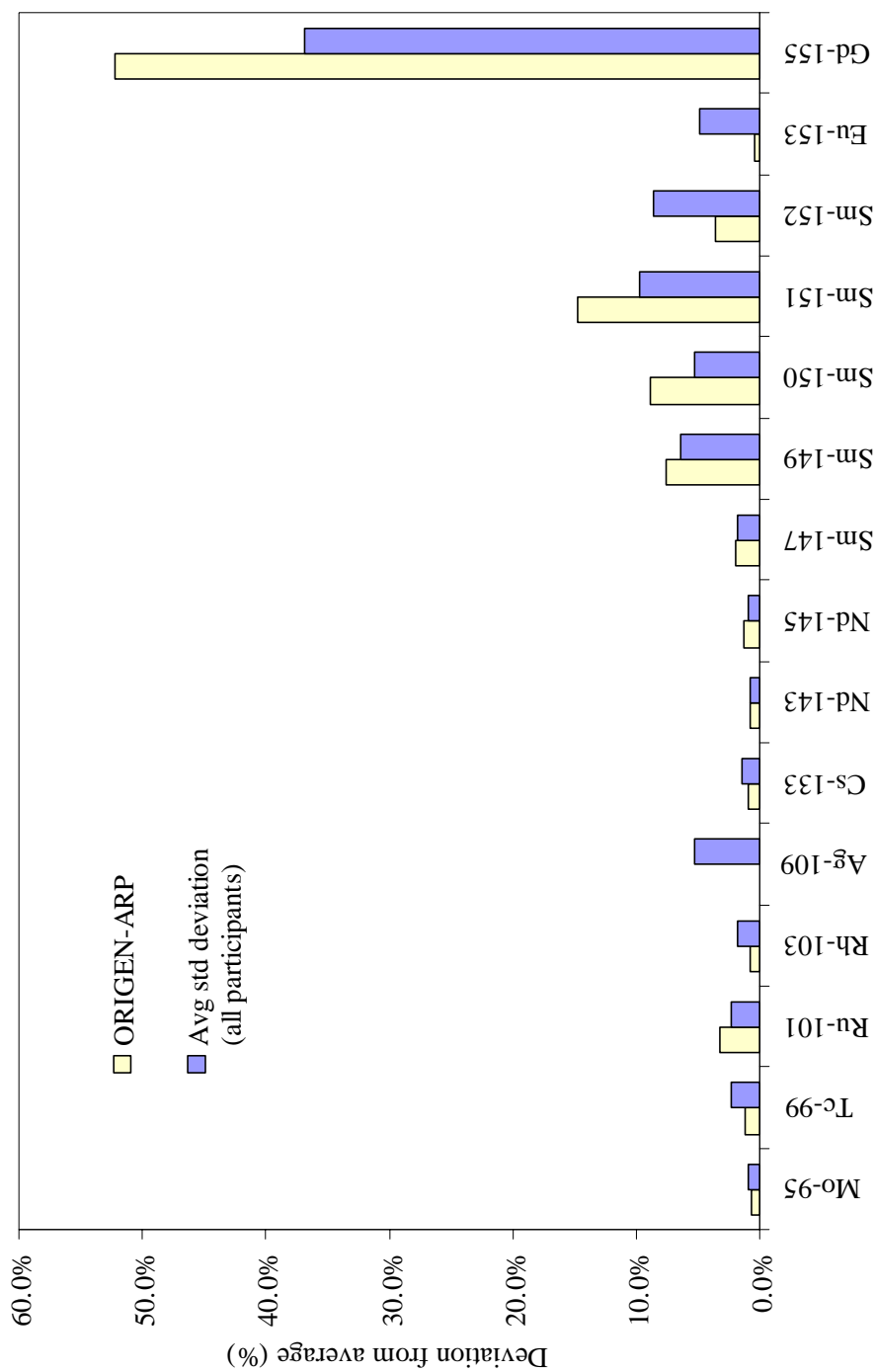
Fig. 14. Fission product results for the OECD Phase IV-B RG MOX assembly benchmark.

6.2 ARIANE MOX BENCHMARKS

Actinide and fission-product inventories in irradiated MOX fuel samples were measured as part of the ARIANE International Program, coordinated by Begonucleaire, in Belgium. The ARIANE program was designed to provide a large set of experimental data on irradiation fuel nuclide compositions for use in code validation. The nuclides that were selected for measurement were those of primary importance in burnup credit (criticality), decay heat, and radiation source terms. The program included measurements of MOX fuel samples obtained from assemblies irradiated in two different reactors: the Beznau PWR in Switzerland, and the Dodewaard BWR operated in the Netherlands prior to its permanent shutdown in 1997.

The Dodewaard BWR MOX assembly was a 6×6 design and contained only two MOX fuel rods, with the remaining rods being UO_2 fuel and gadolium burnable poison rods. The proportion of MOX fuel rods in the assembly is considerably smaller than most assembly designs currently in use, and the Dodewaard samples were therefore considered to be uncharacteristic of commercial MOX fuel. The assembly-averaged Pu content was less than 1%, well outside the range considered in Table 1. For this reason, only the Beznau PWR MOX samples from the ARIANE program were analyzed in this report.

A summary of the specifications for the three Beznau PWR MOX fuel samples, BM1, BM5, and BM6, is given in Table 11. The quantities reported in this benchmark study are the calculated-to-experimental (C/E) comparisons for the nuclide concentrations.

The Beznau samples were obtained from the high Pu content MOX rods in the assembly. The intermediate and low Pu content regions of the assembly were 3.36 and 4.28 wt % Pu, respectively. The burnup of the samples were in the range of 40 to 60 GWd/tHM.

Radiochemical analyses were performed for 17 actinides from ^{234}U to ^{249}Cm. The concentrations for a number of important fission products were also determined, including isotopes of cesium (Cs), neodymium (Nd), samarium (Sm), europium (Eu), gadolinium (Gd), and the isotopes ^{90}Sr, ^{95}Mo, ^{99}Tc, ^{101}Ru, ^{106}Rh, ^{103}Rh, ^{109}Ag, ^{125}Sb, ^{129}I, and ^{144}Ce. The isotope of ^{137}Cs is important gamma ray source in MOX fuel for cooling times up to 100 years, and ^{244}Cm is the dominant spontaneous fission neutron source. These isotopes are therefore particularly important for safeguarded materials verification.

It is well known that many of the fission product elements (e.g., Tc, Mo, Ru, and Rh) segregate in irradiated fuel into metallic particulate that is extremely difficult to dissolve, and therefore difficult to measure. For this group of metallic fission products, separate measurements were performed on the main dissolved fuel solutions and on the undissolved residues in order to account for all material. The measured concentrations for these nuclides were back-calculated to the time of discharge to avoid the difficulty of combining the results of measurements performed at different decay times. For all other nuclides the comparisons were performed using the actual date of the measurements.

Table 11. Summary of Beznau MOX fuel sample characteristics

Parameter	MOX sample		
	BM1	BM5	BM6
Reactor and type	Beznau PWR		
Assembly type	14×14		
Fuel diameter (mm)	9.293		
Fuel density (g/cm^3)	95% TD		
Cladding diameter (mm)	10.72		
Fuel rod pitch (mm)	14.12		
Fuel rods per assembly	179		
Assembly pitch (cm)	19.82		
Moderator density (g/cm^3)	0.75		
^{235}U / U wt %	0.237	0.231	
Pu / HM wt %	6.011	5.5	
^{238}Pu / (Pu + ^{241}Am) wt %	1.003	0.603	
^{239}Pu / (Pu + ^{241}Am) wt %	61.672	66.086	
^{240}Pu / (Pu + ^{241}Am) wt %	23.530	23.198	
^{241}Pu / (Pu + ^{241}Am) wt %	8.834	6.554	
^{242}Pu / (Pu + ^{241}Am) wt %	3.906	2.643	
^{241}Am / (Pu + ^{241}Am) wt %	1.055	0.916	
End of irradiation	04/93	06/96	
Sample burnup (GWd/tHM)	45.6	57.3	39.6

The MOX samples from the ARIANE program were previously analyzed at ORNL using the 2-D HELIOS reactor physics code. HELIOS uses a collision probability technique to solve the transport equation, and allowed explicit simulation of the variation of the different MOX fuel rod compositions within the assembly (i.e., zoning). The analysis results for selected samples have been reported previously in Refs. 15 and 16. The HELIOS results, using ENDF/B-VI cross sections, are also presented in this report for comparison with the results obtained using ORIGEN-ARP. In addition, the results obtained using the 1-D SAS2H code of SCALE are also presented for comparison. Because SAS2H was used to generate the basic MOX cross sections used in the ORIGEN-ARP simulations, any differences between SAS2H and ORIGEN-ARP can be attributed to the interpolation methods used by ARP, and differences between the fuel assembly design and reactor conditions used in the two calculations.

A limitation of the ORIGEN-ARP methods as applied to the analysis of the ARIANE MOX samples, is that the measurements were performed for a single fuel rod within a zoned MOX assembly, whereas the cross-section libraries developed for ORIGEN-ARP simulate the assembly-averaged compositions. Because ORIGEN-ARP uses a point-depletion model for the assembly (i.e., only one fuel material can be specified) the entire assembly was assumed to have the same composition as that of the assayed rod. This representation introduces a bias in the calculations that would otherwise not be present in ORIGEN-ARP simulations for an entire assembly. However, because of the limited quantity of measurements available for MOX fuel, the Beznau samples were analyzed using ORIGEN-ARP, with the awareness that the biases may be larger than those that would be observed for a MOX fuel assembly.

Several MOX samples underwent independent radiochemical analysis at the Paul Scherrer Institute (PSI) in Wurenlingen, Switzerland, and at the SCK-CEN laboratory in Mol, Belgium. The nuclide comparisons for samples BM1 and BM5 presented in this report were based on the measurements made at SCK-CEN, and comparisons for sample BM6 were based on the measurements made at PSI. The burnup value used for each sample in the simulations was the value determined experimentally from the ^{148}Nd concentration. A more detailed discussion on the measurements and the measurement uncertainties can be found in Ref. 15.

The C/E comparisons for the actinides in samples BM1, BM5, and BM6 are presented in Fig. 15, Fig. 16, and Fig. 17, respectively. The fission product results for these same samples are presented in Fig. 18, Fig. 19, and Fig. 20. The ORIGEN-ARP input files used to generate the results presented in this report are listed in Appendix A for reference.

The actinide results are generally consistent between the different calculations. The ORIGEN-ARP results are in good agreement with the other codes. In particular, the ORIGEN-ARP results generally follow very closely the results from the more rigorous HELIOS reactor physics calculations. The differences between the ORIGEN-ARP calculations and SAS2H are attributed mainly to the fact that the SAS2H calculations were performed using the detailed reactor information (e.g., dimensions, fuel temperatures, etc.) whereas the ORIGEN-ARP calculations used MOX libraries developed using generic conditions. The ORIGEN-ARP results for ^{244}Cm, the dominant neutron source nuclide in irradiated MOX fuel, are typically within 5% of the measured concentration. The measurement uncertainties reported by SCK-CEN and PSI for ^{244}Cm are about $\pm 3\%$.

Fig. 15. BM1 MOX sample C/E ratios for the actinides.

Legend:
- HELIOS
- ORIGEN-ARP
- SAS2H

C/E axis: 0.4, 0.6, 0.8, 1, 1.2, 1.4, 1.6, 1.8

Categories: U-234, U-235, U-236, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Am-241, Am242m, Am-243, Cm-242, Cm-243, Cm-244, Cm-245, Cm-246
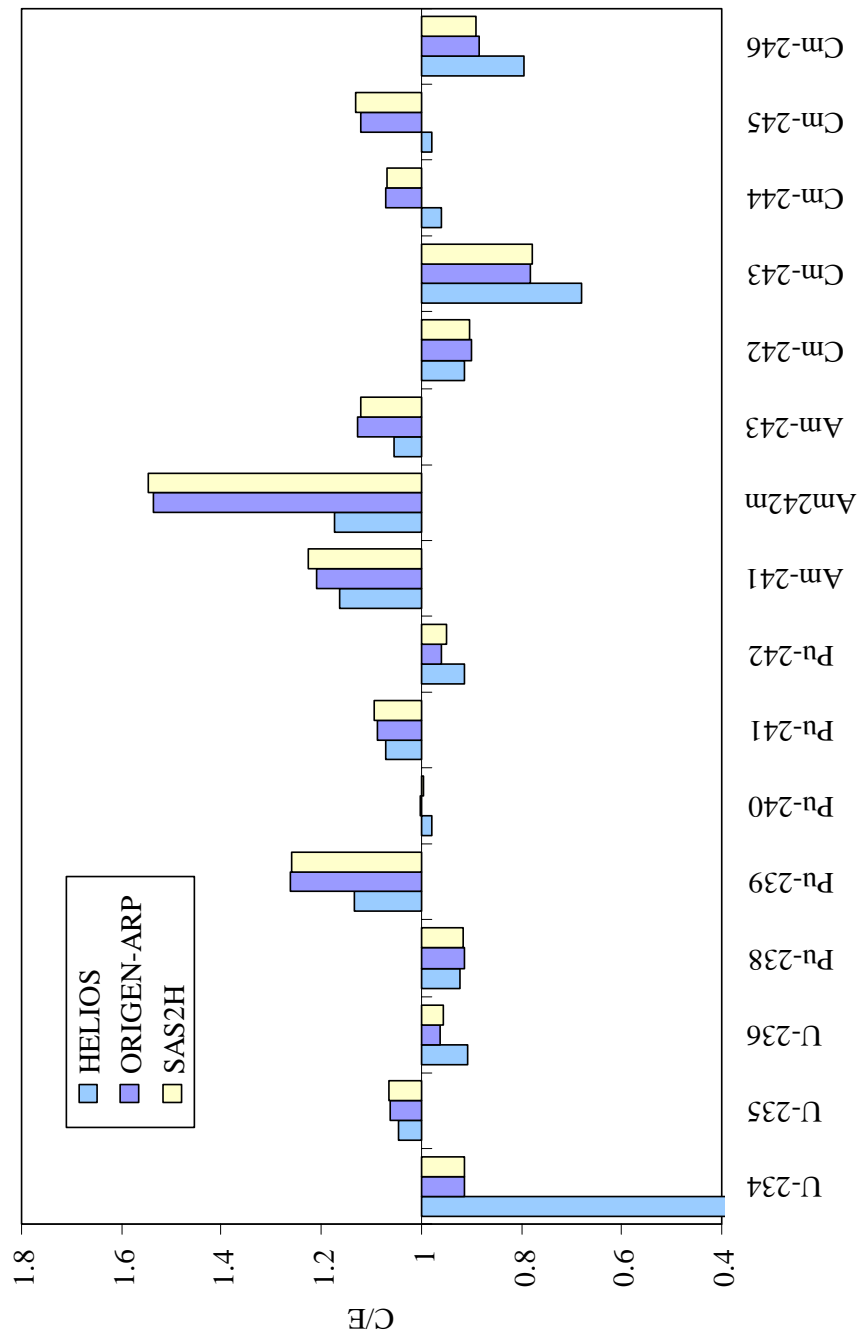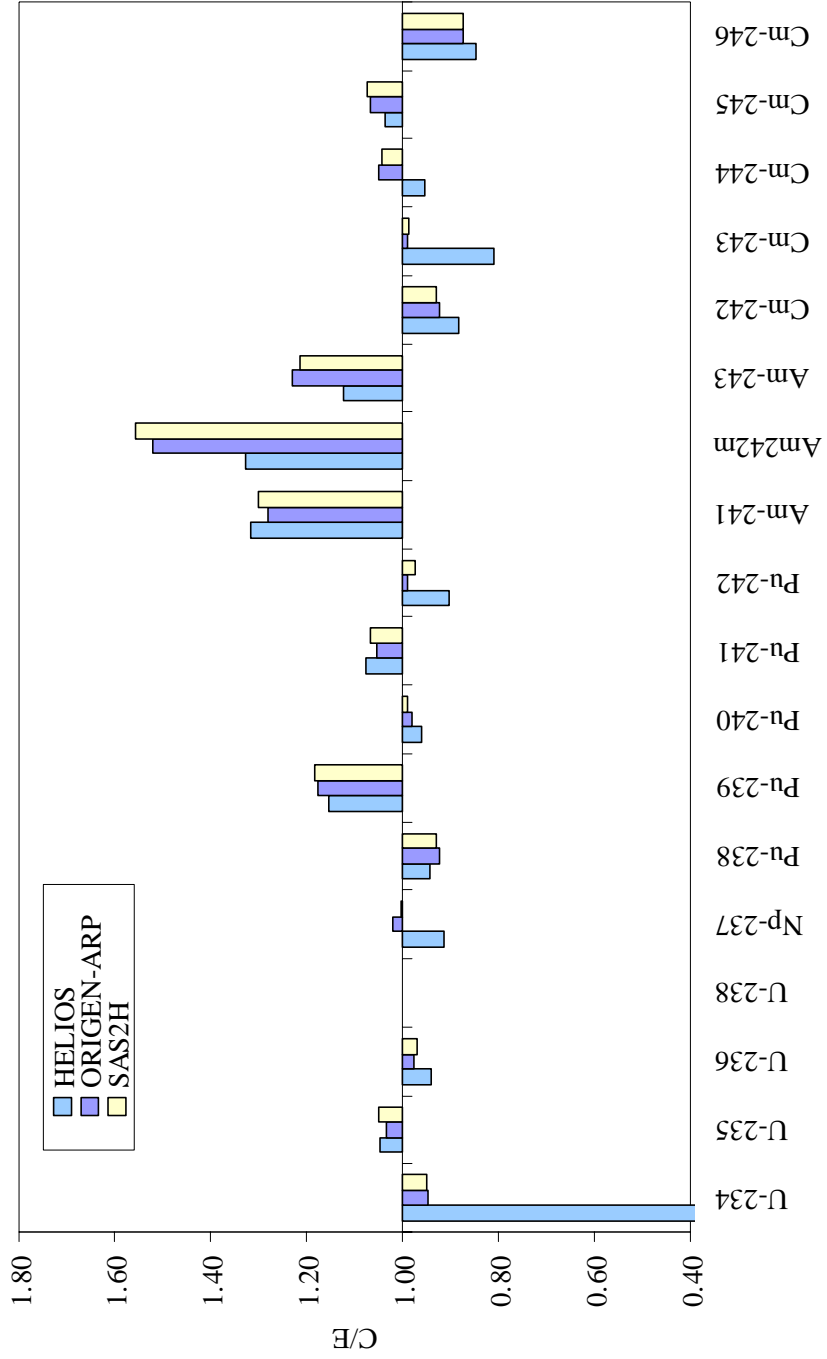
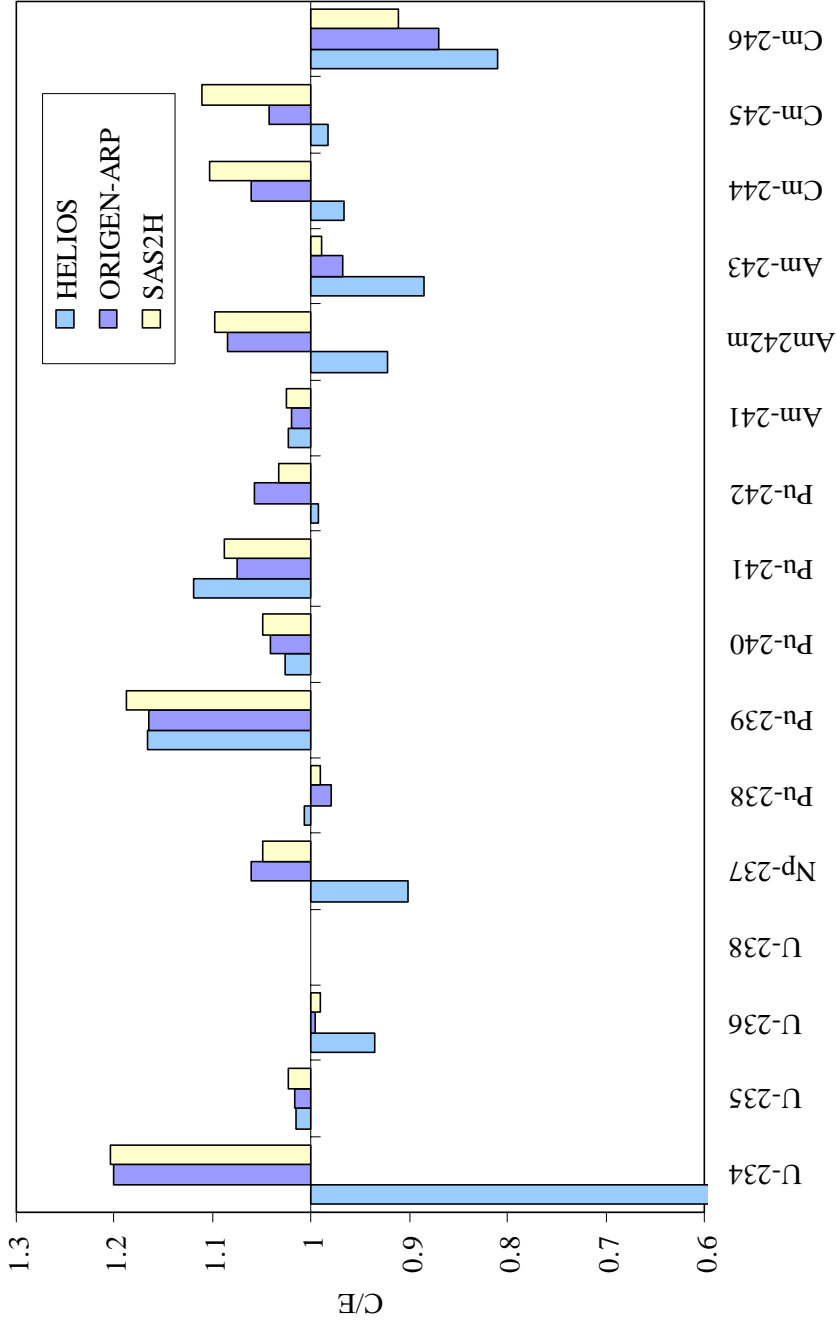**Fig. 16. BM5 MOX sample C/E ratios for the actinides.**

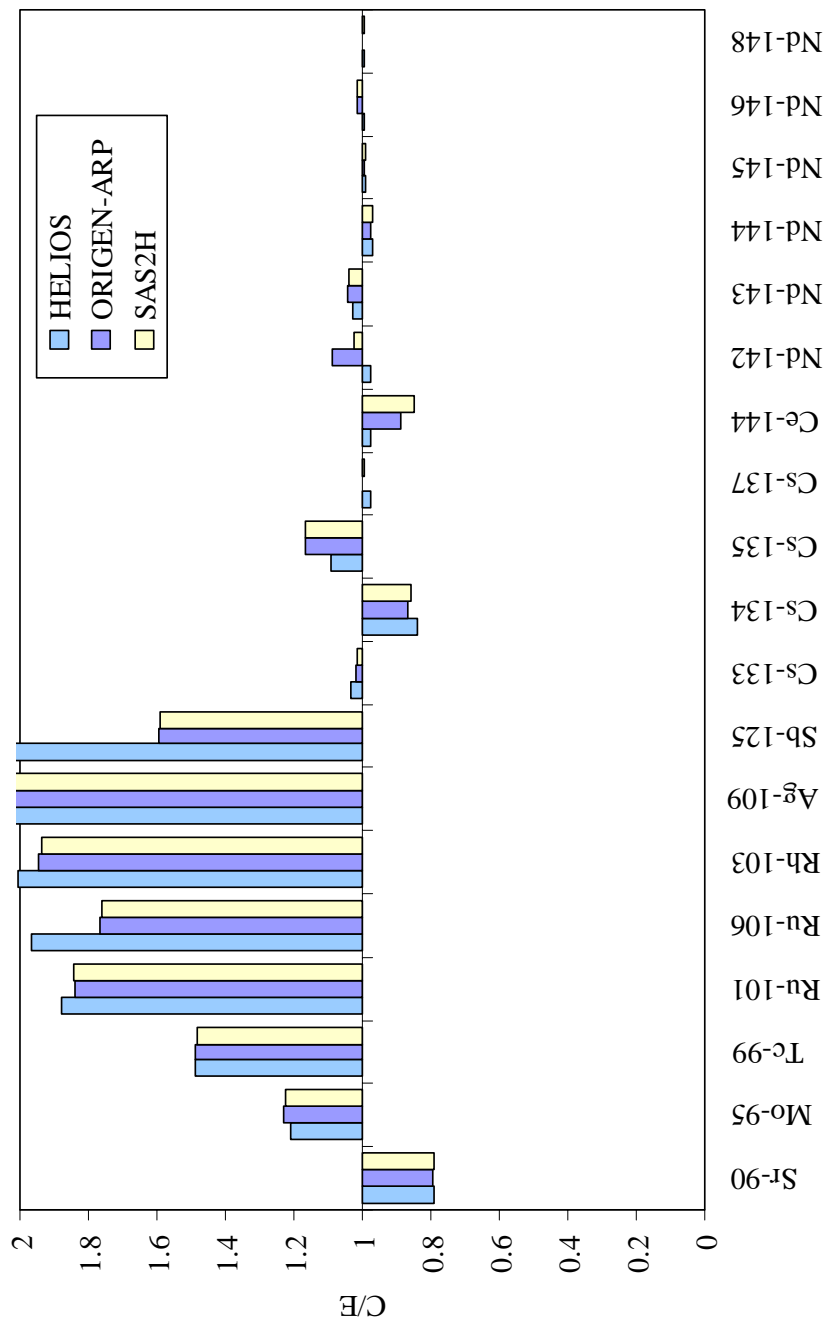**Fig. 17. BM6 MOX sample C/E ratios for the actinides.**

56

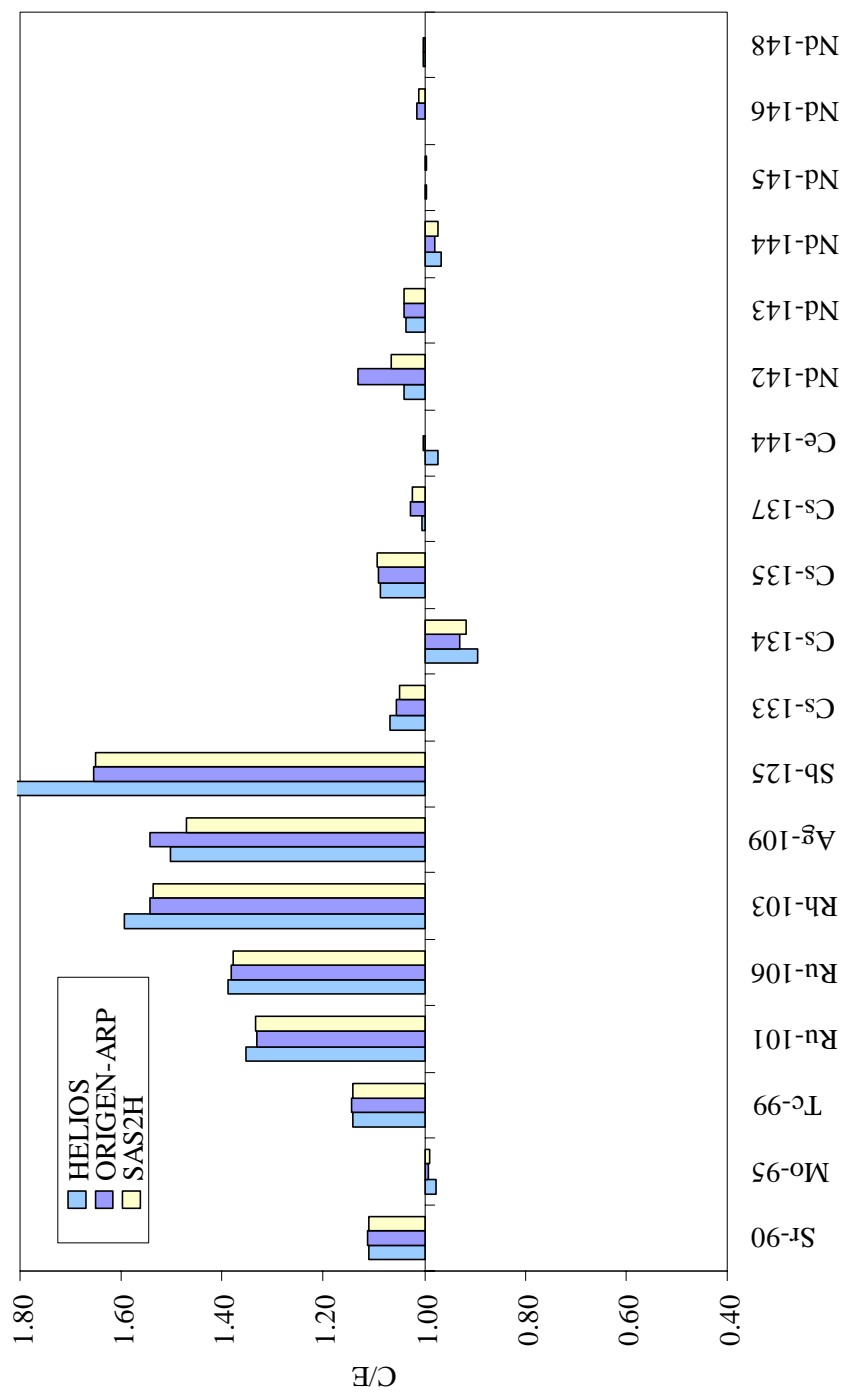**Fig. 18. BM1 MOX sample C/E ratios for selected fission products.**

Fig. 19. BM5 MOX sample C/E ratios for selected fission products.
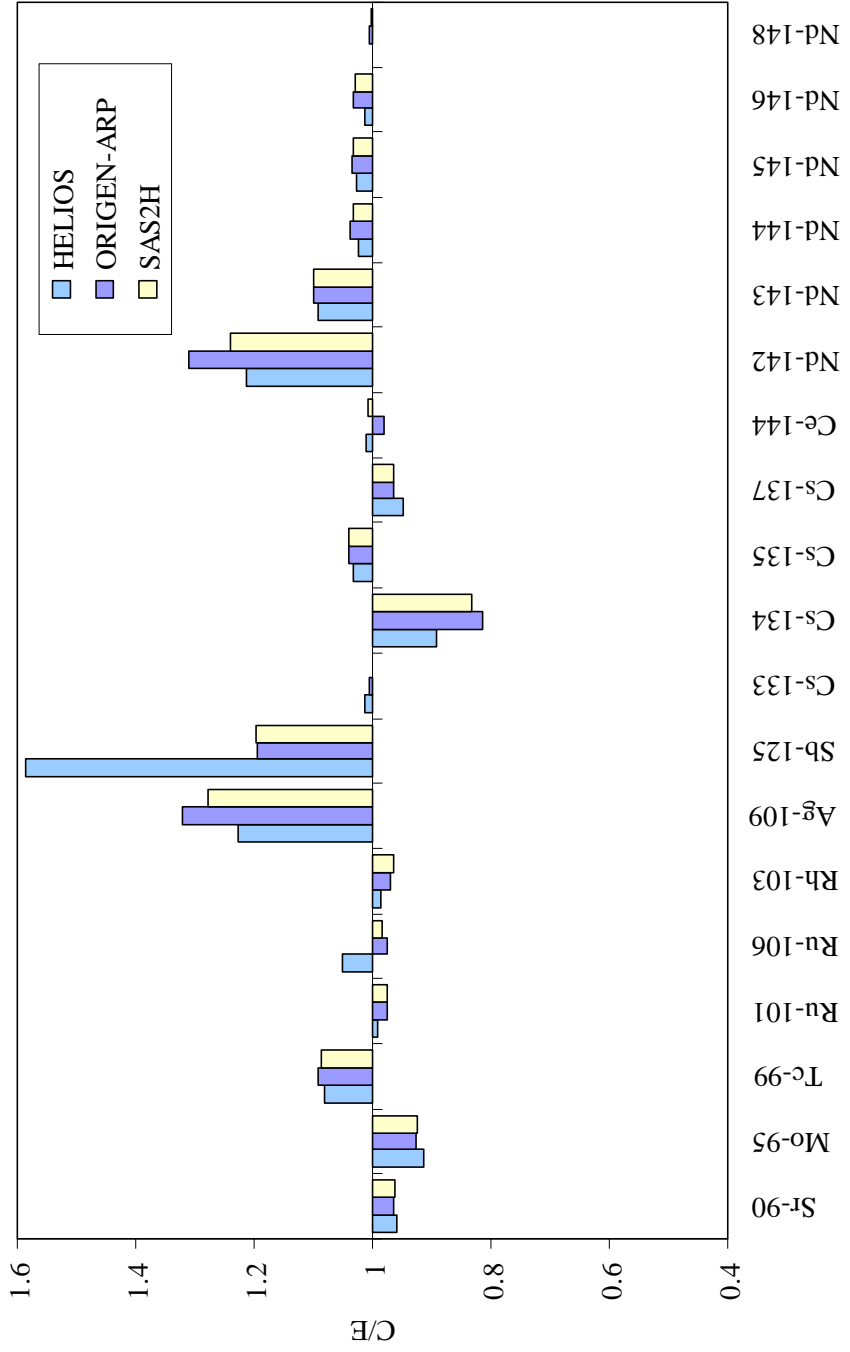
Fig. 20. BM6 MOX sample C/E ratios for selected fission products.

The deviations between calculations and measurements are largest for many of the metallic fission products, particularly ^{99}Tc, ^{101}Ru, ^{106}Ru, ^{103}Rh, ^{109}Ag, and ^{125}Sb, for samples BM1 and BM5 measured by SCK-CEN. Because these nuclides precipitate as undissolved residue, they are particularly difficult to measure and consequently have larger uncertainties. This is evident in the larger discrepancies between the independent measurements performed by PSI and SCK-CEN as discussed in Ref. 15. The deviations in the comparisons for sample BM6 for the metallic fission products measured by PSI are not as large as those observed for samples BM1 and BM5.

The results for the Cs, Ce, and Nd isotopes are seen to be in generally good agreement with experiment. Results for ^{137}Cs, a dominant gamma-ray source in spent fuel, are within 1% of experiment. The overall level of agreement between the calculations and measurements is encouraging. In general, the calculated results from ORIGEN-ARP exhibit biases similar to the other codes considered in the comparison. The calculated concentrations for ^{244}Cm and ^{137}Cs, the nuclides important to the neutron and gamma radiation sources, are in excellent agreement with measured concentrations. However, in general, the predicted concentrations (from all codes) are not as good as previously observed for measurements of spent UO_2 fuels,[17,18] and significant discrepancies are observed for several actinides. Most notably, the concentration of ^{239}Pu is overpredicted by all codes.

Previous work done with the APOLLO reactor physics code in France also refers to the trend of overpredicting ^{239}Pu in MOX fuel.[19,20] This research suggested that the overprediction occurs with MOX assemblies in a PWR mixed-loading core as a result of interface effects and significant mutual self-shielding between the LEU and MOX assemblies. Such effects are currently not treated in either the HELIOS or SCALE code systems. Modifications made to the APOLLO code to simulate these effects have been reported to correct many of the discrepancies.

7   SUMMARY AND CONCLUSIONS

The objectives of this work were to develop and implement an interpolation methodology for MOX fuel that can be used within the framework of ORIGEN-ARP, develop a set of MOX cross-section libraries for the major MOX assembly designs used in Europe, and demonstrate the accuracy and reliability of the methods and data. The numerical and experimental benchmark calculations performed and documented in this report demonstrate that the ARP interpolation strategy implemented for MOX fuels generates cross sections for use in ORIGEN-S burnup calculations of sufficient accuracy such that the nuclide compositions predicted using ORIGEN-ARP are in excellent agreement with results using the SCALE SAS2H code. However, the computing times required to perform the burnup and decay calculations using ORIGEN-ARP are about 1% of the time required by SAS2H. This is achieved by creating the MOX cross-section libraries in advance of the ORIGEN-S calculation and using the ARP code to interpolate appropriate cross sections from these libraries. The libraries described in this report cover a wide range of anticipated MOX fuel compositions and operating conditions.

Benchmarking calculations were performed using an OECD numerical benchmark problem, and experimental data from the ARIANE International Program. The OECD Phase IV-B numerical benchmark for MOX fuel indicates that the ORIGEN-ARP results are generally consistent with the results of more rigorous state-of-the-art reactor physics codes. This is also observed in the comparisons of the ORIGEN-ARP results with those of HELIOS for the ARIANE MOX fuel experiments. However, in comparisons with the measured nuclide concentrations from the ARIANE program, some significant discrepancies are observed, particularly for ^{239}Pu and the metallic fission products. This level of discrepancy has not been observed previously in benchmarks involving UO_2 fuels. Recent work with the APOLLO code has suggested that a more rigorous treatment of the interface and mutual self-shielding effects from LEU and MOX assemblies that reside together in mixed cores is required to correct the problem. The MOX cross-section libraries developed using SCALE does not consider these effects. Further studies are needed to investigate the discrepancies observed in the ARIANE benchmark, and to understand the complex physics phenomena associated with MOX cores that may improve the predictions. As noted previously, the limitations in the accuracy of physics methods to simulate MOX cores are common to nearly all reactor physics codes currently in use. It is anticipated that MALIBU a program currently underway at Belgonucleaire to measure nuclide compositions in high burnup MOX samples, will provide additional experimental data for code validation. MALIBU will also provide measurements for a full BWR MOX fuel.

A key element of future work for this project is to incorporate the computational methods and cross-section libraries described in this report within the PC Windows-based graphical user interface called OrigenArp. The OrigenArp program is used to automatically create input for ORIGEN-ARP, the execute case, and perform post-analysis processing of results. OrigenArp is already publicly available[a] and widely used for commercial UO_2 spent fuel assembly calculations. The OrigenArp program allows burnup calculations to be performed rapidly on a portable laptop computer and requires minimal user input. The graphical user interface also interacts with a detailed post-processor and data visualization program that can rapidly display specific irradiated (or non-irradiated) fuel properties in the units and formats need by inspectors.

---

[a] Version for uranium fuel is available at http://www.ornl.gov/scale/download.html.

In addition to extending the OrigenArp program for MOX fuel, additional libraries will be developed for different MOX fuel types as needed.

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APPENDIX A

**INPUT MODELS USED FOR ANALYSIS OF MOX FUEL SAMPLES
FROM THE ARIANE INTERNATIONAL PROGRAMME**

Input 1: MOX Sample BM6

```
=arp
mox14x14
' beznau-1, ariane sample bm-6
 5.5 67.00 1
 6
 6r317.4434 6r20.81 6r1
 1
 ft33f001
end
=origens
 -1$$ 200000  e
 0$$  a3 74  a4 33  a8 26  a11 71  e
 t

 3$$ 33  a3 1  a16 2  a33 18 e
 4**  a4  1.00000-31  e
 54$$ 5 11r 0  e
 t
 t
 56$$ 10 10 a10 0 a13 13 a15 3 a18 1 e
 57** 0 a3 1e-05 0.1666667 e
 t
mox fuel - 5.5wt%  pu in mox 14x14 asmby, beznau-1 reactor, bm-6
single reactor assembly
 58** 19.068 19.068 19.068 19.068 19.068 19.068 19.068 19.068 19.068
19.068
 60** 31.74434 63.48868 95.23302 126.9774 158.7217 190.466 222.2104
 253.9547 285.6991 317.4434
 66$$ a1 2 a5 2 a9 2 e
 73$$ 80000 400000 410000 500000 922340 922350 922380 942380 942390
 942400 942410 942420 952410 e
 74**  1.34000+05  2.21000+05  7.10000+02  3.60000+03  1.89002+01
 2.18295+03  9.42798+05  3.3165+02  3.63473+04  1.27589+04  3.6047+03
 1.45365+03  5.03800+02  e
 75$$ 4r 4 9r 2 e
 t
 54$$ a8 1 a11 0 e
 56$$ a2 9 a6 3 a10 10 a15 3 a17 4 e
 57** 0 a3 1e-05 e
 t
mox fuel - 5.5wt%  pu in mox 14x14 asmby, beznau-1 reactor, bm-6
1 mtu
60** 0.01 0.03 0.1 0.3 1 3 10 30 56.01942
61** f0.05
65$$
'Gram-Atoms   Grams   Curies   Watts-All   Watts-Gamma
 3z   1   0   0   3z   3z   3z   6z
 3z   1   0   0   3z   3z   3z   6z
 3z   1   0   0   3z   3z   3z   6z
t

3$$ 33 a3 2 27 a33 18 e t
35$$ 0 t
56$$ 10 10 a10 9 a15 3 a18 1 e
57** 0 a3 1e-05 0.1666667 e t
Cycle 2 -beznau-1 bm-6
1 mtu
58** 19.068 19.068 19.068 19.068 19.068 19.068 19.068 19.068 19.068
19.068
```

```
60** 31.74434 63.48868 95.23302 126.9774 158.7217 190.466 222.2104
 253.9547 285.6991 317.4434
66$$ a1 2 a5 2 a9 2 e t
54$$ a8 1 a11 0 e
56$$ a2 9 a6 3 a10 10 a15 3 a17 4 e
57** 0 a3 1e-05 e  t
Decay - beznau-1 bm-6
1 mtu
60** 0.01 0.03 0.1 0.3 1 3 10 30 56.01942
61** f0.05
65$$
'Gram-Atoms   Grams   Curies   Watts-All   Watts-Gamma
 3z   1   0   0   3z   3z   3z   6z
 3z   1   0   0   3z   3z   3z   6z
 3z   1   0   0   3z   3z   3z   6z
t

3$$ 33 a3 3 27 a33 18 e t
35$$ 0 t
56$$ 10 10 a10 9 a15 3 a18 1 e
57** 0 a3 1e-05 0.1666667 e t
Cycle 3 -beznau-1 bm-6
1 mtu
58** 19.068 19.068 19.068 19.068 19.068 19.068 19.068 19.068 19.068
19.068
60** 31.74434 63.48868 95.23302 126.9774 158.7217 190.466 222.2104
 253.9547 285.6991 317.4434
66$$ a1 2 a5 2 a9 2 e t
54$$ a8 1 a11 0 e
56$$ a2 9 a6 3 a10 10 a15 3 a17 4 e
57** 0 a3 1e-05 e  t
Decay - beznau-1 bm-6
1 mtu
60** 0.01 0.03 0.1 0.3 1 3 10 30 56.01942
61** f0.05
65$$
'Gram-Atoms   Grams   Curies   Watts-All   Watts-Gamma
 3z   1   0   0   3z   3z   3z   6z
 3z   1   0   0   3z   3z   3z   6z
 3z   1   0   0   3z   3z   3z   6z
t

3$$ 33 a3 4 27 a33 18 e t
35$$ 0 t
56$$ 10 10 a10 9 a15 3 a18 1 e
57** 0 a3 1e-05 0.1666667 e t
Cycle 4 -beznau-1 bm-6
1 mtu
58** 19.068 19.068 19.068 19.068 19.068 19.068 19.068 19.068 19.068
19.068
60** 31.74434 63.48868 95.23302 126.9774 158.7217 190.466 222.2104
 253.9547 285.6991 317.4434
66$$ a1 2 a5 2 a9 2 e t
54$$ a8 1 a11 0 e
56$$ a2 9 a6 3 a10 10 a15 3 a17 4 e
57** 0 a3 1e-05 e  t
Decay - beznau-1 bm-6
1 mtu
60** 0.01 0.03 0.1 0.3 1 3 10 30 56.01942
61** f0.05
65$$
'Gram-Atoms   Grams   Curies   Watts-All   Watts-Gamma
 3z   1   0   0   3z   3z   3z   6z
```

```
 3z   1   0   0   3z   3z   3z   6z
 3z   1   0   0   3z   3z   3z   6z
t

3$$ 33 a3 5 27 a33 18 e t
35$$ 0 t
56$$ 10 10 a10 9 a15 3 a18 1 e
57** 0 a3 1e-05 0.1666667 e t
Cycle 5 -beznau-1 bm-6
1 mtu
58** 19.068 19.068 19.068 19.068 19.068 19.068 19.068 19.068 19.068
19.068
60** 31.74434 63.48868 95.23302 126.9774 158.7217 190.466 222.2104
 253.9547 285.6991 317.4434
66$$ a1 2 a5 2 a9 2 e t
54$$ a8 1 a11 0 e
56$$ a2 9 a6 3 a10 10 a15 3 a17 4 e
57** 0 a3 1e-05 e   t
Decay - beznau-1 bm-6
1 mtu
60** 0.01 0.03 0.1 0.3 1 3 10 30 56.01942
61** f0.05
65$$
'Gram-Atoms   Grams   Curies   Watts-All   Watts-Gamma
 3z   1   0   0   3z   3z   3z   6z
 3z   1   0   0   3z   3z   3z   6z
 3z   1   0   0   3z   3z   3z   6z
t

3$$ 33 a3 6 0 a33 0 e t
35$$ 0 t
56$$ 10 10 a10 9 a15 3 a18 1 e
57** 0 a3 1e-05 0.1666667 e t
Cycle 6 -beznau-1 bm-6
1 mtu
58** 19.068 19.068 19.068 19.068 19.068 19.068 19.068 19.068 19.068
19.068
60** 31.74434 63.48868 95.23302 126.9774 158.7217 190.466 222.2104
 253.9547 285.6991 317.4434
66$$ a1 2 a5 2 a9 2 e t
54$$ a8 1 a11 0 e
56$$ a2 9 a6 1 a10 10 a14 4 a15 3 a17 2 e
57** 0 a3 1e-05 e   t
Cycle 6 Down - beznau-1 bm-6
1 mtu
60** 1 100 300 600 1063 1174 1249 1273 2051
61** f0.05
65$$
'Gram-Atoms   Grams   Curies   Watts-All   Watts-Gamma
 3z   1   0   0   3z   3z   3z   6z
 3z   1   0   0   3z   3z   3z   6z
 3z   1   0   0   3z   3z   3z   6z
 t
56$$ a2 0 a10 1 e t
56$$ a2 0 a10 5 e t
56$$ a2 0 a10 6 e t
56$$ a2 0 a10 7 e t
56$$ a2 0 a10 8 e t
56$$ a2 0 a10 9 e t
56$$ f0 t
end
```

Input 2: MOX Sample BM1

```
=arp
mox14x14
' beznau-1, ariane sample bm-1, 45,600 mwd/t
 6.011 62.3296 1
 5
 300 312 311 369 211
 30.44 14.77 36.56 36.92 32.54  5r1
 1
 ft33f001
end
=origen
 -1$$ 200000  e
 0$$  a3 74  a4 33  a8 26  a11 71  e
 t

 3$$ 33  a3 1  a16 2  a33 18  e
 4**  a4  1.00000-31  e
 54$$ 5 11r 0  e
 t
 t
 56$$ 5  a2 5  a6 3  a13 14  a15 3  a16 74  a17 4  a18 1  e
 57** 2r  0.00000+00  1.00000-08  1.99601-01  e
 t
mox fuel - 6.011wt% pu in mox 14x14 asmby, beznau-1 reactor, bm-1
single reactor assembly
 58** 4r  3.0440+01  3.03393-14  e
 60**  7.50000+01  1.50000+02  2.25000+02  3.00000+02  3.51000+02  e
 66$$ 2  a5 2  e
 73$$ 80000 400000 410000 500000 922340 922350 922360 922380 942380
  942390 942400 942410 942420 952410  e
 74**  1.34000+05  2.21000+05  7.10000+02  3.60000+03  9.39900+00
 2.25600+03  9.39880+00  9.37605+05  6.02465+02  3.70694+04  1.41431+04
 5.30983+03  2.34794+03  6.34182+02  e
 75$$ 4r 4 10r 2 e
 t

 3$$ 33  a3 2  a33 18  e
 4**  a4  1.00000-31  e
 54$$ 5 11r 0  e
 t
 t
 56$$ 5  a2 5  a6 3  a10 5  a15 3  a16 74  a17 4  a18 1  e
 57**  3.51000+02  0.00000+00  1.00000-08  2.07585-01  e
 t
mox fuel - 6.011wt% pu in mox 14x14 asmby, beznau-1 reactor, bm-1
single reactor assembly
 58** 4r  1.4770+01  3.03393-14  e
 60**  4.29000+02  5.07000+02  5.85000+02  6.63000+02  7.14000+02  e
 66$$ 1  a5 1  e
 t

 3$$ 33  a3 3  a33 18  e
 4**  a4  1.00000-31  e
 54$$ 5 11r 0  e
 t
 t
 56$$ 5  a2 5  a6 3  a10 5  a15 3  a16 74  a17 4  a18 1  e
 57**  7.14000+02  0.00000+00  1.00000-08  2.06919-01  e
 t
mox fuel - 6.011wt% pu in mox 14x14 asmby, beznau-1 reactor, bm-1
single reactor assembly
```

```
 58** 4r  3.656+01  3.03393-14  e
 60** 7.91750+02  8.69500+02  9.47250+02  1.02500+03  1.08600+03  e
 66$$ 1  a5 1  e
 t

 3$$ 33  a3 4  a33 18  e
 4**  a4  1.00000-31  e
 54$$ 5 11r 0  e
 t
 t
 56$$ 5  a2 5  a6 3  a10 5  a15 3  a16 74  a17 4  a18 1  e
 57** 1.08600+03  0.00000+00  1.00000-08  2.45509-01  e
 t
mox fuel - 6.011wt% pu in mox 14x14 asmby, beznau-1 reactor, bm-1
single reactor assembly
 58** 4r  3.6920+01  3.03393-14  e
 60** 1.17825+03  1.27050+03  1.36275+03  1.45500+03  1.51700+03  e
 66$$ 1  a5 1  e
 t

 3$$ 33  a3 5 0  a33 0  e
 4**  a4  1.00000-31  e
 54$$ 5 11r 0  e
 t
 t
 56$$ 4  a2 4  a6 1  a10 5  a15 3  a16 74  a17 4  a18 1  e
 57** 1.51700+03  0.00000+00  1.00000-08  1.40386-01  e
 t
mox fuel - 6.011wt% pu in mox 14x14 asmby, beznau-1 reactor, bm-1
single reactor assembly
 58** 4r  3.2540+01  e
 60** 1.56975+03  1.62250+03  1.67525+03  1.72800+03  e
 66$$ 1  a5 1  e
 t
 56$$  a2 10  a5 5  a6 1  a10 4  a15 3  a16 74  a17 2  a18 1  e
 57** 2r  0.00000+00  1.00000-03  1.40386-01  e
 t
mox fuel - 6.011wt% pu in mox 14x14 asmby, beznau-1 reactor, bm-1
single reactor assembly
 60** 1 30 100 300 600 1000 1429 1446 1469 1525
 66$$ 1  a5 1  e
 61** 3r  7.00000-07 4r  7.00000-09  e
 65$$ 3r 0 1 3r 0 1 2r 0 1 0 1 8r 0 2r 1 0 2r 1 2r 0 1 2r 0 1 0 1 11r 0
1 3r 0 1 2r 0 1 0 2r 1 7r 0  e
 t
 56$$  2r 0 a10 1 e t
 56$$  2r 0 a10 7 e t
 56$$  2r 0 a10 8 e t
 56$$  2r 0 a10 9 e t
 56$$  2r 0 a10 10 e t
 56$$ 20r 0  e
 t
end
```

Input 3: MOX Sample BM5

```
=arp
mox14x14
' beznau-1, ariane sample bm-5, 57,300 mwd/t
 5.5 66.697 1
 6
 311 369 211 343 333 334
 6r30.142 6r1
 1
ft33f001
end
=origen
 -1$$ 200000  e
 0$$  a3 74  a4 33  a8 26  a11 71  e
 t

 3$$ 33  a3 1  a16 2  a33 18  e
 4**  a4  1.00000-31  e
 54$$ 5 11r 0  e
 t
 t
 56$$ 5  a2 5  a6 3  a13 13  a15 3  a16 74  a17 4  a18 1  e
 57** 2r  0.00000+00  1.00000-08  1.63598-01  e
 t
mox fuel - 5.5wt% pu in mox 14x14 asmby, beznau-1 reactor, bm-5
single reactor assembly
 58** 4r  3.01420+01  3.01420-14  e
 60**  7.77500+01  1.55500+02  2.33250+02  3.11000+02  3.62000+02  e
 66$$ 1  a5 1  e
 73$$ 80000 400000 410000 500000 922340 922350 922380 942380 942390
942400 942410 942420 952410 e
 74**  1.34000+05  2.21000+05  7.10000+02  3.60000+03  1.89002+01
 2.18295+03  9.42798+05  3.3165+02  3.63473+04  1.27589+04  3.6047+03
 1.45365+03  5.03800+02  e
 75$$ 4r 4 9r 2 e
 t

 3$$ 33  a3 2  a33 18  e
 4**  a4  1.00000-31  e
 54$$ 5 11r 0  e
 t
 t
 56$$ 5  a2 5  a6 3  a10 5  a15 3  a16 74  a17 4  a18 1  e
 57**  3.62000+02  0.00000+00  1.00000-08  1.94108-01  e
 t
mox fuel - 5.5wt% pu in mox 14x14 asmby, beznau-1 reactor, bm-5
single reactor assembly
 58** 4r  3.01420+01  3.01420-14  e
 60**  4.54250+02  5.46500+02  6.38750+02  7.31000+02  7.93000+02  e
 66$$ 1  a5 1  e
 t

 3$$ 33  a3 3  a33 18  e
 4**  a4  1.00000-31  e
 54$$ 5 11r 0  e
 t
 t
 56$$ 5  a2 5  a6 3  a10 5  a15 3  a16 74  a17 4  a18 1  e
 57**  7.93000+02  0.00000+00  1.00000-08  1.10994-01  e
 t
mox fuel - 5.5wt% pu in mox 14x14 asmby, beznau-1 reactor, bm-5
single reactor assembly
```

```
 58** 4r  3.01420+01  3.01420-14  e
 60**  8.45750+02  8.98500+02  9.51250+02  1.00400+03  1.10300+03  e
 66$$ 1  a5 1  e
 t

 3$$ 33  a3 4  a33 18  e
 4**  a4  1.00000-31  e
 54$$ 5 11r 0  e
 t
 t
 56$$ 5  a2 5  a6 3  a10 5  a15 3  a16 74  a17 4  a18 1  e
 57**  1.10300+03  0.00000+00  1.00000-08  1.80431-01  e
 t
mox fuel - 5.5wt% pu in mox 14x14 asmby, beznau-1 reactor, bm-5
single reactor assembly
 58** 4r  3.01420+01  3.01420-14  e
 60**  1.18875+03  1.27450+03  1.36025+03  1.44600+03  1.49100+03  e
 66$$ 1  a5 1  e
 t

 3$$ 33  a3 5  a33 18  e
 4**  a4  1.00000-31  e
 54$$ 5 11r 0  e
 t
 t
 56$$ 5  a2 5  a6 3  a10 5  a15 3  a16 74  a17 4  a18 1  e
 57**  1.49100+03  0.00000+00  1.00000-08  1.75171-01  e
 t
mox fuel - 5.5wt% pu in mox 14x14 asmby, beznau-1 reactor, bm-5
single reactor assembly
 58** 4r  3.01420+01  3.01420-14  e
 60**  1.57425+03  1.65750+03  1.74075+03  1.82400+03  1.85400+03  e
 66$$ 1  a5 1  e
 t

 3$$ 33  a3 6 0  a33 0  e
 4**  a4  1.00000-31  e
 54$$ 5 11r 0  e
 t
 t
 56$$ 4  a2 4  a6 1  a10 5  a15 3  a16 74  a17 4  a18 1  e
 57**  1.85400+03  0.00000+00  1.00000-08  1.75697-01  e
 t
mox fuel - 5.5wt% pu in mox 14x14 asmby, beznau-1 reactor, bm-5
single reactor assembly
 58** 4r  3.01420+01  e
 60**  1.93750+03  2.02100+03  2.10450+03  2.18800+03  e
 66$$ 1  a5 1  e
 t
 56$$  a2 10  a5 5  a6 1  a10 4  a15 3  a16 74  a17 2  a18 1  e
 57** 2r  0.00000+00  1.00000-03  1.75697-01  e
 t
mox fuel - 5.5wt% pu in mox 14x14 asmby, beznau-1 reactor, bm-5
single reactor assembly
 60**  1 100 300 600 1098 1200 1243 1270 1382 1418
 66$$ 1  a5 1  e
 61** 3r  7.00000-07 4r  7.00000-09  e
 65$$ 3r 0 1 3r 0 1 2r 0 1 0 1 8r 0 2r 1 0 2r 1 2r 0 1 2r 0 1 0 1 11r 0
 1 3r 0 1 2r 0 1 0 2r 1 7r 0  e
 t
 56$$  0 0 a10 1 e t
 56$$  0 0 a10 5 e t
 56$$  0 0 a10 6 e t
```

73

```
 56$$   0  0  a10  7  e  t
 56$$   0  0  a10  8  e  t
 56$$   0  0  a10  9  e  t
 56$$   0  0  a10  10  e  t
 56$$  20r  0   e
 t
end
```

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