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# **Analysis of Experimental Data for High Burnup PWR Spent Fuel Isotopic Validation—Calvert Cliffs, Takahama, and Three Mile Island Reactors**

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# **Analysis of Experimental Data for High Burnup PWR Spent Fuel Isotopic Validation—Calvert Cliffs, Takahama, and Three Mile Island Reactors**

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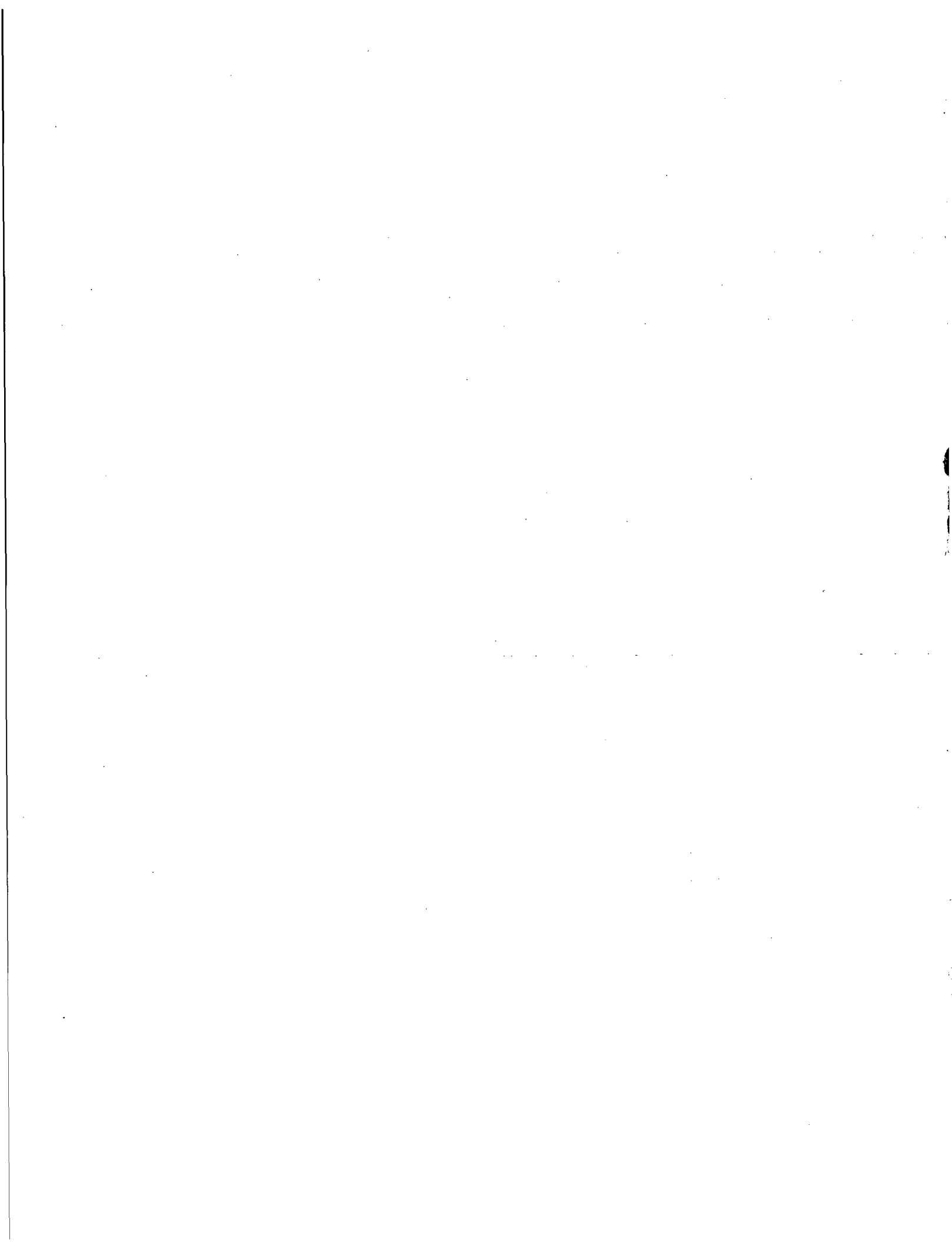
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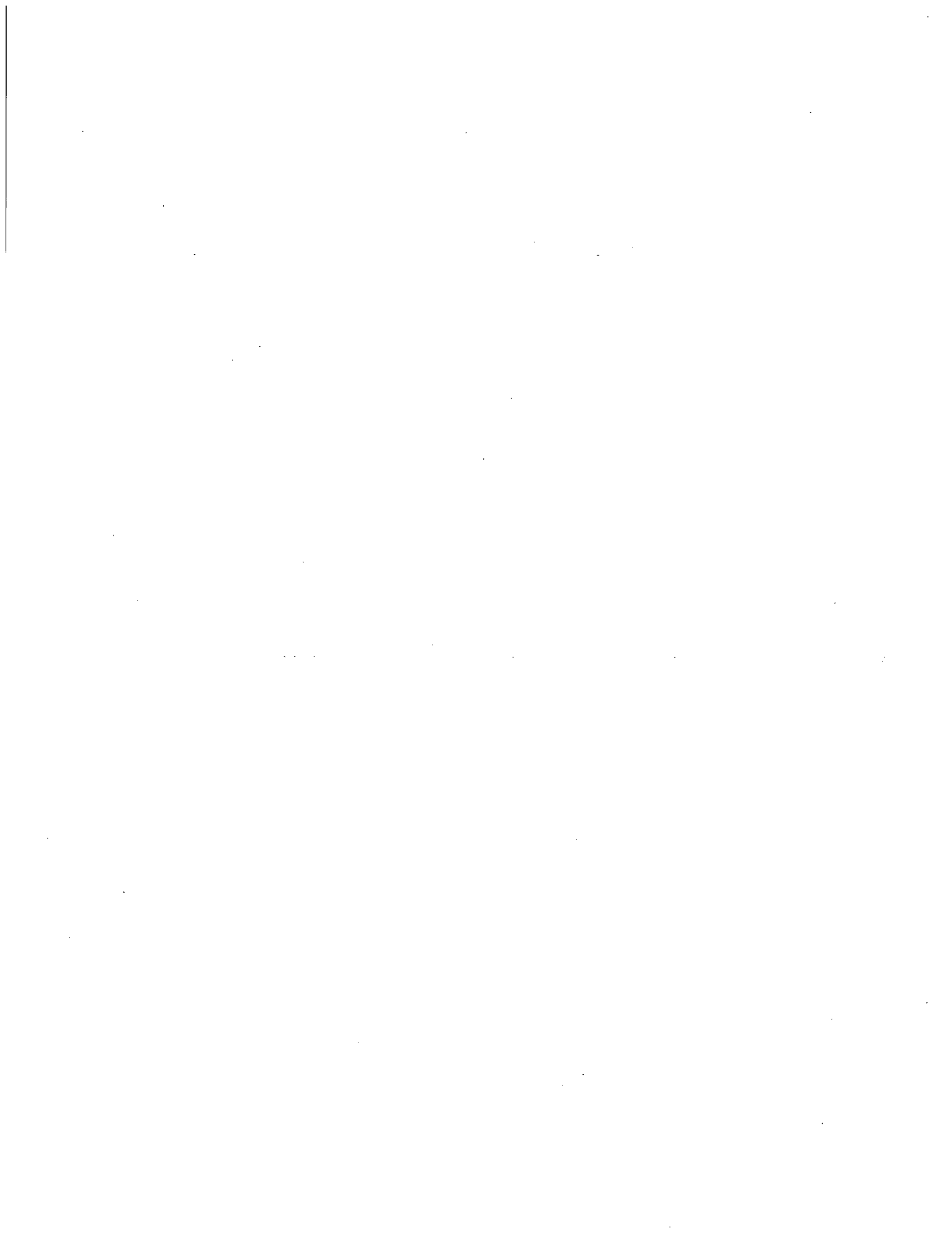
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## ABSTRACT

This report is part of a report series designed to document benchmark-quality radiochemical isotopic assay data against which computer code accuracy can be quantified to establish the uncertainty and bias associated with the code predictions. The experimental data included in the report series were acquired from domestic and international programs and include spent fuel samples that cover a large burnup range. The measurements analyzed in the current report, for which experimental data is publicly available, include 38 spent fuel samples selected from fuel rods with a 2.6 to 4.7 wt %  $^{235}\text{U}$  initial enrichment, which were irradiated in three pressurized water reactors operated in the United States and Japan and achieved burnup values from 14 to 56 GWd/MTU. The analysis of the measurements was performed by employing the two-dimensional depletion sequence of the TRITON module in the SCALE code system.



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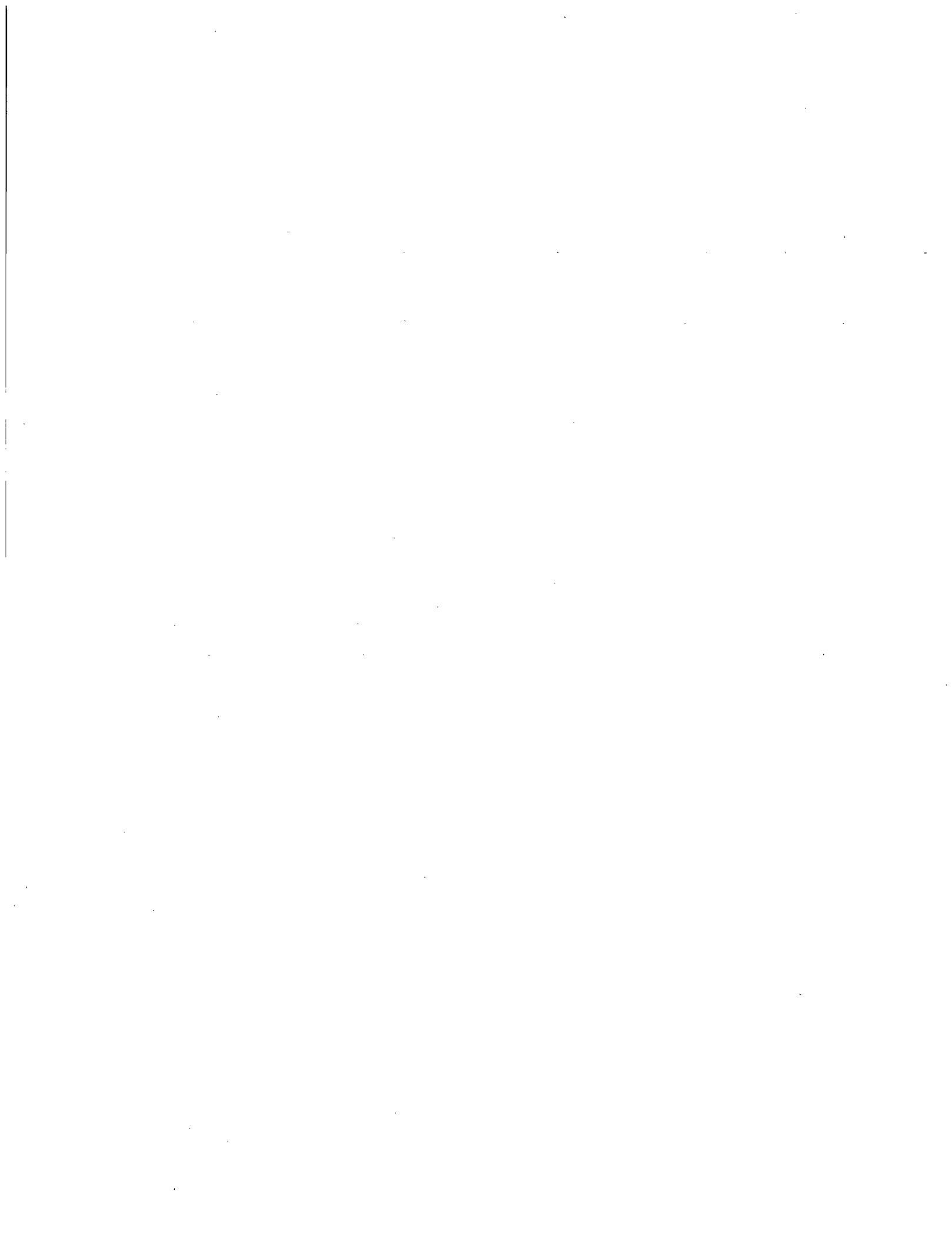
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## ACRONYMS

ANL	Argonne National Laboratory
ARIANE	<u>A</u> ctinides <u>R</u> esearch <u>I</u> n <u>A</u> <u>N</u> uclear <u>E</u> lement
ATM	Approved Testing Material
BOC	beginning of cycle
BPR	burnable poison rod
CE	Combustion Engineering
CEA	Commissariat à l'Énergie Atomique
C/E	calculated-to-experimental
DOE	U.S. Department of Energy
EFPD	effective full power days
EOC	end of cycle
EPRI	Electric Power Research Institute
GE-VNC	General Electric-Vallecitos Nuclear Center
GKN II	Gemeinschaftskernkraftwerk Unit II
ICP-MS	inductively coupled plasma mass spectrometry
ID-MS	isotope dilution mass spectrometry
ITU	Institute for Transuranium Elements
JAERI	Japanese Atomic Energy Research Institute
KRI	Khoplin Radium Institute
LANL	Los Alamos National Laboratory
LA	luminescent analysis
LWR	light water reactor
MALIBU	<u>MOX</u> and <u>UOX</u> <u>L</u> WR Fuels <u>I</u> rradiated to High <u>B</u> urnup
MOX	mixed oxide
MS	mass spectrometry
MTU	metric ton uranium ( $10^6$ grams)
NEA	Nuclear Energy Agency
NRC	U.S. Nuclear Regulatory Commission
OECD	Organization for Economic Cooperation and Development
ORNL	Oak Ridge National Laboratory
PNNL	Pacific Northwest National Laboratory
PSI	Paul Scherrer Institute
PWR	pressurized water reactor
REBUS	<u>R</u> eactivity Tests for a Direct Evaluation of the <u>B</u> urnup Credit on <u>S</u> electd irradiated LWR fuel bundles
RSD	relative standard deviation
SCALE	Standardized Computer Analyses for Licensing Evaluations
SCK-CEN	Studiecentrum voor Kernenergie - Centre d'étude de l'Énergie Nucléaire
SFCOMPO	Spent Fuel Isotopic Composition Database
TIMS	thermal ionization mass spectrometry
TMI	Three Mile Island
YMP	Yucca Mountain Project





# 1 INTRODUCTION

The current trend toward extended irradiation cycles and higher fuel enrichments of up to 5 wt %  $^{235}\text{U}$  has led to an increase of the burnup range for discharged nuclear fuel assemblies in the United States that is expected to exceed 60 GWd/MTU. Accurate analysis and evaluation of the uncertainties in the predicted isotopic composition for spent nuclear fuel in the high burnup regime requires rigorous computational tools and experimental data against which these tools can be benchmarked. However, the majority of isotopic assay measurements available to date involve spent fuel with burnups of less than 40 GWd/MTU and enrichments below 4 wt %  $^{235}\text{U}$ , limiting the ability to directly validate computer code predictions and accurately quantify the uncertainties of isotopic analyses for modern, high-burnup fuel.

This report is part of a report series that documents high-quality radiochemical assay data against which computer code predictions of the isotopic composition in high burnup fuel can be validated. Quantifying and evaluating these uncertainties is fundamental for understanding and reducing the uncertainties associated with predicting the high burnup fuel characteristics for spent fuel transportation and storage applications involving decay heat, radiation sources, and criticality safety evaluations with burnup credit, as well as for reactor safety studies and accident consequence analysis. The report series presents a compilation of recently available isotopic measurements involving high burnup pressurized water reactor (PWR) fuel as well as older isotopic measurements for low- and medium-range burnup fuel that can be used for code validation purposes. Previous experiments were selected primarily on the basis of having extensive fission product measurements.

The experimental data included in the report series were compiled from domestic and international programs. The isotopic assay measurements include data for a total of 45 spent fuel samples selected from fuel rods enriched from 2.6 to 4.7 wt %  $^{235}\text{U}$  and irradiated in five different PWRs operated in Germany, Japan, Switzerland, and the United States. The samples cover a large burnup range, from 14 to 70 GWd/MTU. A summary of the experimental programs and measured fuel characteristics is listed in Table 1.1.

The current report includes the experimental data and analysis of measurements for which information is publicly available and was not obtained through multi-collaborative international programs. Data for 38 fuel sample measurements are presented in this report: 22 of domestic origin and 16 from experiments carried out in Japan. The burnup range for these samples is 14 to 56 GWd/MTU. The Japanese experimental data is publicly available in the Spent Fuel Isotopic Composition Database (SFCOMPO), originally developed by the Japanese Atomic Energy Research Institute (JAERI) and now administered by the Nuclear Energy Agency (NEA), a specialized agency within the Organization for Economic Cooperation and Development (OECD). As indicated in Table 1.1, a second report documents the analysis of experimental data acquired by Oak Ridge National Laboratory (ORNL) through participation in two international programs: (1) "Actinides Research In A Nuclear Element" (ARIANE) and (2) "Reactivity Tests for a Direct Evaluation of the Burnup Credit on Selectd Irradiated LWR Fuel Bundles" (REBUS), both coordinated by the Belgian company Belgonucleaire. A third report presents the analysis of experimental data obtained by ORNL through participation in the MALIBU international program coordinated by Belgonucleaire. Each of the three reports mentioned in Table 1.1 present information on the radiochemical analysis methods and uncertainties, assembly design description and irradiation history, and computational models and results obtained using the "Standardized Computer Analyses for Licensing Evaluations" (SCALE) code system.<sup>1</sup>

Section 2 of the current report presents a summary of the experimental programs evaluated. The radiochemical methods employed and the associated experimental uncertainties are provided in Section 3.

Information on the assembly design data and irradiation history is presented in Section 4, and details on the computational models developed and simulation methodology used are shown in Section 5. A comparison of the experimental results to the results obtained from code simulations with SCALE are presented in Section 6.

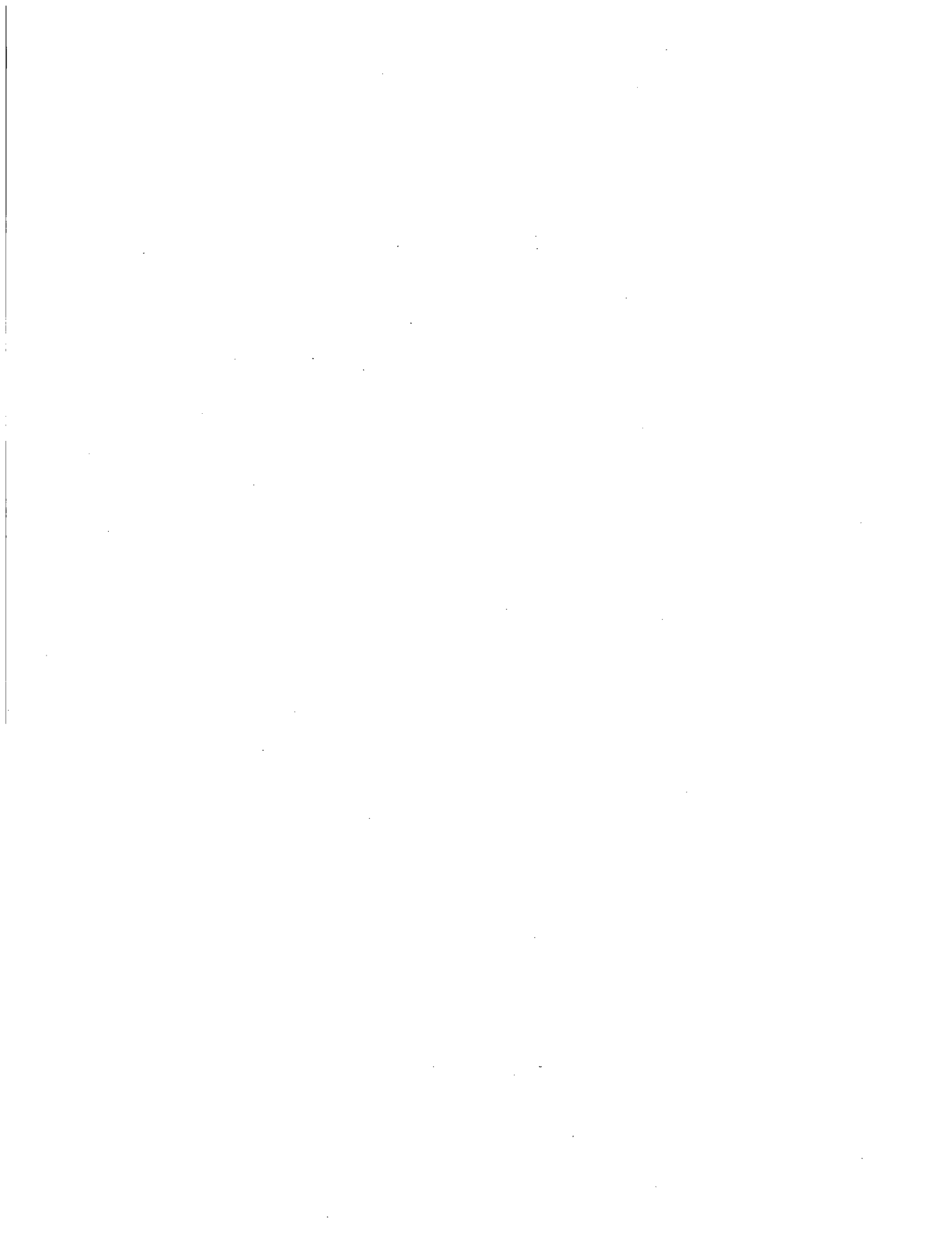
**Table 1.1 Summary of spent fuel measurements**

Reactor (country)	Measurement facility	Experimental program name	Assembly design	Enrichment (wt % <sup>235</sup> U)	No. of samples	Measurement methods	Burnup(s) (GWd/MTU)
TMI-1 <sup>a</sup> (USA)	ANL (USA)	YMP	15 × 15	4.013	11	ICP-MS, α-spec, γ-spec	44.8 – 55.7
TMI-1 <sup>a</sup> (USA)	GE-VNC (USA)	YMP	15 × 15	4.657	8	TIMS, α-spec, γ-spec	22.8 – 29.9
Calvert Cliffs <sup>a</sup> (USA)	PNNL, KRI (USA, Russia)	ATM	14 × 14 CE	3.038	3	ID-MS, LA, α-spec, γ-spec	27.4 – 44.3
Takahama 3 <sup>a</sup> (Japan)	JAERI (Japan)	JAERI	17 × 17	2.63, 4.11	16	ID-MS, α-spec, γ-spec	14.3 – 47.3
Gösgen <sup>b</sup> (Switzerland)	SCK-CEN, ITU (Belgium, Germany)	ARIANE	15 × 15	3.5, 4.1	3	TIMS, ICP-MS, α-spec, β-spec, γ-spec	29.1, 52.5, 59.7
GKN II <sup>b</sup> (Germany)	SCK-CEN (Belgium)	REBUS	18 × 18	3.8	1	TIMS, ICP-MS α-spec, γ-spec	54.0
Gösgen <sup>c</sup> (Switzerland)	CEA, PSI, SCK-CEN (France, Switzerland, Belgium)	MALIBU	15 × 15	4.3	3	TIMS, ICP-MS, α-spec, γ-spec	46.0, 50.8, 70.4

<sup>a</sup> Documented in current report.

<sup>b</sup> Documented in G. Ilas, I. C. Gauld, and B. D. Murphy, *Analysis of Experimental Data for High Burnup PWR Spent Fuel Isotopic Validation—ARIANE and REBUS Programs (UO<sub>2</sub> Fuel)*, NUREG/CR-6969 (ORNL/TM-2008/072), Oak Ridge National Laboratory, Oak Ridge, Tennessee (May 2008).

<sup>c</sup> Documented in G. Ilas, and I. C. Gauld, and B. D. Murphy, *Analysis of Experimental Data for High Burnup PWR Spent Fuel Isotopic Validation—MALIBU Program (UO<sub>2</sub> Fuel)*, NUREG/CR-6970 (ORNL/TM-2008/13), Oak Ridge National Laboratory, Oak Ridge, Tennessee (May 2008).



## 2 EXPERIMENTAL PROGRAMS

This section provides a brief overview of the measured isotopic assay data compiled in this report for code validation and a summary of the experimental programs from which they were acquired. A description of the measurement techniques and experimental data and uncertainties is provided in Section 3.

### 2.1 DOMESTIC PROGRAMS

#### 2.1.1 TMI-1

Measurements on 19 spent fuel samples from the Three Mile Island (TMI) Unit 1 reactor were performed under the auspices of the U.S. Department of Energy (DOE) Yucca Mountain Project (YMP). Fuel rods were obtained from two separate assemblies, identified as NJ05YU and NJ070G. Radiochemical analyses were performed at two independent experimental facilities: Argonne National Laboratory (ANL) and General Electric–Vallecitos Nuclear Center (GE-VNC). Measurements on 11 of the TMI-1 samples from rod H6 of assembly NJ05YU were performed in 1998 and 2000 at ANL;<sup>2</sup> whereas, the other eight TMI-1 samples, from rods O1, O12, and O13 of assembly NJ070G, were analyzed in 1999 at GE-VNC.<sup>3</sup> Fuel rod H6 had an initial enrichment of 4.013 wt % <sup>235</sup>U and achieved local sample burnups from 45 to 56 GWd/MTU over two irradiation cycles (cycles 9 and 10). Rods O1, O12, and O13 had an initial enrichment of 4.657 wt % <sup>235</sup>U and achieved burnups between 22 and 30 GWd/MTU in one irradiation cycle (cycle 10).

Previous benchmark calculations performed using these measurements have yielded uncharacteristically large deviations in isotopic results in comparison with past experience: YMP has published results indicating deviations in the predicted <sup>239</sup>Pu concentrations that ranged up to 30–40% higher than the measurements.<sup>4</sup> Past experience with other spent fuel samples evaluated by ORNL (and YMP) have yielded lower deviations as compared to measurements.<sup>5</sup> The large deviations obtained by YMP were inconsistent with the results observed for similar burnup samples from the Takahama-3 reactor<sup>6</sup> and also differed from literature results for spent fuel validation for the French Gravelines reactor<sup>7</sup> obtained using French codes and data.

Investigations have been performed by Electric Power Research Institute (EPRI), following indications of fuel leakage during TMI-1 cycle 10, to examine the causes of fuel rod failure, as it is mentioned in the abstract for the TR-108784-V1 report.<sup>8</sup> As the fuel failure phenomena introduce additional uncertainties related to the actual operating conditions of the fuel that may affect the accuracy of code predictions, these type of uncertainties and their importance to the fuel simulations would need to be accounted for in a comparison of predicted and experimental isotopic assay data. Because no details are publicly available on the actual location or description of the failed fuel rods in cycle 10 and their relationship with the fuel rods for which measured isotopic assay data is presented here, no assessment of the impact of the failed fuel on the calculated results can be made based on the currently available unrestricted information.

#### 2.1.2 Calvert Cliffs

The measurements on three spent fuel samples from Calvert Cliffs Unit 1 reactor considered in this report were carried out at the Material Characterization Center at Pacific Northwest National Laboratory (PNNL) for the Approved Testing Material (ATM) Program<sup>9</sup> designed to characterize medium-burnup spent fuel representative of reactors operating in the United States. Lanthanide measurements for the same three samples have been also performed at Khoplin Radium Institute (KRI) in Russia.<sup>10</sup> These three

samples were selected from rod MKP-109 of assembly D047 that was irradiated in the reactor for four consecutive cycles. The assembly had an initial fuel enrichment of 3.038 wt %  $^{235}\text{U}$ , and the samples under consideration covered a burnup range from 27 to 44 GWd/MTU.

The PNNL data served as the basis of a benchmark for validating irradiated fuel used in criticality calculations<sup>11,12</sup> and was used for the OECD/NEA burnup credit criticality safety calculation benchmark Phase I-B.<sup>13</sup>

## **2.2 INTERNATIONAL PROGRAMS**

### **2.2.1 JAERI (Takahama-3)**

From 1990 to 1999, JAERI carried out a series of projects focused on obtaining high-quality experimental isotopic assay and criticality data to support the development of burnup credit for storage and transportation of spent fuel. The measurements included destructive radiochemical analyses of spent fuel samples, axial gamma scanning of spent fuel rods, and exponential experiments on spent fuel assemblies. The measured data were used by JAERI for evaluating the accuracy of depletion or criticality computational tools.

Sixteen samples selected from three fuel rods irradiated in assemblies NT3G23 and NT3G24 of the Takahama-3 reactor were included for destructive isotopic analyses. Five of these samples belonged to a  $\text{UO}_2\text{-Gd}_2\text{O}_3$  fuel rod with a 2.63 wt %  $^{235}\text{U}$  initial enrichment; whereas, the other 11 samples were from two  $\text{UO}_2$  fuel rods with an initial enrichment of 4.11 wt %  $^{235}\text{U}$ . The burnup of these samples was between 14 and 47 GWd/MTU.

### 3 ISOTOPIC MEASUREMENTS

#### 3.1 TMI-1 SAMPLES

##### 3.1.1 ANL Measurements

The radiochemical analysis at ANL considered 11 samples from fuel rod H6 of TMI-1 assembly identified as NJ05YU, cut from rod segments provided by GE-VNC. The samples for analysis were prepared by dissolution of an approximately 0.1–0.2 g aliquot of homogenized fuel sample powder. Analyses were carried out by using inductively coupled plasma mass spectrometry (ICP-MS),  $\gamma$ -spectrometry, and  $\alpha$ -spectrometry to determine the isotopic mass of 31 nuclides. The results were reported relative to the measured  $^{238}\text{U}$  content in the sample, as g/g  $^{238}\text{U}$ . Two measures of the experimental uncertainty, a within-sample precision and a bias uncertainty, were provided by ANL. The within-sample precision was estimated by ANL as one standard deviation through repeated measurements of samples, whereas the bias uncertainty was estimated from deviations of quality control standard solutions measured before and after fuel samples; the bias uncertainty included the propagation of error for normalization to  $^{238}\text{U}$ .<sup>2</sup>

The main experimental techniques used for each nuclide and the reported corresponding experimental uncertainties<sup>2</sup> are presented in Table 3.1. In addition to the bias values shown in the table, a bias uncertainty of 3.8% was reported for  $^{238}\text{U}$ ; but no explanation was provided on the significance of this value; it is assumed here that it refers to the  $^{238}\text{U}$  concentration measured directly. The within-sample precision shown in the fifth column of the table was calculated so that it accounted for error propagation due to normalization of the concentration to the  $^{238}\text{U}$  content, as:

$$\sigma_{i,\text{within-sample}} = \sqrt{\left(\sigma_{i,\text{within-sample}}^{\text{reported}}\right)^2 + \left(\sigma_{^{238}\text{U},\text{within-sample}}^{\text{reported}}\right)^2} \quad (3-1)$$

where  $i$  identifies the nuclide. The total uncertainty for the measured concentration of a nuclide  $i$  expressed relative to the  $^{238}\text{U}$  content is shown in the sixth column of Table 3.1 and was obtained by combining the within-sample uncertainty, calculated as in Eq. 3-1, and the reported bias, as:

$$\sigma_{i,\text{total}} = \sqrt{\left(\sigma_{i,\text{within-sample}}\right)^2 + \left(\sigma_{i,\text{bias}}^{\text{reported}}\right)^2} \quad (3-2)$$

The total uncertainty is 3.7% for  $^{235}\text{U}$ , in the range 5–8% for plutonium nuclides, and about 5 - 7% for neodymium isotopes.

The reported results of the radiochemical analyses performed on TMI-1 samples at ANL<sup>2</sup> are shown in Table 3.2. In order to be compared with measured data obtained from other experimental programs, the experimental results were also expressed in units of g/g  $U_{\text{initial}}$ , as shown in Table 3.3, using the initial uranium content in the sample as a basis. The concentration in g/g  $U_{\text{initial}}$  of nuclide  $i$  was determined as:<sup>14</sup>

$$\frac{m_i}{\sum_k m_{U_k} + \sum_l m_{Pu_l} + \sum_m m_{Am_m} + \sum_n m_{Cm_n} + 238 \frac{m_{^{148}\text{Nd}}}{148\bar{Y}}} \quad (3-3)$$

where  $m_i$  is the mass of isotope  $i$  as reported in g/g  $^{238}\text{U}$  measured. The denominator in Eq. (3-3) is an estimate of the initial uranium content as a sum of the actinide (uranium, plutonium, americium, curium) weights in the measured sample and the weight loss in initial uranium due to burnup. The reduction in heavy metal mass due to burnup is approximated by  $238 \frac{m_{^{148}\text{Nd}}}{148\bar{Y}}$ , where  $\bar{Y}$  is the average fission yield of  $^{148}\text{Nd}$ . A value  $\bar{Y} = 0.0176$  is recommended for PWR  $\text{UO}_2$  fuel.<sup>14</sup> Note that  $m_{\text{U}_{238}} = 1$  in Eq. (3-3). The relative standard deviations associated to the nuclide concentrations shown in Table 3.3 are assumed to be similar to the total uncertainty values in Table 3.1. No error propagation was carried out on the ratio in Eq. (3-3).

### 3.1.2 GE-VNC Measurements

The measurements performed at GE-VNC<sup>3</sup> considered eight samples selected from three fuel rods from assembly NJ070G. Most of the 32 nuclides for which isotopic concentrations were measured at GE-VNC were determined by using thermal ionization mass spectrometry (TIMS) and some through  $\gamma$ - or  $\alpha$ -spectrometry. The nuclide concentrations in the samples measured by TIMS were determined from measurements of spiked and unspiked samples. The nuclide content was reported as g/g  $^{238}\text{U}$ . The main experimental techniques used for each nuclide and the corresponding experimental uncertainty as reported are presented in Table 3.4. The experimental errors, reported by GE-VNC as relative uncertainty at a 95% confidence level, are shown in the third column of the table. The relative standard deviation (RSD) shown in the fourth column of the table was obtained as half of the reported uncertainty at a 95% confidence level. The RSD for the GE-VNC measurements is 0.6% for all plutonium nuclides except for  $^{238}\text{Pu}$ , 0.5% for  $^{235}\text{U}$ , and 0.8% for neodymium isotopes.

The reported results of the radiochemical analyses performed on TMI-1 samples at GE-VNC<sup>3</sup> are shown in Table 3.5. The measured results, expressed using the initial content of uranium in the sample as a basis, are presented in Table 3.6. The unit conversion was done by using Eq. (3-3).



**Table 3.1 Experimental techniques and uncertainties for  
TMI-1 samples measurements at ANL**

Nuclide ID	Method <sup>a</sup>	Reported within-sample precision (%)	Reported bias uncertainty (%)	Within-sample precision <sup>b</sup> accounting for normalization to <sup>238</sup> U (%)	Total <sup>c</sup> uncertainty (%)
U-234	ICP-MS	3.0	2.7	3.4	4.4
U-235	ICP-MS	1.5	2.9	2.3	3.7
U-236	ICP-MS	4.6	3.1	4.9	5.8
U-238	ICP-MS	1.7			4.2
Np-237	ICP-MS	4.1	3.4	4.4	5.6
Pu-238	α-spec	6.8	3.6	7.0	7.9
Pu-239	ICP-MS	4.3	3.3	4.6	5.7
Pu-240	ICP-MS	5.1	3.1	5.4	6.2
Pu-241	ICP-MS	3.2	2.9	3.6	4.6
Pu-242	ICP-MS	5.9	2.8	6.1	6.7
Am-241	γ-spec	6.1	3.1	6.3	7.1
Am-242m	ICP-MS	NA	3.1		3.1
Am-243	ICP-MS	4.2	3.8	4.5	5.9
Mo-95	ICP-MS	1.7	3.4	2.4	4.2
Tc-99	ICP-MS	2.7	7.3	3.2	8.0
Ru-101	ICP-MS	1.6	5.3	2.3	5.8
Rh-103	ICP-MS	1.5	3.1	2.3	3.8
Ag-109	ICP-MS	4.7	3.1	5.0	5.9
Cs-137	γ-spec	3.6	2.7	4.0	4.8
Nd-143	ICP-MS	3.5	3.9	3.9	5.5
Nd-145	ICP-MS	4.8	3.5	5.1	6.2
Nd-148	ICP-MS	4.2	5.5	4.5	7.1
Sm-147	ICP-MS	3.3	9.4	3.7	10.1
Sm-149	ICP-MS	7.1	3.5	7.3	8.1
Sm-150	ICP-MS	3.5	3.2	3.9	5.0
Sm-151	ICP-MS	6.1	3.2	6.3	7.1
Sm-152	ICP-MS	2.7	3.2	3.2	4.5
Eu-151	ICP-MS	12.0	2.9	12.1	12.5
Eu-153	ICP-MS	3.9	3.0	4.3	5.2
Eu-155	γ-spec	6.4	2.7	6.6	7.2
Gd-155	ICP-MS	6.8	3.8	7.0	8.0

<sup>a</sup> Main technique is listed; some nuclides require multiple techniques to eliminate interferences.

<sup>b</sup> Calculated as shown in Eq. 3-1.

<sup>c</sup> Calculated as shown in Eq. 3-2.

Table 3.2 Experimental results (g/g <sup>238</sup>U) for TMI-1 samples from assembly NJ05YU

Sample ID	A1B	D2	B2	C1	D1A4	A2	C3	C2B	B3J	B1B	D1A2
Burnup <sup>a</sup> (GWd/MTU)	44.8	44.8	50.1	50.2	50.5	50.6	51.3	52.6	53.0	54.5	55.7
U-234	2.21E-04	2.07E-04	2.02E-04	2.14E-04	2.14E-04	2.07E-04	2.00E-04	1.96E-04	1.99E-04	2.04E-04	2.10E-04
U-235	9.26E-03	7.94E-03	6.71E-03	7.13E-03	8.11E-03	6.84E-03	6.77E-03	6.75E-03	6.63E-03	6.94E-03	7.59E-03
U-236	5.50E-03	5.74E-03	5.84E-03	5.92E-03	5.81E-03	5.95E-03	5.77E-03	5.62E-03	5.92E-03	5.87E-03	5.94E-03
Pu-238	4.34E-04	3.50E-04	3.40E-04	3.57E-04	4.06E-04	3.83E-04	2.72E-04	4.97E-04	4.32E-04	4.69E-04	4.15E-04
Pu-239	5.45E-03	5.84E-03	5.72E-03	5.85E-03	5.85E-03	5.78E-03	5.97E-03	5.41E-03	5.52E-03	5.55E-03	5.94E-03
Pu-240	2.52E-03	2.87E-03	2.95E-03	2.98E-03	2.84E-03	3.01E-03	3.08E-03	2.76E-03	2.88E-03	2.86E-03	2.95E-03
Pu-241	1.30E-03	1.47E-03	1.50E-03	1.54E-03	1.55E-03	1.47E-03	1.52E-03	1.44E-03	1.48E-03	1.48E-03	1.60E-03
Pu-242	7.31E-04	8.55E-04	9.89E-04	9.74E-04	1.02E-03	9.99E-04	1.00E-03	1.01E-03	1.20E-03	1.04E-03	1.05E-03
Np-237	6.50E-04	7.27E-04	7.48E-04	7.62E-04	7.42E-04	7.51E-04	7.39E-04	7.44E-04	7.66E-04	7.62E-04	7.69E-04
Am-241	3.73E-04	3.72E-04	3.69E-04	4.08E-04	5.70E-04	3.27E-04	3.28E-04	5.50E-04	5.49E-04	3.13E-04	3.65E-04
Am-242m	1.00E-05	1.00E-05	1.00E-05	1.00E-05	9.09E-07	1.00E-05	1.00E-05	1.82E-06	1.35E-06	1.12E-06	6.63E-07
Am-243	1.34E-04	2.07E-04	2.76E-04	2.66E-04	2.00E-04	2.75E-04	2.67E-04	2.12E-04	2.29E-04	2.22E-04	2.24E-04
Nd-143	1.06E-03	9.83E-04	1.08E-03	1.06E-03	1.17E-03	1.03E-03	1.03E-03	1.12E-03	1.15E-03	1.18E-03	1.21E-03
Nd-145	9.17E-04	8.92E-04	9.80E-04	9.71E-04	1.04E-03	9.50E-04	9.71E-04	1.02E-03	1.06E-03	1.07E-03	1.09E-03
Nd-148	5.24E-04	5.24E-04	5.89E-04	5.90E-04	5.94E-04	5.96E-04	6.04E-04	6.20E-04	6.25E-04	6.44E-04	6.60E-04
Cs-137	1.81E-03	1.74E-03	1.89E-03	1.96E-03	1.79E-03	1.91E-03	1.84E-03	1.91E-03	1.88E-03	1.91E-03	1.67E-03
Sm-147	2.43E-04	1.96E-04	2.01E-04	2.02E-04	2.55E-04	2.13E-04	1.97E-04	2.48E-04	2.69E-04	2.77E-04	2.74E-04
Sm-149	3.35E-06	3.33E-06	3.53E-06	3.45E-06	3.90E-06	4.13E-06	3.14E-06	3.64E-06	3.46E-06	3.72E-06	4.20E-06
Sm-150	3.85E-04	3.75E-04	4.06E-04	4.15E-04	4.47E-04	4.05E-04	3.92E-04	4.54E-04	4.91E-04	5.08E-04	4.93E-04
Sm-151	1.39E-05	1.36E-05	1.45E-05	1.35E-05	1.53E-05	1.36E-05	1.36E-05	1.44E-05	1.60E-05	1.63E-05	1.69E-05
Sm-152	1.31E-04	1.30E-04	1.40E-04	1.37E-04	1.45E-04	1.43E-04	1.36E-04	1.41E-04	1.54E-04	1.56E-04	1.55E-04
Eu-151	7.98E-07	7.57E-07	8.58E-07	7.42E-07	7.23E-07	9.56E-07	9.18E-07	7.62E-07	8.11E-07	6.19E-07	7.21E-07
Eu-153	1.58E-04	1.68E-04	1.81E-04	1.81E-04	1.89E-04	1.85E-04	1.74E-04	1.87E-04	1.99E-04	2.02E-04	2.06E-04
Eu-155	1.08E-05	1.32E-05	1.42E-05	1.55E-05	1.37E-05	1.39E-05	1.38E-05	1.08E-05	1.12E-05	1.68E-05	1.07E-05

**Table 3.2 Experimental results (g/g <sup>238</sup>U) for TMI-1 samples from assembly NJ05YU (continued)**

Sample ID	A1B	D2	B2	C1	D1A4	A2	C3	C2B	B3J	B1B	D1A2
Burnup <sup>a</sup> (GWd/MTU)	44.8	44.8	50.1	50.2	50.5	50.6	51.3	52.6	53.0	54.5	55.7
Gd-155	8.85E-06	6.02E-06	7.08E-06	6.88E-06	1.51E-05	6.56E-06	7.22E-06	1.02E-05	1.13E-05	1.09E-05	1.11E-05
Mo-95	1.12E-03	9.90E-04	1.22E-03	1.19E-03	1.18E-03	1.21E-03	1.09E-03	1.19E-03	1.22E-03	1.25E-03	1.21E-03
Tc-99	1.53E-03	1.05E-03	1.18E-03	1.17E-03	1.29E-03	1.17E-03	1.12E-03	1.47E-03	1.35E-03	1.43E-03	1.24E-03
Ru-101	1.20E-03	1.02E-03	1.30E-03	1.26E-03	1.19E-03	1.25E-03	1.11E-03	1.27E-03	1.27E-03	1.29E-03	1.23E-03
Rh-103	6.41E-04	5.55E-04	6.80E-04	6.69E-04	6.53E-04	6.70E-04	5.93E-04	6.66E-04	6.73E-04	6.81E-04	6.72E-04
Ag-109	5.50E-05	5.01E-05	5.71E-05	5.80E-05	9.17E-05	6.46E-05	1.00E-04	7.08E-05	8.45E-05	4.78E-05	5.02E-05

<sup>a</sup>As reported in J. M. Scaglione, *Three Mile Island Unit 1 Radiochemical Assay Comparisons to SAS2H Calculations*, Yucca Mountain Project Report CAL-UDC-NU-000011, Rev. A (April 2002).

Table 3.3 Experimental results (g/g  $U_{initial}$ ) for TMI-1 samples from assembly NJ05YU

Sample ID	A1B	D2	B2	CI	DIA4	A2	C3	C2B	B3J	B1B	DIA2
Burnup <sup>a</sup> (GWd/MTU)	44.8	44.8	50.1	50.2	50.5	50.6	51.3	52.6	53.0	54.5	55.7
U-234	2.06E-04	1.93E-04	1.87E-04	1.98E-04	1.98E-04	1.92E-04	1.85E-04	1.81E-04	1.84E-04	1.88E-04	1.93E-04
U-235	8.62E-03	7.39E-03	6.22E-03	6.60E-03	7.50E-03	6.34E-03	6.27E-03	6.24E-03	6.13E-03	6.40E-03	6.99E-03
U-236	5.12E-03	5.35E-03	5.41E-03	5.48E-03	5.38E-03	5.51E-03	5.34E-03	5.20E-03	5.47E-03	5.42E-03	5.47E-03
Pu-238	4.04E-04	3.26E-04	3.15E-04	3.31E-04	3.76E-04	3.55E-04	2.52E-04	4.60E-04	3.99E-04	4.33E-04	3.82E-04
Pu-239	5.08E-03	5.44E-03	5.30E-03	5.42E-03	5.41E-03	5.35E-03	5.53E-03	5.00E-03	5.10E-03	5.12E-03	5.47E-03
Pu-240	2.35E-03	2.67E-03	2.73E-03	2.76E-03	2.63E-03	2.79E-03	2.85E-03	2.55E-03	2.66E-03	2.64E-03	2.71E-03
Pu-241	1.21E-03	1.37E-03	1.39E-03	1.43E-03	1.43E-03	1.36E-03	1.41E-03	1.33E-03	1.37E-03	1.37E-03	1.47E-03
Pu-242	6.81E-04	7.96E-04	9.17E-04	9.02E-04	9.44E-04	9.25E-04	9.26E-04	9.34E-04	1.11E-03	9.60E-04	9.66E-04
Np-237	6.05E-04	6.77E-04	6.93E-04	7.06E-04	6.87E-04	6.96E-04	6.84E-04	6.88E-04	7.08E-04	7.03E-04	7.08E-04
Am-241	3.47E-04	3.46E-04	3.42E-04	3.78E-04	5.27E-04	3.03E-04	3.04E-04	5.09E-04	5.07E-04	2.89E-04	3.36E-04
Am-242m	9.31E-06	9.31E-06	9.27E-06	9.26E-06	8.41E-07	9.26E-06	9.26E-06	1.68E-06	1.25E-06	1.03E-06	6.10E-07
Am-243	1.25E-04	1.93E-04	2.56E-04	2.46E-04	1.85E-04	2.55E-04	2.47E-04	1.96E-04	2.12E-04	2.05E-04	2.06E-04
Nd-143	9.87E-04	9.15E-04	1.00E-03	9.82E-04	1.08E-03	9.54E-04	9.53E-04	1.04E-03	1.06E-03	1.09E-03	1.11E-03
Nd-145	8.54E-04	8.31E-04	9.08E-04	8.99E-04	9.62E-04	8.80E-04	8.99E-04	9.43E-04	9.80E-04	9.87E-04	1.00E-03
Nd-148	4.88E-04	4.88E-04	5.46E-04	5.47E-04	5.50E-04	5.52E-04	5.59E-04	5.73E-04	5.78E-04	5.94E-04	6.07E-04
Cs-137	1.69E-03	1.62E-03	1.75E-03	1.82E-03	1.66E-03	1.77E-03	1.70E-03	1.77E-03	1.74E-03	1.76E-03	1.54E-03
Sm-147	2.26E-04	1.83E-04	1.86E-04	1.87E-04	2.36E-04	1.97E-04	1.82E-04	2.29E-04	2.49E-04	2.56E-04	2.52E-04
Sm-149	3.12E-06	3.10E-06	3.27E-06	3.20E-06	3.61E-06	3.83E-06	2.91E-06	3.37E-06	3.20E-06	3.43E-06	3.87E-06
Sm-150	3.59E-04	3.49E-04	3.76E-04	3.84E-04	4.14E-04	3.75E-04	3.63E-04	4.20E-04	4.54E-04	4.69E-04	4.54E-04
Sm-151	1.29E-05	1.27E-05	1.34E-05	1.25E-05	1.42E-05	1.26E-05	1.26E-05	1.33E-05	1.48E-05	1.50E-05	1.56E-05
Sm-152	1.22E-04	1.21E-04	1.30E-04	1.27E-04	1.34E-04	1.32E-04	1.26E-04	1.30E-04	1.42E-04	1.44E-04	1.43E-04
Eu-151	6.95E-07	7.05E-07	7.95E-07	6.87E-07	6.69E-07	8.85E-07	8.50E-07	7.05E-07	7.49E-07	5.71E-07	6.64E-07
Eu-153	1.47E-04	1.56E-04	1.68E-04	1.68E-04	1.75E-04	1.71E-04	1.61E-04	1.73E-04	1.84E-04	1.86E-04	1.90E-04
Eu-155	1.01E-05	1.23E-05	1.32E-05	1.44E-05	1.27E-05	1.29E-05	1.28E-05	9.99E-06	1.03E-05	1.55E-05	9.85E-06

**Table 3.3 Experimental results (g/g U<sub>initial</sub>) for TMI-1 samples from assembly NJ05YU (continued)**

Sample ID	A1B	D2	B2	C1	D1A4	A2	C3	C2B	B3J	B1B	D1A2
<b>Burnup<sup>a</sup> (GWd/MTU)</b>	<b>44.8</b>	<b>44.8</b>	<b>50.1</b>	<b>50.2</b>	<b>50.5</b>	<b>50.6</b>	<b>51.3</b>	<b>52.6</b>	<b>53.0</b>	<b>54.5</b>	<b>55.7</b>
Gd-155	8.24E-06	5.61E-06	6.56E-06	6.37E-06	1.40E-05	5.23E-06	6.68E-06	9.43E-06	1.04E-05	1.01E-05	1.02E-05
Mo-95	1.04E-03	9.22E-04	1.13E-03	1.10E-03	1.09E-03	1.12E-03	1.01E-03	1.10E-03	1.13E-03	1.15E-03	1.11E-03
Tc-99	1.42E-03	9.78E-04	1.09E-03	1.08E-03	1.19E-03	1.08E-03	1.04E-03	1.36E-03	1.25E-03	1.32E-03	1.14E-03
Ru-101	1.12E-03	9.50E-04	1.21E-03	1.17E-03	1.10E-03	1.16E-03	1.03E-03	1.17E-03	1.17E-03	1.19E-03	1.13E-03
Rh-103	5.97E-04	5.17E-04	6.30E-04	6.20E-04	6.04E-04	6.21E-04	5.49E-04	6.16E-04	6.22E-04	6.28E-04	6.18E-04
Ag-109	5.12E-05	4.67E-05	5.29E-05	5.37E-05	8.48E-05	5.98E-05	9.26E-05	6.55E-05	7.81E-05	4.41E-05	4.62E-05

<sup>a</sup> As reported in J. M. Scaglione, *Three Mile Island Unit 1 Radiochemical Assay Comparisons to SAS2H Calculations*, Yucca Mountain Project Report, CAL-UDC-NU-000011, Rev. A (April 2002).

**Table 3.4 Experimental techniques and uncertainties for TMI-1 samples measurements at GE-VNC**

Nuclide ID	Method <sup>a</sup>	Reported uncertainty at 95% confidence (%)	RSD <sup>b</sup> (%)
U-234	TIMS	1.0	0.5
U-235	TIMS	1.0	0.5
U-236	TIMS	1.0	0.5
U-238	TIMS	1.0	0.5
Np-237	$\alpha$ -spec	5.8	2.9
Pu-238	$\alpha$ -spec	5.0	2.5
Pu-239	TIMS	1.2	0.6
Pu-240	TIMS	1.2	0.6
Pu-241	TIMS	1.2	0.6
Pu-242	TIMS	1.2	0.6
Am-241	TIMS, $\alpha$ -spec	7.0	3.5
Am-242m	TIMS, $\alpha$ -spec	7.0	3.5
Am-243	TIMS, $\alpha$ -spec	7.0	3.5
Cm-242	TIMS, $\alpha$ -spec	20.0	10.0
Cm-243	TIMS, $\alpha$ -spec	5.5	2.75
Cm-244	TIMS, $\alpha$ -spec	5.5	2.75
Cm-245	TIMS, $\alpha$ -spec	5.5	2.75
Cs-134	$\gamma$ -spec	3.5	1.75
Cs-137	$\gamma$ -spec	3.5	1.75
Nd-143	TIMS	1.5	0.75
Nd-145	TIMS	1.5	0.75
Nd-146	TIMS	1.5	0.75
Nd-148	TIMS	1.5	0.75
Nd-150	TIMS	1.5	0.75
Sm-147	TIMS	1.7	0.85
Sm-149	TIMS	1.8	0.9
Sm-150	TIMS	1.7	0.85
Sm-151	TIMS	1.7	0.85
Sm-152	TIMS	1.7	0.85
Eu-151	TIMS	1.7	0.85
Eu-153	TIMS	1.8	0.9
Gd-155	TIMS	2.7	1.35

<sup>a</sup> Main technique is listed; some nuclides require multiple techniques to eliminate interferences.

<sup>b</sup> Relative standard deviation; calculated here as half of the uncertainty reported at a 95% confidence level.

**Table 3.5 Experimental results (g/g <sup>238</sup>U) for TMI-1 samples from assembly NJ070G**

Sample ID	O13S7	O12S4	O12S6	O1S1	O13S8	O12S5	O1S3	O1S2
<b>Burnup<sup>a</sup> (GWd/MTU)</b>	<b>22.8</b>	<b>23.7</b>	<b>24.0</b>	<b>25.8</b>	<b>26.3</b>	<b>26.5</b>	<b>26.7</b>	<b>29.9</b>
U-234	3.65E-04	3.55E-04	3.48E-04	3.48E-04	3.40E-04	3.34E-04	3.35E-04	3.25E-04
U-235	2.53E-02	2.51E-02	2.55E-02	2.35E-02	2.34E-02	2.33E-02	2.32E-02	2.05E-02
U-236	4.49E-03	4.58E-03	4.68E-03	4.83E-03	4.89E-03	4.93E-03	4.99E-03	5.34E-03
Pu-238	6.41E-05	6.68E-05	8.29E-05	7.67E-05	9.29E-05	9.40E-05	1.00E-04	1.16E-04
Pu-239	5.77E-03	5.79E-03	6.60E-03	5.81E-03	6.28E-03	6.41E-03	6.44E-03	5.98E-03
Pu-240	1.46E-03	1.48E-03	1.61E-03	1.62E-03	1.73E-03	1.76E-03	1.83E-03	1.98E-03
Pu-241	7.04E-04	7.34E-04	8.54E-04	8.04E-04	8.79E-04	8.97E-04	9.56E-04	9.79E-04
Pu-242	1.54E-04	1.58E-04	1.76E-04	1.92E-04	2.16E-04	2.20E-04	2.36E-04	3.04E-04
Np-237	3.01E-04	3.23E-04	3.50E-04	3.24E-04	3.71E-04	3.72E-04	3.89E-04	4.23E-04
Am-241	1.73E-04	1.62E-04	1.47E-04	1.22E-04	2.16E-04	2.22E-04	1.83E-04	2.12E-04
Am-242m	3.36E-07	3.77E-07	3.97E-07	2.93E-07	4.99E-07	5.18E-07	4.50E-07	4.53E-07
Am-243	1.71E-05	1.80E-05	1.76E-05	1.60E-05	2.85E-05	2.96E-05	2.74E-05	3.75E-05
Cm-242 <sup>b</sup>	7.45E-09	1.97E-08	2.00E-08	1.89E-08	1.25E-08	1.20E-08	2.90E-08	1.75E-08
Cm-243	5.97E-08	6.36E-08	6.99E-08	5.50E-08	1.01E-07	1.07E-07	1.04E-07	1.25E-07
Cm-244	2.62E-06	2.89E-06	3.22E-06	2.66E-06	5.23E-06	5.51E-06	5.32E-06	7.68E-06
Cm-245	1.14E-07	1.24E-07	1.67E-07	1.19E-07	2.74E-07	2.90E-07	2.81E-07	4.02E-07
Nd-143	7.41E-04	7.51E-04	7.66E-04	7.95E-04	8.11E-04	8.16E-04	8.28E-04	8.92E-04
Nd-145	5.51E-04	5.59E-04	5.64E-04	6.00E-04	6.08E-04	6.11E-04	6.21E-04	6.87E-04
Nd-146	5.04E-04	5.12E-04	5.26E-04	5.56E-04	5.72E-04	5.76E-04	5.87E-04	6.58E-04
Nd-148	2.77E-04	2.81E-04	2.88E-04	3.05E-04	3.12E-04	3.14E-04	3.21E-04	3.58E-04
Nd-150	1.25E-04	1.26E-04	1.31E-04	1.38E-04	1.42E-04	1.43E-04	1.47E-04	1.64E-04
Cs-134	1.76E-05	2.22E-05	2.44E-05	2.51E-05	2.27E-05	2.27E-05	2.90E-05	2.76E-05
Cs-137	8.92E-04	9.05E-04	9.18E-04	9.71E-04	1.01E-03	1.00E-03	1.03E-03	1.17E-03
Sm-147	1.86E-04	1.81E-04	1.79E-04	1.91E-04	1.99E-04	2.01E-04	1.94E-04	2.20E-04
Sm-149	4.23E-06	4.32E-06	4.73E-06	4.32E-06	4.42E-06	4.44E-06	4.72E-06	4.36E-06
Sm-150	2.06E-04	2.11E-04	2.17E-04	2.30E-04	2.38E-04	2.41E-04	2.47E-04	2.78E-04
Sm-151	1.35E-05	1.38E-05	1.58E-05	1.36E-05	1.51E-05	1.51E-05	1.53E-05	1.47E-05
Sm-152	8.47E-05	8.62E-05	8.41E-05	9.23E-05	9.19E-05	9.27E-05	9.54E-05	1.07E-04
Eu-151	4.48E-07	4.29E-07	4.89E-07	4.15E-07	4.99E-07	5.02E-07	4.61E-07	4.74E-07
Eu-153	7.13E-05	7.37E-05	7.69E-05	8.05E-05	8.61E-05	8.65E-05	8.80E-05	1.01E-04
Gd-155	2.10E-06	2.03E-06	2.33E-06	2.46E-06	2.70E-06	2.68E-06	2.82E-06	3.09E-06

<sup>a</sup> As reported in J. M. Scaglione, *Three Mile Island Unit 1 Radiochemical Assay Comparisons to SAS2H Calculations*, Yucca Mountain Project Report, CAL-UDC-NU-000011, Rev. A (April 2002).

<sup>b</sup> Average of the two values measured by TIMS and  $\gamma$ -spectrometry.

**Table 3.6 Experimental results (g/g U<sub>initial</sub>) for TMI-1 samples from assembly NJ070G**

Sample ID	O13S7	O12S4	O12S6	O1S1	O13S8	O12S5	O1S3	O1S2
<b>Burnup<sup>a</sup> (GWd/MTU)</b>	<b>22.8</b>	<b>23.7</b>	<b>24.0</b>	<b>25.8</b>	<b>26.3</b>	<b>26.5</b>	<b>26.7</b>	<b>29.9</b>
U-234	3.43E-04	3.34E-04	3.26E-04	3.27E-04	3.19E-04	3.13E-04	3.14E-04	3.04E-04
U-235	2.38E-02	2.36E-02	2.39E-02	2.21E-02	2.19E-02	2.18E-02	2.17E-02	1.92E-02
U-236	4.22E-03	4.30E-03	4.39E-03	4.53E-03	4.58E-03	4.62E-03	4.67E-03	5.00E-03
Pu-238	6.03E-05	6.28E-05	7.77E-05	7.20E-05	8.71E-05	8.81E-05	9.37E-05	1.09E-04
Pu-239	5.42E-03	5.44E-03	6.19E-03	5.45E-03	5.89E-03	6.01E-03	6.03E-03	5.60E-03
Pu-240	1.37E-03	1.39E-03	1.51E-03	1.52E-03	1.62E-03	1.65E-03	1.71E-03	1.85E-03
Pu-241	6.62E-04	6.90E-04	8.01E-04	7.55E-04	8.24E-04	8.41E-04	8.95E-04	9.16E-04
Pu-242	1.45E-04	1.48E-04	1.65E-04	1.80E-04	2.03E-04	2.06E-04	2.21E-04	2.85E-04
Np-237	2.83E-04	3.04E-04	3.28E-04	3.04E-04	3.48E-04	3.49E-04	3.64E-04	3.96E-04
Am-241	1.63E-04	1.52E-04	1.38E-04	1.15E-04	2.03E-04	2.08E-04	1.71E-04	1.98E-04
Am-242m	3.16E-07	3.54E-07	3.72E-07	2.75E-07	4.68E-07	4.86E-07	4.21E-07	4.24E-07
Am-243	1.61E-05	1.69E-05	1.65E-05	1.50E-05	2.67E-05	2.77E-05	2.57E-05	3.51E-05
Cm-242 <sup>b</sup>	7.00E-09	1.85E-08	1.88E-08	1.77E-08	0.00E+00	1.12E-08	2.72E-08	1.64E-08
Cm-243	5.61E-08	5.98E-08	6.56E-08	5.16E-08	9.47E-08	1.00E-07	9.74E-08	1.17E-07
Cm-244	2.46E-06	2.72E-06	3.02E-06	2.50E-05	4.90E-06	5.16E-06	4.98E-06	7.19E-06
Cm-245	1.07E-07	1.17E-07	1.57E-07	1.12E-07	2.57E-07	2.72E-07	2.63E-07	3.76E-07
Nd-143	6.97E-04	7.06E-04	7.18E-04	7.46E-04	7.60E-04	7.65E-04	7.76E-04	8.35E-04
Nd-145	5.18E-04	5.25E-04	5.29E-04	5.63E-04	5.70E-04	5.73E-04	5.82E-04	6.43E-04
Nd-146	4.74E-04	4.81E-04	4.93E-04	5.22E-04	5.36E-04	5.40E-04	5.50E-04	6.16E-04
Nd-148	2.60E-04	2.64E-04	2.70E-04	2.86E-04	2.93E-04	2.94E-04	3.01E-04	3.35E-04
Nd-150	1.18E-04	1.18E-04	1.23E-04	1.30E-04	1.33E-04	1.34E-04	1.38E-04	1.53E-04
Cs-134	1.65E-05	2.09E-05	2.29E-05	2.36E-05	2.13E-05	2.13E-05	2.72E-05	2.58E-05
Cs-137	8.38E-04	8.50E-04	8.61E-04	9.12E-04	9.47E-04	9.37E-04	9.65E-04	1.10E-03
Sm-147	1.75E-04	1.70E-04	1.68E-04	1.79E-04	1.87E-04	1.88E-04	1.82E-04	2.06E-04
Sm-149	3.98E-06	4.06E-06	4.44E-06	4.06E-06	4.14E-06	4.16E-06	4.42E-06	4.08E-06
Sm-150	1.94E-04	1.98E-04	2.04E-04	2.16E-04	2.23E-04	2.07E-04	2.31E-04	2.60E-04
Sm-151	1.27E-05	1.30E-05	1.48E-05	1.28E-05	1.42E-05	1.42E-05	1.43E-05	1.38E-05
Sm-152	7.96E-05	8.10E-05	7.89E-05	8.66E-05	8.62E-05	8.69E-05	8.94E-05	1.00E-04
Eu-151	4.21E-07	4.03E-07	4.59E-07	3.90E-07	4.68E-07	4.71E-07	4.32E-07	4.44E-07
Eu-153	6.70E-05	6.93E-05	7.21E-05	7.56E-05	8.07E-05	8.11E-05	8.24E-05	9.45E-05
Gd-155	1.97E-06	1.91E-06	2.19E-06	2.31E-06	2.53E-06	2.51E-06	2.64E-06	2.89E-06

<sup>a</sup> As reported in J. M. Scaglione, *Three Mile Island Unit 1 Radiochemical Assay Comparisons to SAS2H Calculations*, Yucca Mountain Project Report, CAL-UDC-NU-000011, Rev. A (April 2002).

<sup>b</sup> Average of the two values measured by TIMS and  $\gamma$ -spectrometry.



## 3.2 CALVERT CLIFFS SAMPLES

The three samples from the Calvert Cliffs reactor considered in this report belonged to a fuel rod of a  $14 \times 14$  fuel assembly of Combustion Engineering (CE) design. The burnup of the samples covers the range 27 to 44 GWd/MTU. The samples were identified as 87-81, 87-72, and 87-63.

### 3.2.1 PNNL Measurements

The measurements at PNNL were performed by using the following main spectrometric methods:<sup>11</sup>

- $\gamma$ -spectrometry for  $^{137}\text{Cs}$ ;
- $\alpha$ -spectrometry for  $^{241}\text{Am}$  and  $^{237}\text{Np}$ ;
- $\beta$ -spectrometry for  $^{99}\text{Tc}$  and  $^{90}\text{Sr}$ ;
- isotope dilution mass spectrometry (ID-MS) for neodymium, uranium, and plutonium nuclides, using a calibrated triple spike of  $^{150}\text{Nd}$ ,  $^{233}\text{U}$ , and  $^{242}\text{Pu}$ ;
- mass spectrometry (MS) after elemental separation of cesium for  $^{133}\text{Cs}$  and  $^{135}\text{Cs}$ ;
- ICP-MS measurements relative to  $^{143}\text{Nd}$  and  $^{145}\text{Nd}$  for lanthanide elements: samarium, europium, gadolinium.

The lanthanide measurements were carried out by ICP-MS in general without previous chemical separation into individual elements. Therefore, there was an interference issue for data corresponding to nuclides with mass numbers 147 (Pm, Sm), 150 (Nd, Sm), 151 (Sm, Eu), and 155 (Eu, Gd). The data corresponding to these four mass numbers were adjusted by PNNL based on calculations in order to infer information for individual isotopes. The PNNL lanthanide data are not considered in this report for code validation purposes because of the large dependence of the reported measurement data on additional calculated results.

Isotopic measured concentrations were reported as g/g fuel, g/MTU, or Ci/g fuel depending on the reporting reference and the nuclide under consideration.<sup>10,11,12,13,15</sup> A summary of the measured nuclides, methods used, and reported measurement uncertainties are summarized in Table 3.7. The magnitude of the experimental errors varies with the method and the nuclide. For example, it is less than 1% for  $^{143}\text{Nd}$  and  $^{145}\text{Nd}$  and 1.6% for uranium and plutonium isotopes. These uncertainties, except for lanthanides, represent one relative standard deviation that is based on experience at the PNNL experimental facility. For some isotopes, the measurement errors were not explicitly specified ( $^{133}\text{Cs}$ ,  $^{144}\text{Nd}$ ,  $^{146}\text{Nd}$ , and  $^{148}\text{Nd}$ ). It was stated though that the measurements for all neodymium nuclides provided very good quality data, as a chemical separation for neodymium was performed prior to ID-MS. The measurement errors reported for lanthanides were inferred by PNNL<sup>11</sup> based on additional lanthanide measurement data on sample identified as 87-81: ICP-MS measurements by PNNL and Los Alamos National Laboratory (LANL) and MS with luminescent analysis (LA) by KRI.

The measured nuclide concentrations in g/g fuel as reported in Refs. 9, 10, and 15 are presented in Table 3.8. Data for  $^{134}\text{Cs}$  was found only in Ref. 15. Data for  $^{90}\text{Sr}$  is shown in Table 3.8 both in Ci/g fuel, as reported in Ref. 9, and in g/g fuel, calculated as:

$$m_{^{90}\text{Sr}} (g / g_{\text{fuel}}) = \frac{\Lambda}{\lambda} \frac{M}{N_A} \quad (3-4)$$

where  $\Lambda = 3.7 \times 10^{10} m_{\text{Sr},90}(\text{Ci/g fuel})$  reported radioactivity in units of Bq/s/g fuel  
 $\lambda = 7.62759 \times 10^{-10} \text{ s}^{-1}$  decay constant (half-life = 28.79 years)

$M = 89.99$  atomic mass  
 $N_A = 6.022 \times 10^{23} \text{ mol}^{-1}$  Avogadro's number

The PNNL data are also shown in units of g/g  $U_{\text{initial}}$  in Table 3.9; the unit conversion was performed as:

$$m(g/g_{U_{\text{initial}}}) = 1.1345m(g/g_{\text{fuel}}) \quad (3-5)$$

### 3.2.2 KRI Measurements

Additional lanthanide analysis was performed for the same three samples at KRI in St. Petersburg, Russia.<sup>10</sup> The measurements included:

- Chemical separation of rare earth elements and transuranics followed by chemical separation of lanthanides into individual elements;
- ID-MS for neodymium and gadolinium isotopes using a spike of  $^{142}\text{Nd}$  and  $^{160}\text{Gd}$ ;
- Luminescent analysis—laser-induced fluorometry for absolute measurement of europium and samarium content in the sample; the content was determined by comparison of the sample luminescence intensity with that of standard solutions containing known quantities of europium and samarium;
- MS for europium and samarium nuclides to determine relative isotope ratios;
- $\gamma$ -spectrometry for  $^{154}\text{Eu}$  and  $^{155}\text{Eu}$ .

As chemical separations were performed, the KRI measurements were not subject to mass interference from different elements, as it was the case with the PNNL measurements. The experimental results were reported by KRI as the ratio of nuclide mass to  $^{145}\text{Nd}$  mass or as the nuclide mass percentage relative to the corresponding element total mass. The measured nuclides and corresponding measurement error range are shown in Table 3.10. The reported results of the radiochemical analyses performed by KRI, as well as the reported experimental errors for each nuclide and sample are presented in Table 3.11. The concentration values shown in Table 3.11 for  $^{152}\text{Sm}$ ,  $^{154}\text{Gd}$ ,  $^{155}\text{Gd}$ ,  $^{156}\text{Gd}$ , and  $^{158}\text{Gd}$  for sample 87-81 in g/g  $^{145}\text{Nd}$  units were taken from Ref. 16. The values provided in Ref. 10 for these isotopes were different, as follows:  $0.115 \pm 0.005$ ,  $0.0108 \pm 0.0004$ ,  $0.110 \pm 0.0002$ ,  $<0.00007$ , and  $0.0236 \pm 0.0005$ , respectively. The values shown in italics in Table 3.11 for nuclide concentrations in g/g  $^{145}\text{Nd}$  units were derived based on the available data. For example, concentration for each of the measured gadolinium nuclides except for  $^{155}\text{Gd}$ , for which concentration relative to  $^{145}\text{Nd}$  was available, was calculated as:

$$m_{\text{Gd}}(g/g^{145}\text{Nd}) = \frac{m_{\text{Gd}}(g/g\text{Gd})}{m_{^{155}\text{Gd}}(g/g\text{Gd})} m_{^{155}\text{Gd}}(g/g^{145}\text{Nd}) \quad (3-6)$$

In the current report, the experimental data reported by KRI are also expressed in units of g/g  $U_{\text{initial}}$  (see Table 3.13) in order to be used in a consistent comparison with other sets of data from different experiments. As no absolute concentration values were reported by KRI, the  $^{145}\text{Nd}$  values provided by PNNL were used to renormalize the KRI experimental results. A study of the KRI and PNNL data, both expressed relative to  $^{145}\text{Nd}$  concentration, showed that the difference in data for those neodymium nuclides measured in all three samples at both experimental facilities were within one standard deviation, as shown in Table 3.12. Therefore, the use of the  $^{145}\text{Nd}$  concentrations determined at PNNL to renormalize the KRI data would not introduce additional large uncertainties. The uncertainties shown in Tables 3.12 and 3.13 include the error propagation due to renormalization.

### 3.2.3 Experimental Data Used for Code Validation

The two sets of PNNL and KRI measured data are combined into one set for code validation purposes. The combined set of experimental data is presented in Table 3.14. As previously mentioned, the samarium, europium, and gadolinium data reported by PNNL are not included in this set in order to minimize the associated uncertainties because these data were derived by adjusting the measured isotope ratios using calculated values; for these nuclides, the KRI data are used. The neodymium data in Table 3.14 correspond to PNNL measurements. The measured concentrations for the  $^{154}\text{Eu}$  and  $^{155}\text{Eu}$  isotopes shown in Table 3.14 were obtained by combining the two values shown in Table 3.13, obtained by ID-MS and  $\gamma$ -spectrometry, respectively, at KRI.

**Table 3.7 Experimental techniques and uncertainties for Calvert Cliffs samples—PNNL data**

Nuclide ID	Method <sup>a</sup>	RSD <sup>b</sup> (%)
U-234	ID-MS	1.6
U-235	ID-MS	1.6
U-236	ID-MS	1.6
U-238	ID-MS	1.6
Pu-238	ID-MS	1.6
Pu-239	ID-MS	1.6
Pu-240	ID-MS	1.6
Pu-241	ID-MS	1.6
Pu-242	ID-MS	1.6
Np-237	$\alpha$ -spec	1.9
Am-241	$\alpha$ -spec	4.9
Cs-133	MS	NA
Cs-134 <sup>c</sup>	NA	NA
Cs-135	MS	14.0
Cs-137	$\gamma$ -spec	3.5
Nd-143	ICP-MS	< 1.0
Nd-144	ICP-MS	NA
Nd-145	ICP-MS	< 1.0
Nd-146	ICP-MS	NA
Nd-148	ICP-MS	NA
Nd-150	ICP-MS	NA
Sm-147	ICP-MS	4.0
Sm-149	ICP-MS	18.0
Sm-150	ICP-MS	2.0
Sm-151	ICP-MS	7.0
Sm-152	ICP-MS	3.0
Eu-151	ICP-MS	NA
Eu-153	ICP-MS	2.0
Eu-155	ICP-MS	29.0
Gd-155	ICP-MS	29.0
Sr-90	$\beta$ -spec	5.7
Tc-99	$\beta$ -spec	3.5

<sup>a</sup> Main technique is listed; some nuclides require multiple techniques to eliminate interferences.

<sup>b</sup> Relative standard deviation.

<sup>c</sup> Measured value only reported in O. W. Hermann, S. M. Bowman, M. C. Brady, and C. V. Parks, *Validation of the SCALE System for PWR Spent Fuel Isotopic Composition Analyses*, ORNL/TM-12667, Oak Ridge National Laboratory, Oak Ridge, Tennessee (March 1995).

**Table 3.8 Experimental results (g/g fuel) for  
Calvert Cliffs samples—PNNL data**

Sample ID	87-81	87-72	87-63
Burnup <sup>a</sup> (GWd/MTU)	27.35	37.12	44.34
U-234	1.60E-04	1.40E-04	1.20E-04
U-235	8.47E-03	5.17E-03	3.54E-03
U-236	3.14E-03	3.53E-03	3.69E-03
U-238	8.43E-01	8.33E-01	8.25E-01
Pu-238	1.01E-04	1.89E-04	2.69E-04
Pu-239	4.26E-03	4.36E-03	4.36E-03
Pu-240	1.72E-03	2.24E-03	2.54E-03
Pu-241	6.81E-04	9.03E-04	1.02E-03
Pu-242	2.89E-04	5.76E-04	8.40E-04
Np-237	2.68E-04	3.56E-04	4.68E-04
Am-241	2.49E-04	3.43E-04	3.81E-04
Cs-133	8.50E-04	1.09E-03	1.24E-03
Cs-134	1.00E-05	2.00E-05	3.00E-05
Cs-135	3.60E-04	4.00E-04	4.30E-04
Cs-137	7.70E-04	1.04E-03	1.25E-03
Nd-143	6.13E-04	7.16E-04	7.63E-04
Nd-144	9.43E-04	1.34E-03	1.64E-03
Nd-145	5.10E-04	6.53E-04	7.44E-04
Nd-146	4.90E-04	6.82E-04	8.30E-04
Nd-148	2.65E-04	3.59E-04	4.28E-04
Nd-150	1.24E-04	1.72E-04	2.08E-04
Sm-147	1.90E-04	2.18E-04	2.30E-04
Sm-148	1.06E-04	1.64E-04	2.22E-04
Sm-149	2.90E-06	3.00E-06	4.70E-06
Sm-150	2.07E-04	2.71E-04	3.61E-04
Sm-151	8.60E-06	8.60E-06	9.00E-06
Sm-152	8.70E-06	1.04E-04	1.21E-04
Eu-151	7.00E-07	7.00E-07	8.00E-07
Eu-153	7.90E-05	1.09E-04	1.48E-04
Eu-155	2.10E-06	3.30E-06	4.50E-06
Gd-155	2.50E-06	3.90E-06	5.30E-06
Tc-99	5.60E-04	7.20E-04	7.80E-04
Sr-90 <sup>b</sup>	4.59E-02	5.90E-02	6.58E-02
Sr-90	3.33E-04	4.28E-04	4.77E-04

<sup>a</sup>As reported in O. W. Hermann, S. M. Bowman, M. C. Brady, and C. V. Parks, *Validation of the SCALE System for PWR Spent Fuel Isotopic Composition Analyses*, ORNL/TM-12667, Oak Ridge National Laboratory, Oak Ridge, Tennessee (March 1995).

<sup>b</sup>In Ci/g fuel, as reported in R.J Guenther et al. *Characterization of LWR Spent Fuel MCC-Approved Testing Material TM-104*, PNL-5109-104 (1991).

**Table 3.9 Experimental results (g/g  $U_{initial}$ ) for Calvert Cliffs samples—PNNL data**

Sample ID	87-81	87-72	87-63
Burnup <sup>a</sup> (GWd/MTU)	27.35	37.12	44.34
U-234	1.82E-04	1.59E-04	1.36E-04
U-235	9.61E-03	5.87E-03	4.02E-03
U-236	3.56E-03	4.00E-03	4.19E-03
U-238	9.56E-01	9.45E-01	9.36E-01
Pu-238	1.15E-04	2.14E-04	3.05E-04
Pu-239	4.83E-03	4.95E-03	4.95E-03
Pu-240	1.95E-03	2.54E-03	2.88E-03
Pu-241	7.73E-04	1.02E-03	1.16E-03
Pu-242	3.28E-04	6.53E-04	9.53E-04
Np-237	3.04E-04	4.04E-04	5.31E-04
Am-241	2.82E-04	3.89E-04	4.32E-04
Cs-133	9.64E-04	1.24E-03	1.41E-03
Cs-134	1.13E-05	2.27E-05	3.40E-05
Cs-135	4.08E-04	4.54E-04	4.88E-04
Cs-137	8.74E-04	1.18E-03	1.42E-03
Nd-143	6.95E-04	8.12E-04	8.66E-04
Nd-144	1.07E-03	1.52E-03	1.86E-03
Nd-145	5.79E-04	7.41E-04	8.44E-04
Nd-146	5.56E-04	7.74E-04	9.42E-04
Nd-148	3.01E-04	4.07E-04	4.86E-04
Nd-150	1.41E-04	1.95E-04	2.36E-04
Sm-147	2.16E-04	2.47E-04	2.61E-04
Sm-148	1.20E-04	1.86E-04	2.52E-04
Sm-149	3.29E-06	3.40E-06	5.33E-06
Sm-150	2.35E-04	3.07E-04	4.10E-04
Sm-151	9.76E-06	9.76E-06	1.02E-05
Sm-152	9.87E-06	1.18E-04	1.37E-04
Eu-151	7.94E-07	7.94E-07	9.08E-07
Eu-153	8.96E-05	1.24E-04	1.68E-04
Eu-155	2.38E-06	3.74E-06	5.11E-06
Gd-155	2.84E-06	4.42E-06	6.01E-06
Tc-99	6.35E-04	8.17E-04	8.85E-04
Sr-90	3.78E-04	4.86E-04	5.41E-04

<sup>a</sup> As reported in O. W. Hermann, S. M. Bowman, M. C. Brady, and C. V. Parks, *Validation of the SCALE System for PWR Spent Fuel Isotopic Composition Analyses*, ORNL/TM-12667, Oak Ridge National Laboratory, Oak Ridge, Tennessee (March 1995).

**Table 3.10 Experimental techniques and  
uncertainties for Calvert Cliffs  
samples—KRI data**

Nuclide ID	Method <sup>a</sup>	RSD <sup>b</sup> (%)
Nd-143	ID-MS	0.7–1.9
Nd-145	ID-MS	NA
Sm-147	MS, LA	2.5–3.3
Sm-149	MS, LA	7.4–20.0
Sm-150	MS, LA	2.3–4.2
Sm-151	MS, LA	3.2–4.7
Sm-152	MS, LA	2.7–4.4
Sm-154	MS, LA	5.7
Eu-151	MS, LA	9.7
Eu-154	MS, LA, $\gamma$ -spec	5.3–8.6
Eu-155	MS, LA, $\gamma$ -spec	2.7–16.7
Gd-155	ID-MS	0.2–3.3

<sup>a</sup> Main technique is listed; some nuclides require multiple techniques to eliminate interferences.

<sup>b</sup> Relative standard deviation.

Table 3.11 Experimental results for Calvert Cliffs samples—KRI data<sup>a</sup>

Sample ID	87-81						87-72				87-63			
Burnup <sup>b</sup> (GWd/MTU)	27.35						37.12				44.34			
ID-MS data	ng/g sample	$\sigma$	$\sigma$ (%)	g/g <sup>145</sup> Nd	$\sigma$	$\sigma$ (%)	g/g element (%)	g/g <sup>145</sup> Nd	$\sigma$	$\sigma$ (%)	g/g element (%)	g/g <sup>145</sup> Nd	$\sigma$	$\sigma$ (%)
Nd-142	287	3	1.0	0.039	0.001	2.6	1.25	<i>0.077</i>		<i>0.9</i>	0.76	<i>0.048</i>		<i>1.9</i>
Nd-143	9100	40	0.4	1.218	0.008	0.7	18.15	1.120	0.010	0.9	16.37	1.040	0.020	1.9
Nd-144	14060	55	0.4	1.882	0.011	0.6	33.93	<i>2.084</i>		<i>0.9</i>	35.34	<i>2.235</i>		<i>1.9</i>
Nd-145	7470	32	0.4	1.000			16.28	1.000			15.81	1.000		
Nd-146	7270	35	0.5	0.973	0.006	0.6	17.12	<i>1.052</i>		<i>0.9</i>	17.87	<i>1.130</i>		<i>1.9</i>
Nd-148	3910	24	0.6	0.523	0.004	0.8	8.96	<i>0.550</i>		<i>0.9</i>	9.24	<i>0.584</i>		<i>1.9</i>
Nd-150	1850	150	8.1	0.248	0.020	0.8	4.32	<i>0.265</i>		<i>0.9</i>	4.59	<i>0.290</i>		<i>1.9</i>
Sm-147	2975	100	3.4	0.398	0.013	3.3	30.57	0.365	0.009	2.5	28	0.365	0.012	3.3
Sm-148	1290	20	1.6	0.173	0.003	1.7	18.3	<i>0.218</i>		<i>2.3</i>	20.39	<i>0.226</i>		<i>3.2</i>
Sm-149	35	5	14.3	0.005	0.001	20.0	0.22	0.0025	0.0003	12.0	0.41	0.0054	0.0004	7.4
Sm-150	2696	110	4.1	0.361	0.015	4.2	32.89	0.391	0.009	2.3	33.06	0.431	0.014	3.2
Sm-151	96	35	36.5	0.013	0.005	38.5	1.08	0.0127	0.0004	3.1	0.97	0.0127	0.0006	4.7
Sm-152	1160	60	5.2	0.155	0.005	3.2	12.56	0.148	0.004	2.7	12.05	0.157	0.006	3.8
Sm-154	393	20	5.1	0.053	0.003	5.7	4.32	<i>0.051</i>		<i>2.3</i>	5.12	<i>0.067</i>		<i>3.2</i>
Eu-151	23	2	8.7	0.0031	0.0003	9.7	0.74	<i>0.00141</i>		<i>2.7</i>	1.91	<i>0.00407</i>		<i>2.8</i>
Eu-152	11	10	90.9	0.0002	0.0002	100.0	0.04	<i>0.00008</i>		<i>2.7</i>	0.25	<i>0.00053</i>		<i>2.8</i>
Eu-153	1100	20	1.8	0.1472	0.0027	1.8	91.98	<i>0.17551</i>		<i>2.7</i>	90.25	<i>0.19212</i>		<i>2.8</i>
Eu-154	79	7	8.9	0.0105	0.0009	8.6	6.26	<i>0.01195</i>		<i>2.7</i>	6.58	<i>0.01401</i>		<i>2.8</i>
Eu-155	13	2	15.4	0.0018	0.0003	16.7	0.98	0.00187	0.00005	2.7	1.01	0.00215	0.00006	2.8
Gd-154	176	4	2.3	0.0236	0.0005	2.1	13.28	<i>0.0202</i>		<i>3.0</i>	13.27	<i>0.0237</i>		<i>3.4</i>
Gd-155	81	2	2.5	0.0108	0.0004	3.7	6.58	0.0100	0.0003	3.0	6.62	0.0118	0.0004	3.4
Gd-156	825	16	1.9	0.1100	0.002	1.8	65.10	<i>0.0989</i>		<i>3.0</i>	63.20	<i>0.1127</i>		<i>3.4</i>
Gd-157	6	4	75.0	<0.00007			1.84	<i>0.0028</i>		<i>3.0</i>	3.24	<i>0.0058</i>		<i>3.4</i>
Gd-158	180	4	2.2	0.0241	0.0005	2.1	13.20	<i>0.0201</i>		<i>3.0</i>	13.70	<i>0.0244</i>		<i>3.4</i>
Gd-160	19	2	10.5	0.0025	0.0003	12.0								
$\gamma$ -spec data														
Eu-154								<i>0.0117</i>	0.0006	5.1				
Eu-155								<i>0.00182</i>	0.00009	4.9		0.0119	0.0007	5.9
												0.00209	0.00012	5.7

<sup>a</sup> Values shown in italics are inferred based on available data. All other values are as given in M. C. Brady-Raap and R. J. Talbert, *Compilation of Radiochemical Analyses of Spent Nuclear Fuel Samples*, PNNL-13677, Pacific Northwest National Laboratory, Richland, Washington (September 2001); A. A. Rimski-Korsakov, A. V. Stepanov, A. D. Kirikov, *Radiochemical Analysis of Spent Reactor Fuel Sample—Report of Results*, V. G. Khlopin Institute, St. Petersburg, Russia, Communication to PNNL (1993).

<sup>b</sup> As provided in O. W. Herman, S. M. Bowman, M. C. Brady and C. V. Parks, *Validation of the SCALE System for PWR Spent Fuel Isotopic Composition Analyses*, ORNL/TM-12667, Oak Ridge National Laboratory, Oak Ridge, Tennessee (March 1995).

**Table 3.12 Comparison of PNNL and KRI data (relative to  $^{145}\text{Nd}$ )**

Sample ID	Nuclide ID	PNNL data		KRI data		Difference	
		g/g $^{145}\text{Nd}$	$\sigma$	g/g $^{145}\text{Nd}$	$\sigma$	g/g $^{145}\text{Nd}$	$\sigma$
87-81	Nd-143	1.202	0.017	1.218	0.008	-0.016	0.019
87-72	Nd-143	1.096	0.017	1.120	0.010	0.024	0.020
87-63	Nd-143	1.026	0.015	1.040	0.020	-0.014	0.025



**Table 3.13 Experimental results (g/g U<sub>initial</sub>) for Calvert Cliffs samples—KRI data**

Sample ID	87-81		87-72		87-63	
Burnup <sup>a</sup> (Gwd/MTU)	27.35		37.12		44.34	
ID-MS data	g/g U <sub>initial</sub>	RSD <sup>b</sup> (%)	g/g U <sub>initial</sub>	RSD (%)	g/g U <sub>initial</sub>	RSD (%)
Nd-142	2.26E-05	3.2	5.69E-05	2.1	4.06E-05	2.7
Nd-143	7.05E-04	2.0	8.30E-04	2.1	8.78E-04	2.7
Nd-144	1.09E-03	2.0	1.54E-03	2.1	1.89E-03	2.7
Nd-145	5.79E-04	1.9	7.41E-04	1.9	8.44E-04	1.9
Nd-146	5.63E-04	2.0	7.79E-04	2.1	9.54E-04	2.7
Nd-148	3.03E-04	2.0	4.08E-04	2.1	4.93E-04	2.7
Nd-150	1.44E-04	8.3	1.97E-04	2.1	2.45E-04	2.7
Sm-147	2.30E-04	3.8	2.70E-04	3.1	3.08E-04	3.8
Sm-148	1.00E-04	2.6	1.61E-04	3.0	2.24E-04	3.8
Sm-149	2.90E-06	20.1	1.85E-06	12.1	4.56E-06	7.6
Sm-150	2.09E-04	4.6	2.90E-04	3.0	3.64E-04	3.7
Sm-151	7.53E-06	38.5	9.41E-06	3.6	1.07E-05	5.1
Sm-152	8.97E-05	3.7	1.10E-04	3.3	1.33E-04	4.2
Sm-154	3.07E-05	6.0	3.81E-05	3.0	5.63E-05	3.8
Eu-151	1.79E-06	9.9	1.05E-06	3.3	3.43E-06	3.4
Eu-152	1.16E-07	100.0	5.66E-08	3.3	4.49E-07	3.4
Eu-153	8.52E-05	2.6	1.30E-04	3.3	1.62E-04	3.4
Eu-154	6.08E-06	8.8	8.85E-06	3.3	1.18E-05	3.4
Eu-155	1.04E-06	16.8	1.39E-06	3.3	1.81E-06	3.4
Gd-154	1.37E-05	2.8	1.50E-05	3.6	2.00E-05	3.9
Gd-155	6.25E-06	4.2	7.41E-06	3.6	9.96E-06	3.9
Gd-156	6.37E-05	2.6	7.33E-05	3.6	9.51E-05	3.9
Gd-158	1.40E-05	2.8	1.49E-05	3.6	2.06E-05	3.9
Gd-160	1.45E-06	12.1				
<b>γ-spec data</b>						
Eu-154			8.67E-06	5.4	1.00E-05	6.2
Eu-155			1.35E-06	5.3	1.76E-06	6.0

<sup>a</sup> As reported in O. W. Hermann, S. M. Bowman, M. C. Brady and C. V. Parks, *Validation of the SCALE System for PWR Spent Fuel Isotopic Composition Analyses*, ORNL/TM-12667, Oak Ridge National Laboratory, Oak Ridge, Tennessee (March 1995).

<sup>b</sup> Relative standard deviation.

**Table 3.14 Experimental results (g/g  $U_{initial}$ ) for Calvert Cliffs samples used for code validation <sup>a</sup>**

Sample ID	87-81		87-72		87-63	
Burnup <sup>b</sup> (GWd/MTU)	27.35		37.12		44.34	
Nuclide ID	g/g $U_{initial}$	RSD <sup>c</sup> (%)	g/g $U_{initial}$	RSD (%)	g/g $U_{initial}$	RSD (%)
U-234	1.82E-04	2.3	1.59E-04	2.3	1.36E-04	2.3
U-235	9.61E-03	2.3	5.87E-03	2.3	4.02E-03	2.3
U-236	3.56E-03	2.3	4.00E-03	2.3	4.19E-03	2.3
U-238	9.56E-01	2.3	9.45E-01	2.3	9.36E-01	2.3
Pu-238	1.15E-04	2.3	2.14E-04	2.3	3.05E-04	2.3
Pu-239	4.83E-03	2.3	4.95E-03	2.3	4.95E-03	2.3
Pu-240	1.95E-03	2.3	2.54E-03	2.3	2.88E-03	2.3
Pu-241	7.73E-04	2.3	1.02E-03	2.3	1.16E-03	2.3
Pu-242	3.28E-04	2.3	6.53E-04	2.3	9.53E-04	2.3
Np-237	3.04E-04	2.5	4.04E-04	2.5	5.31E-04	2.5
Am-241	2.82E-04	5.2	3.89E-04	5.2	4.32E-04	5.2
Cs-133	9.64E-04		1.24E-03		1.41E-03	
Cs-134	1.13E-05		2.27E-05		3.40E-05	
Cs-135	4.08E-04	14.1	4.54E-04	14.1	4.88E-04	14.1
Cs-137	8.74E-04	3.8	1.18E-03	3.8	1.42E-03	3.8
Nd-143	6.95E-04	1.9	8.12E-04	1.9	8.66E-04	1.9
Nd-144	1.07E-03	NA	1.52E-03	NA	1.86E-03	NA
Nd-145	5.79E-04	1.9	7.41E-04	1.9	8.44E-04	1.9
Nd-146	5.56E-04	NA	7.74E-04	NA	9.42E-04	NA
Nd-148	3.01E-04	NA	4.07E-04	NA	4.86E-04	NA
Nd-150	1.41E-04	NA	1.95E-04	NA	2.36E-04	NA
Sm-147	2.30E-04	3.8	2.70E-04	3.1	3.08E-04	3.8
Sm-148	1.00E-04	2.6	1.61E-04	3.0	2.24E-04	3.8
Sm-149	2.90E-06	20.1	1.85E-06	12.1	4.56E-06	7.6
Sm-150	2.09E-04	4.6	2.90E-04	3.0	3.64E-04	3.8
Sm-151	7.53E-06	38.5	9.41E-06	3.7	1.07E-05	5.1
Sm-152	8.97E-05	3.7	1.10E-04	3.3	1.33E-04	4.3
Sm-154	3.07E-05	6.0	3.81E-05	3.0	5.63E-05	3.8
Eu-151	1.79E-06	9.9	1.05E-06	3.3	3.43E-06	3.4
Eu-152	1.16E-07	100.0	5.66E-08	3.3	4.49E-07	3.4
Eu-153	8.52E-05	2.6	1.30E-04	3.3	1.62E-04	3.4
Eu-154	6.08E-06	8.8	8.76E-06	6.4	1.09E-05	7.0
Eu-155	1.04E-06	16.8	1.37E-06	6.2	1.79E-06	6.9

**Table 3.14 Experimental results (g/g  $U_{initial}$ ) for Calvert Cliffs samples used for code validation (continued)**

Sample ID	87-81		87-72		87-63	
Burnup <sup>b</sup> (GWd/MTU)	27.35		37.12		44.34	
Nuclide ID	g/g $U_{initial}$	RSD (%)	g/g $U_{initial}$	RSD (%)	g/g $U_{initial}$	RSD (%)
Gd-154	1.37E-05	2.8	1.50E-05	3.6	2.00E-05	3.9
Gd-155	6.25E-06	4.2	7.41E-06	3.6	9.96E-06	3.9
Gd-156	6.37E-05	2.6	7.33E-05	3.6	9.51E-05	3.9
Gd-158	1.40E-05	2.8	1.49E-05	3.6	2.06E-05	3.9
Gd-160	1.45E-06	12.1				
Tc-99	6.35E-04	5.9	8.17E-04	5.9	8.85E-04	5.9
Sr-90	3.78E-04	3.8	4.86E-04	3.8	5.41E-04	3.8

<sup>a</sup> Data for Sm, Eu, and Gd isotopes correspond to KRI measurements. The other isotope data correspond to PNNL measurements.

<sup>b</sup> As reported in O. W. Hermann, S. M. Bowman, M. C. Brady, and C. V. Parks, *Validation of the SCALE System for PWR Spent Fuel Isotopic Composition Analyses*, ORNL/TM-12667, Oak Ridge National Laboratory, Oak Ridge, Tennessee (March 1995).

<sup>c</sup> Relative standard deviation.

### 3.3 TAKAHAMA-3 SAMPLES

The 16 samples that were measured at JAERI were cut from three fuel rods irradiated in the Takahama-3 reactor operated in Japan. After sample cutting, the elements were separated by using exchange separation methods. The following experimental techniques were used to determine the nuclide concentrations:<sup>17</sup>

- ID-MS
  - major actinides: uranium, plutonium
  - lanthanides: neodymium, samarium
- $\alpha$ -spectrometry plus MS
  - americium, curium
- $\gamma$ -spectrometry
  - <sup>106</sup>Ru, <sup>134</sup>Cs, <sup>137</sup>Cs, <sup>144</sup>Ce, <sup>154</sup>Eu, <sup>125</sup>Sb
- $\alpha$ -spectrometry
  - <sup>237</sup>Np

A summary of the nuclides measured, methods used and corresponding experimental uncertainties are presented in Table 3.15. The reported experimental uncertainties were not specific for each sample measurement, but were typical values based on previous measurement experience at JAERI. Not all nuclides shown in the table were measured in each of the samples. The reported experimental RSD is less than 0.5% for all measured plutonium, samarium, and neodymium isotopes, as well as for <sup>235</sup>U and <sup>238</sup>U. For minor actinides measured by MS and  $\alpha$ -spectrometry the experimental errors are larger, in the 2 to 10% range. The nuclides determined through  $\gamma$ -spectrometry have measurement errors between 3 and 10%.

The experimental results of the radiochemical analyses for the 16 samples from fuel rods identified as SF95, SF96, and SF97 were reported as g/MTU initial. These data were reported at discharge time, except for samarium nuclides in samples from rod SF97 that were reported at 3.96 years after discharge. The measured data are presented in Tables 3.16-3.18 in g/g U<sub>initial</sub>.

**Table 3.15 Experimental techniques and uncertainties for Takahama-3 samples**

Nuclide ID	Method <sup>a</sup>	RSD <sup>b</sup> (%)
U-234	ID-MS	< 1.0
U-235	ID-MS	< 0.1
U-236	ID-MS	< 2.0
U-238	ID-MS	< 0.1
Pu-238	ID-MS	< 0.5
Pu-239	ID-MS	< 0.3
Pu-240	ID-MS	< 0.3
Pu-241	ID-MS	< 0.3
Pu-242	ID-MS	< 0.3
Np-237	$\alpha$ -spec	< 10.0
Am-241	MS, $\alpha$ -spec	< 2.0
Am-242m	MS, $\alpha$ -spec	< 10.0
Am-243	MS, $\alpha$ -spec	< 5.0
Cm-242	MS, $\alpha$ -spec	< 10.0
Cm-243	MS, $\alpha$ -spec	< 2.0
Cm-244	MS, $\alpha$ -spec	< 2.0
Cm-245	MS, $\alpha$ -spec	< 2.0
Cm-246	MS, $\alpha$ -spec	< 5.0
Cs-134	$\gamma$ -spec	< 3.0
Cs-137	$\gamma$ -spec	< 3.0
Ce-144	$\gamma$ -spec	< 10.0
Nd-142	ID-MS	< 0.1
Nd-143	ID-MS	< 0.1
Nd-144	ID-MS	< 0.1
Nd-145	ID-MS	< 0.1
Nd-146	ID-MS	< 0.1
Nd-148	ID-MS	< 0.1
Nd-150	ID-MS	< 0.1
Sm-147	ID-MS	< 0.1
Sm-148	ID-MS	< 0.1
Sm-149	ID-MS	< 0.1
Sm-150	ID-MS	< 0.1
Sm-151	ID-MS	< 0.1
Sm-152	ID-MS	< 0.1
Sm-154	ID-MS	< 0.1
Eu-154	$\gamma$ -spec	< 3.0
Ru-106	$\gamma$ -spec	< 5.0
Sb-125	$\gamma$ -spec	< 10.0

<sup>a</sup> Main technique is listed; some nuclides require multiple techniques to eliminate interferences.

<sup>b</sup> Relative standard deviation. As reported ( $1\sigma$ ) in Y. Nakahara, Y. Suyama, and T. Suzuki, *Technical Development on Burnup Credit for Spent LWR Fuels*, JAERI-Tech 2000-071 (ORNL/TR-2001/01), English Translation, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2002).

**Table 3.16 Experimental results (g/g U<sub>initial</sub>) for Takahama-3 samples from rod SF95**

Sample ID	SF95-1	SF95-2	SF95-3	SF95-4	SF95-5
<b>Burnup<sup>a</sup> (GWd/MTU)</b>	<b>14.30</b>	<b>24.35</b>	<b>35.42</b>	<b>36.69</b>	<b>30.40</b>
U-234	2.987E-04	2.850E-04	1.873E-04	1.870E-04	2.829E-04
U-235	2.674E-02	1.927E-02	1.326E-02	1.230E-02	1.544E-02
U-236	2.672E-03	4.024E-03	4.911E-03	4.999E-03	4.566E-03
U-238	9.499E-01	9.424E-01	9.338E-01	9.335E-01	9.388E-01
Pu-238	1.718E-05	7.102E-05	1.539E-04	1.588E-04	1.020E-04
Pu-239	4.227E-03	5.655E-03	6.194E-03	6.005E-03	5.635E-03
Pu-240	7.802E-04	1.539E-03	2.186E-03	2.207E-03	1.821E-03
Pu-241	3.690E-04	9.578E-04	1.486E-03	1.466E-03	1.153E-03
Pu-242	3.790E-05	1.844E-04	4.516E-04	4.803E-04	2.976E-04
Am-241	1.378E-05	2.344E-05	3.310E-05	2.351E-05	2.840E-05
Am-242m	1.840E-07	5.201E-07	7.877E-07	7.282E-07	5.687E-07
Am-243	2.682E-06	2.289E-05	8.047E-05	8.472E-05	4.400E-05
Cm-242	1.510E-06	7.672E-06	1.964E-05	2.328E-05	1.006E-05
Cm-243	1.451E-08	1.240E-07	3.720E-07	3.976E-07	2.293E-07
Cm-244	2.712E-07	5.042E-06	2.562E-05	2.837E-05	1.064E-05
Cm-245	5.519E-09	1.962E-07	1.396E-06	1.587E-06	4.839E-07
Cm-246	2.560E-10	1.190E-08	1.049E-07	1.251E-07	1.952E-08
Nd-142	3.429E-06	8.887E-06	2.116E-05	2.222E-05	1.371E-05
Nd-143	4.631E-04	7.149E-04	9.299E-04	9.373E-04	8.303E-04
Nd-144	3.276E-04	6.046E-04	9.347E-04	1.024E-03	7.928E-04
Nd-145	3.328E-04	5.384E-04	7.392E-04	7.598E-04	6.518E-04
Nd-146	2.809E-04	4.925E-04	7.340E-04	7.624E-04	6.185E-04
Nd-148	1.592E-04	2.736E-04	3.979E-04	4.126E-04	3.401E-04
Nd-150	7.200E-05	1.258E-04	1.895E-04	1.959E-04	1.572E-04
Cs-134	2.343E-05	7.012E-05	1.404E-04	1.471E-04	1.014E-04
Cs-137	5.405E-04	9.336E-04	1.347E-03	1.400E-03	1.148E-03
Ce-144	1.937E-04	3.160E-04	4.560E-04	4.301E-04	3.868E-04
Eu-154	4.093E-06	1.306E-05	2.525E-05	2.657E-05	1.817E-05
Ru-106	4.447E-05	8.340E-05	1.360E-04	1.401E-04	1.208E-04
Sb-125	1.471E-06	2.900E-06	3.733E-06	3.169E-06	3.262E-06

<sup>a</sup> As reported in Y. Nakahara, Y. Suyama, and T. Suzaki, *Technical Development on Burnup Credit for Spent LWR Fuels*, JAERI-Tech 2000-071 (ORNL/TR-2001/01), English Translation, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2002).

**Table 3.17 Experimental results (g/g  $U_{initial}$ ) for Takahama-3 samples from rod SF96**

Sample ID	SF96-1	SF96-2	SF96-3	SF96-4	SF96-5
Burnup <sup>a</sup> (GWd/MTU)	7.79	16.44	28.20	28.91	24.19
U-234	1.805E-04	1.522E-04	1.251E-04	1.250E-04	1.354E-04
U-235	1.944E-02	1.408E-02	8.638E-03	8.064E-03	9.937E-03
U-236	1.421E-03	2.411E-03	3.244E-03	3.302E-03	3.013E-03
U-238	9.660E-01	9.580E-01	9.476E-01	9.475E-01	9.522E-01
Pu-238	8.536E-06	4.172E-05	1.206E-04	1.248E-04	7.978E-05
Pu-239	3.781E-03	5.459E-03	6.001E-03	5.819E-03	5.519E-03
Pu-240	6.764E-04	1.494E-03	2.303E-03	2.327E-03	1.964E-03
Pu-241	2.622E-04	8.684E-04	1.498E-03	1.480E-03	1.203E-03
Pu-242	2.440E-05	1.615E-04	5.103E-04	5.411E-04	3.551E-04
Np-237	6.125E-05	1.323E-04	2.168E-04	2.252E-04	1.875E-04
Am-241	5.985E-06	1.735E-05	2.845E-05	3.094E-05	2.149E-05
Am-242m	1.218E-07	4.579E-07	6.413E-07	6.793E-07	5.647E-07
Am-243	1.147E-06	1.728E-05	8.872E-05	9.598E-05	5.078E-05
Cm-242	8.502E-07	5.781E-06	1.628E-05	1.679E-05	1.115E-05
Cm-244	9.560E-08	3.092E-06	2.862E-05	3.128E-05	1.280E-05
Nd-143	2.521E-04	4.778E-04	7.158E-04	7.184E-04	6.433E-04
Nd-144	1.536E-04	3.588E-04	7.292E-04	7.513E-04	5.927E-04
Nd-145	1.800E-04	3.575E-04	5.766E-04	5.880E-04	5.095E-04
Nd-146	1.536E-04	3.266E-04	5.795E-04	5.948E-04	4.910E-04
Nd-148	8.770E-05	1.851E-04	3.201E-04	3.280E-04	2.733E-04
Nd-150	4.130E-05	8.972E-05	1.591E-04	1.628E-04	1.331E-04
Cs-134	8.609E-06	3.759E-05	1.002E-04	1.047E-04	7.146E-05
Cs-137	2.813E-04	5.983E-04	1.018E-03	1.053E-03	8.572E-04
Ce-144	1.179E-04	2.250E-04	3.362E-04	3.453E-04	3.145E-04
Eu-154	2.309E-06	8.538E-06	1.973E-05	1.992E-05	1.423E-05
Ru-106	2.830E-05	6.053E-05	1.402E-04	1.291E-04	1.344E-04
Sb-125	1.433E-06	2.829E-06	3.658E-06	4.645E-06	3.690E-06

<sup>a</sup> As reported in Y. Nakahara, Y. Suyama, and T. Suzuki, *Technical Development on Burnup Credit for Spent LWR Fuels*, JAERI-Tech 2000-071 (ORNL/TR-2001/01), English Translation, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2002).

**Table 3.18 Experimental results (g/g  $U_{initial}$ ) for Takahama-3 samples from rod SF97**

Sample ID	SF97-1	SF97-2	SF97-3	SF97-4	SF97-5	SF97-6
Burnup <sup>a</sup> (GWd/MTU)	17.69	30.73	42.16	47.03	47.25	40.79
U-234	2.939E-04	2.348E-04	2.010E-04	1.872E-04	1.865E-04	2.057E-04
U-235	2.347E-02	1.571E-02	1.030E-02	8.179E-03	7.932E-03	1.016E-02
U-236	3.115E-03	4.560E-03	5.312E-03	5.528E-03	5.532E-03	5.272E-03
U-238	9.493E-01	9.377E-01	9.282E-01	9.246E-01	9.247E-01	9.310E-01
Pu-238	2.370E-05	1.250E-04	2.581E-04	3.199E-04	3.188E-04	2.175E-04
Pu-239	3.844E-03	5.928E-03	6.217E-03	6.037E-03	5.976E-03	5.677E-03
Pu-240	9.347E-04	1.871E-03	2.471E-03	2.668E-03	2.648E-03	2.326E-03
Pu-241	4.237E-04	1.235E-03	1.689E-03	1.770E-03	1.754E-03	1.494E-03
Pu-242	6.185E-05	3.152E-04	6.517E-04	8.246E-04	8.341E-04	5.977E-04
Np-237	1.521E-04	4.034E-04	5.845E-04	6.604E-04	6.701E-04	5.570E-04
Am-241	1.492E-05	4.017E-05	4.909E-05	5.311E-05	5.327E-05	4.297E-05
Am-242m	2.270E-07	8.838E-07	1.179E-06	1.233E-06	1.200E-06	9.756E-07
Am-243	4.448E-06	5.132E-05	1.410E-04	1.924E-04	1.935E-04	1.170E-04
Cm-242	2.134E-06	1.049E-05	1.839E-05	2.044E-05	1.903E-05	1.616E-05
Cm-243	2.483E-08	2.773E-07	6.921E-07	8.721E-07	8.670E-07	5.600E-07
Cm-244	4.981E-07	1.384E-05	5.696E-05	8.810E-05	8.823E-05	4.221E-05
Cm-245	1.087E-08	6.848E-07	3.735E-06	6.042E-06	5.915E-06	2.363E-06
Cm-246	3.866E-10	4.222E-07	3.648E-07	7.440E-07	7.549E-07	2.481E-07
Cm-247	NA	4.043E-10	4.974E-09	1.098E-08	1.075E-08	3.139E-09
Nd-143	5.450E-04	8.307E-04	1.008E-03	1.048E-03	1.049E-03	9.736E-04
Nd-144	4.661E-04	8.843E-04	1.331E-03	1.567E-03	1.599E-03	1.311E-03
Nd-145	4.045E-04	6.480E-04	8.387E-04	9.118E-04	9.179E-04	8.247E-04
Nd-146	3.502E-04	6.304E-04	8.929E-04	1.008E-03	1.014E-03	8.586E-04
Nd-148	1.945E-04	3.389E-04	4.662E-04	5.204E-04	5.226E-04	4.504E-04
Nd-150	8.570E-05	1.582E-04	2.234E-04	2.516E-04	2.518E-04	2.130E-04
Cs-134	2.983E-05	1.030E-04	1.829E-04	2.139E-04	2.144E-04	1.632E-04
Cs-137	6.617E-04	1.151E-03	1.582E-03	1.749E-03	1.761E-03	1.531E-03
Ce-144	2.026E-04	3.061E-04	3.720E-04	3.756E-04	3.750E-04	3.714E-04
Eu-154	5.253E-06	1.973E-05	3.293E-05	3.739E-05	3.707E-05	2.859E-05
Ru-106	5.163E-05	1.162E-04	1.829E-04	1.936E-04	1.162E-04	1.959E-04
Sb-125	2.462E-06	5.118E-06	4.966E-06	6.090E-06	7.507E-06	4.546E-06
Sm-147 <sup>b</sup>	1.529E-04	2.050E-04	2.355E-04	2.468E-04	2.479E-04	2.371E-04
Sm-148	4.092E-05	1.194E-04	1.978E-04	2.338E-04	2.357E-04	1.809E-04
Sm-149	2.935E-06	3.976E-06	4.259E-06	3.943E-06	3.799E-06	3.843E-06
Sm-150	1.323E-04	2.499E-04	3.599E-04	4.074E-04	4.113E-04	3.409E-04
Sm-151	9.324E-06	1.351E-05	1.503E-05	1.491E-05	1.465E-05	1.294E-05
Sm-152	6.526E-05	9.546E-05	1.191E-04	1.298E-04	1.319E-04	1.207E-04
Sm-154	1.425E-05	2.977E-05	4.536E-05	5.252E-05	5.298E-05	4.231E-05

<sup>a</sup> As reported in Y. Nakahara, Y. Suyama, and T. Suzuki, *Technical Development on Burnup Credit for Spent LWR Fuels*, JAERI-Tech 2000-071 (ORNL/TR-2001/01), English Translation, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2002).

<sup>b</sup> Measured data for samarium isotopes were reported at 3.96 years after discharge; at discharge time for all other isotopes.



## 4 ASSEMBLY AND IRRADIATION HISTORY DATA

This section presents information on the fuel assembly geometry, irradiation history, and sample burnup necessary for developing a computational model to determine the isotopic composition of the samples under consideration.

### 4.1 TMI-1 SAMPLES

The samples considered were selected from two different fuel assemblies, identified as NJ05YU and NJ070G, irradiated in the TMI-1 reactor. Details related to the geometry, material composition, and irradiation history were taken from Ref. 4. Both assemblies are a  $15 \times 15$  design, with 208 fuel rods, 16 guide tubes, and one instrument tube, as illustrated in Figures 4.1 and 4.2.

The fuel assembly geometry and material information for the two assemblies are presented in Table 4.1. Assembly NJ05YU was irradiated in the reactor for two consecutive cycles, cycle 9 and cycle 10. It contained 16 burnable poison rods (BPRs) with  $\text{Al}_2\text{O}_3\text{-B}_4\text{C}$  absorber, which were removed at the end of the cycle 9. All the fuel rods in this assembly had an initial fuel enrichment of 4.013 wt %  $^{235}\text{U}$ . Assembly NJ070G was present in the reactor during cycle 10 only. It also contained 16 BPRs during this cycle. Four of its fuel rods had 2.0 wt %  $\text{Gd}_2\text{O}_3$  poison, and their initial fuel enrichment was 4.19 wt %  $^{235}\text{U}$ . The other 204 regular fuel rods had an initial enrichment of 4.657 wt %  $^{235}\text{U}$ . Guide and instrument tube data were used as given elsewhere.<sup>18</sup> The locations of the  $\text{Gd}_2\text{O}_3$  poison rods in the assembly were provided by AREVA.

Eleven of the 19 TMI-1 samples, those measured at ANL, were selected from a fuel rod identified as H6, located in assembly NJ05YU. The other eight TMI-1 samples, analyzed at GE-VNC, were selected from the rods identified as O1, O12, and O13, located in assembly NJ070G. The location of the measured fuel rods in the assembly is illustrated in Figures 4.1 and 4.2. Note that all three measured fuel rods from assembly NJ070G were located at the edge of the assembly; the rod identified as O1 was located at the corner of the assembly.

Two sets of burnup values were specified in Ref. 4 for each sample: cumulative burnup based on operational data provided at end of cycle (EOC) for cycles 9 and 10, and total measured burnup, determined based on isotopic measurements, corresponding to EOC-10. The specific average powers for cycle  $P_9$  and  $P_{10}$  used for the calculations in the current work were obtained as:

$$P_9 = \frac{B_9}{\Delta t_9} \frac{B_{\text{meas}}}{B_{10}} \quad P_{10} = \frac{B_{10} - B_9}{\Delta t_{10}} \frac{B_{\text{meas}}}{B_{10}} \quad (4-1)$$

where  $B_9$  and  $B_{10}$  are the nominal burnup values at EOC-9 and EOC-10,  $B_{\text{meas}}$  is the sample measured burnup at EOC-10, and  $\Delta t_9$  and  $\Delta t_{10}$  is the cycle duration for cycles 9 and 10, respectively.

The effective full power days (EFPD) for cycle 9 and 10 are 639.4 days and 660.3 days, respectively. The down time between cycles 9 and 10, not available in Ref. 4, was assumed to be 30 days. Burnup and power data for each sample, as well as moderator density data are presented in Table 4.2. The variations with time of the soluble boron concentration in moderator and of the fuel temperature for assemblies NJ05YU and NJ070G are shown in Tables 4.3 and 4.4, respectively. Cooling time values corresponding to the measurement date for each sample are provided in Table 4.5.

Data available<sup>18</sup> on the assemblies surrounding assembly NJ070G are illustrated in Figure 4.3. As the samples from this assembly are expected to be subjected to edge effects given their location at the periphery of the assembly, this information may be important for modeling purposes. The sensitivity of the calculated nuclide content to the inclusion of this type of geometry details in the computational model is discussed in detail in Appendix A. The measured fuel rods were located at the east edge of assembly NJ070G that neighbored an assembly from batch 12A with an initial fuel enrichment of 4 wt % <sup>235</sup>U. Assemblies in batch 12 were first irradiated in the core during cycle 10. Assemblies in batch 11 were present in the core since cycle 9; no data were available on the average burnup of these assemblies at BOC-10. It is not known whether assemblies surrounding assembly NJ070G have fuel rods containing gadolinia poison. Also unknown is the exact location of rods O1, O12, and O13 with respect to the assemblies located north and south of assembly NJ070G. However, given the symmetry, as seen in Figure 4.3, this detail is deemed to be of low importance for modeling purposes.

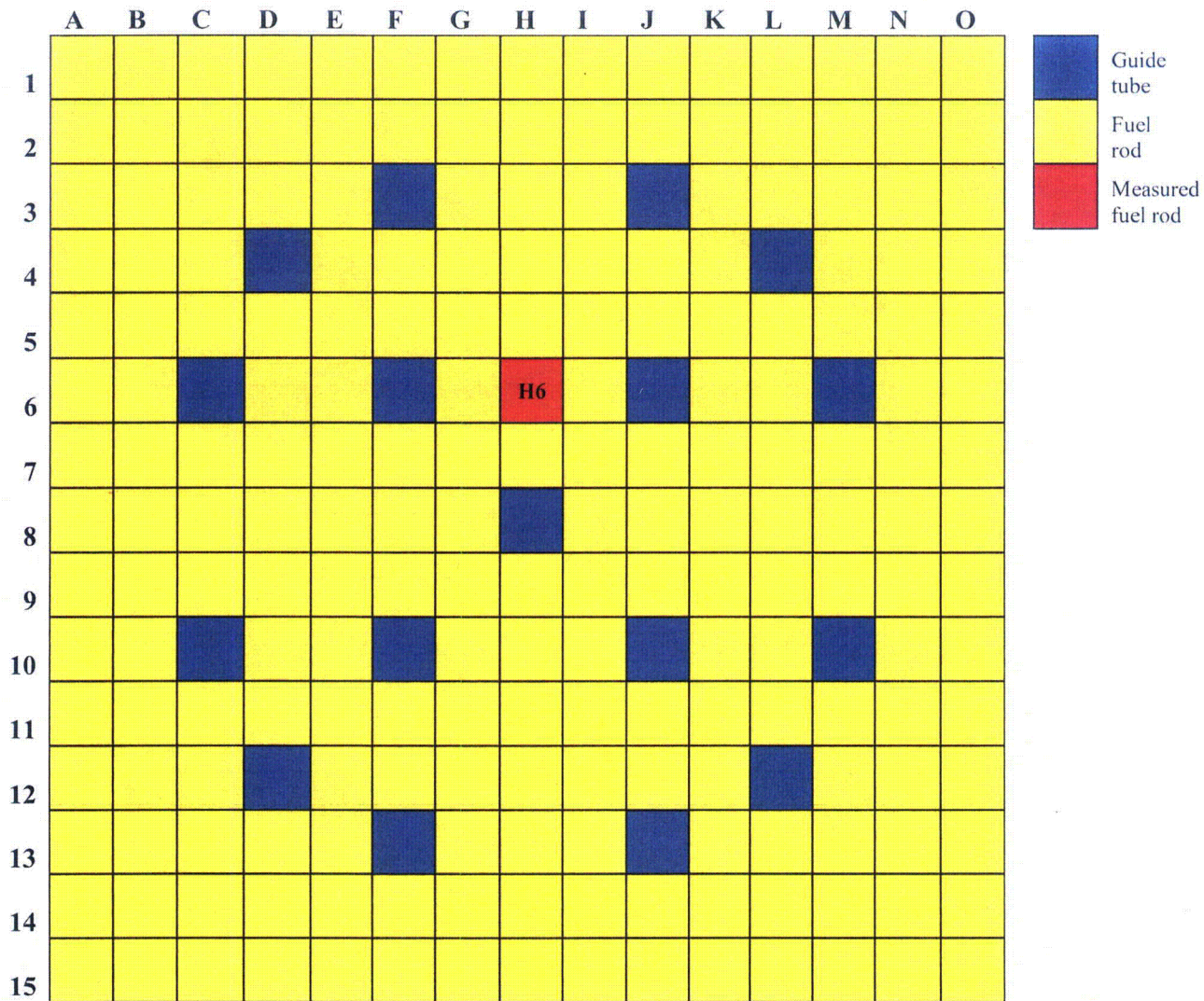


Figure 4.1 Assembly layout for TMI-1 samples—NJ05YU

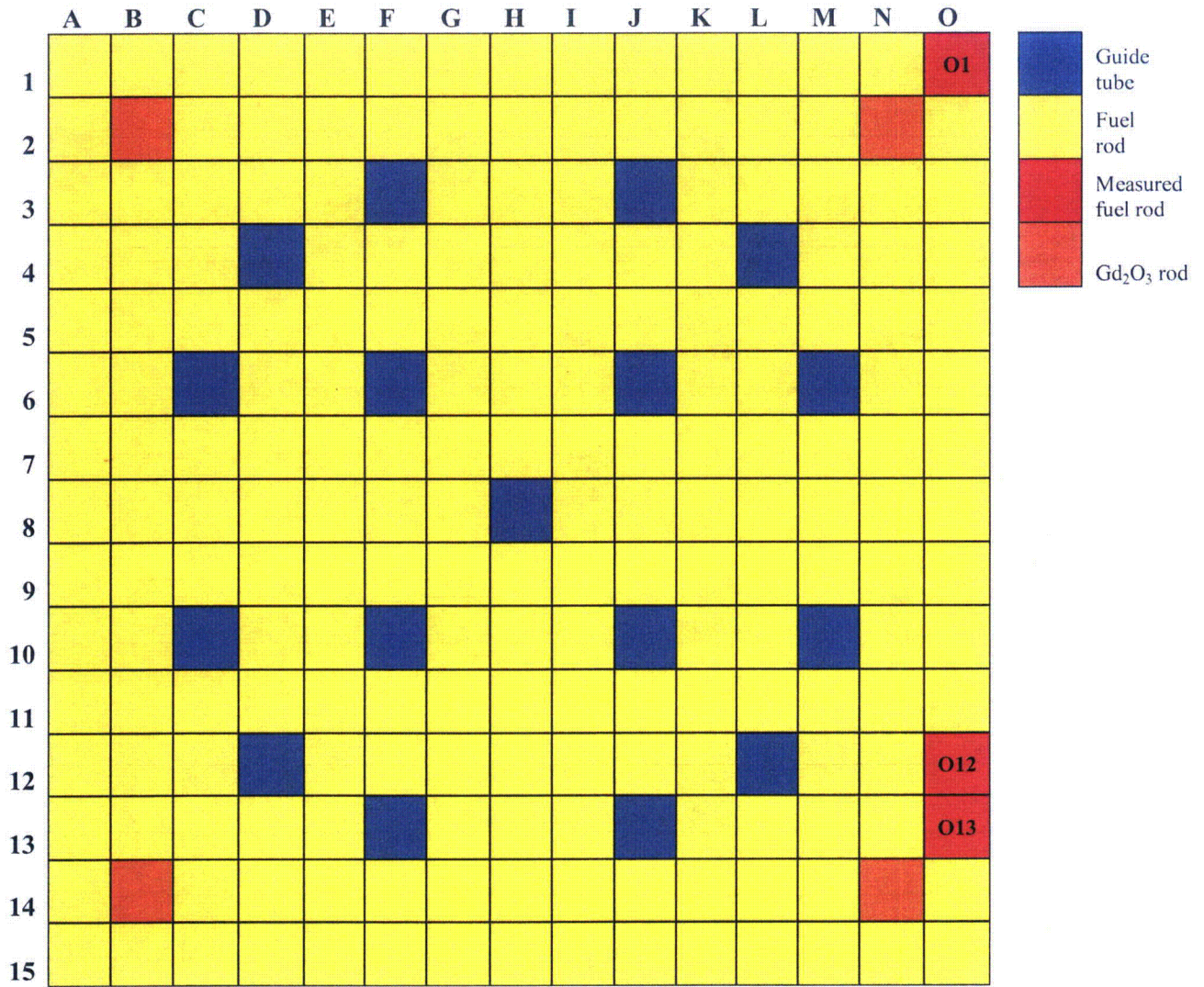


Figure 4.2 Assembly layout for TMI-1 samples—NJ070G

**Table 4.1 Assembly design data for TMI-1 samples**

Parameter	Data for assembly NJ05YU	Data for assembly NJ070G
<b>Assembly and reactor data<sup>a</sup></b>		
Reactor	TMI-1	TMI-1
Lattice geometry	15 × 15	15 × 15
Rod pitch (cm)	1.44272	1.44272
Number of fuel rods	208	208
Number of guide tubes	16	16
Number of instrument tubes	1	1
Assembly pitch (cm)	21.81098	21.81098
<b>Fuel rod data<sup>a</sup></b>		
Fuel material type	UO <sub>2</sub>	UO <sub>2</sub>
Fuel pellet density (g/cm <sup>3</sup> )	10.196	10.217
Fuel pellet diameter (cm)	0.9362	0.9398
Fuel temperature (K)	see Table 4.3	see Table 4.4
Enrichment (wt % <sup>235</sup> U)	4.013	4.657
Clad material	Zircaloy-4	Zircaloy-4
Clad inner diameter (cm)	0.95758	0.95758
Clad outer diameter (cm)	1.0922	1.0922
Average clad temperature (K)	640	640
Number of rods with Gd <sub>2</sub> O <sub>3</sub>	0	4
Gd <sub>2</sub> O <sub>3</sub> content (wt %)	NA	2.0
Initial fuel composition (wt %)		
<sup>234</sup> U	0.040	0.045 (0.0) <sup>b</sup>
<sup>235</sup> U	4.013	4.657 (4.019) <sup>b</sup>
<sup>238</sup> U	95.947	95.298 (95.981) <sup>b</sup>
<b>Moderator data<sup>a</sup></b>		
Moderator density (g/cm <sup>3</sup> )	see Table 4.2	see Table 4.2
Soluble boron in moderator (ppm)	see Table 4.3	see Table 4.4
<b>Burnable poison rod (BPR) data<sup>a</sup></b>		
Absorber diameter (cm)	0.8636	0.8636
Clad inner diameter (cm)	0.9144	0.9144
Clad outer diameter (cm)	1.0922	1.0922
Absorber material	Al <sub>2</sub> O <sub>3</sub> -B <sub>4</sub> C	Al <sub>2</sub> O <sub>3</sub> -B <sub>4</sub> C
Absorber material density (g/cm <sup>3</sup> )	3.7	3.7
B <sub>4</sub> C content (wt %)	1.7	2.1
Cladding material	Zircaloy-4	Zircaloy-4
<b>Guide/instrument tube data<sup>c</sup></b>		
Guide/instrument tube material	Zircaloy-4	Zircaloy-4
Guide tube inner diameter (cm)	1.26492	1.26492
Guide tube outer diameter (cm)	1.3462	1.3462
Instrument tube inner diameter (cm)	1.12014	1.12014
Instrument tube outer diameter (cm)	1.25222	1.25222

<sup>a</sup> As provided in J. M. Scaglione, *Three Mile Island Unit 1 Radiochemical Assay Comparisons to SAS2H Calculations*, Yucca Mountain Project Report, CAL-UDC-NU-000011, Rev. A (April 2002).

<sup>b</sup> Values in parentheses correspond to gadolinia-bearing fuel rods.

<sup>c</sup> As provided in L. B. Wimmer, *Summary Report of Commercial Reactor Criticality Data for Three Mile Island Unit 1*, TDR-UDC-NU-000004 REV 01, Bechtel SAIC Company, LLC, Las Vegas, NV (August 2001).

Table 4.2 Burnup, power and moderator density data for TMI-1 samples

Assembly	Rod ID	Sample ID	Burnup <sup>a</sup> EOC-9 (GWd/MTU)	Burnup <sup>a</sup> EOC-10 (GWd/MTU)	Measured <sup>b</sup> burnup (GWd/MTU)	Calculated <sup>c</sup> power cycle 9 (MW/MTU)	Calculated power cycle 10 (MW/MTU)	Moderator density (g/cm <sup>3</sup> )
NJ05YU	H6	A2	28.338	51.861	50.6	43.242	34.759	0.7314
		B2	28.444	52.089	50.1	42.787	34.442	0.7248
		C1	28.132	51.545	50.2	42.849	34.533	0.6965
		C3	28.230	51.696	51.3	43.813	35.266	0.7151
		D2	26.366	48.569	44.8	38.036	31.016	0.6787
		A1B	24.767	45.687	44.8	37.983	31.067	0.7382
		B1B	28.230	51.696	54.5	46.546	37.466	0.7151
		B3J	28.338	51.861	53.0	45.293	36.407	0.7314
		C2B	28.155	51.563	52.6	44.919	36.164	0.7057
		D1A2	28.115	51.530	55.7	47.529	38.331	0.6934
D1A4	28.034	50.810	50.5	43.577	34.283	0.6875		
NJ070G	O1	O1 S1		27.498	25.8		39.073	0.7382
		O1 S2		31.377	29.9		45.282	0.7057
		O1 S3		30.848	26.7		40.436	0.6875
	O12	O12 S4		25.592	23.7		35.893	0.7382
		O12 S5		29.271	26.5		40.133	0.7057
		O12 S6		28.760	24.0		36.347	0.6875
	O13	O13 S7		25.331	22.8		34.530	0.7382
		O13 S8		29.020	26.3		39.830	0.7057

<sup>a</sup> Based on operating history information.

<sup>b</sup> As provided in J. M. Scaglione, *Three Mile Island Unit 1 Radiochemical Assay Comparisons to SAS2H Calculations*, Yucca Mountain Project Report, CAL-UDC-NU-000011, Rev. A (April 2002).

<sup>c</sup> See Eq. (4-1).

**Table 4.3 Fuel temperature and concentration of soluble boron in moderator for TMI-1 samples from assembly NJ05YU**

Cycle #	Sample ID	A2	B2	C1	C3	D2	A1B	B1B	B3J	C2B	D1A2	D1A4	Boron <sup>a</sup> (ppm)
	Time (days)	Temp. <sup>a</sup> (K)											
9	0.0												1670
	74.2	1051.2	1085.4	1105.7	1098.3	1029.0	948.7	1098.3	1051.2	1106.1	1100.7	1091.2	1481
	141.1	1040.9	1058.8	1069.1	1062.9	1025.2	957.5	1062.9	1040.9	1066.8	1068.4	1065.0	1342
	214.0	1023.3	1030.3	1034.4	1029.4	1009.3	959.3	1029.4	1023.3	1031.2	1035.8	1035.8	1175
	284.9	1002.0	1002.0	1003.2	998.2	995.7	953.5	998.2	1002.0	998.9	1006.2	1009.0	990
	349.7	982.09	976.62	976.01	971.18	982.57	947.65	971.18	982.09	971.2	980.2	985.1	772
	425.0	959.40	950.04	948.93	944.23	963.71	940.48	944.23	959.40	944.2	963.4	959.3	545
	483.9	936.52	925.90	925.46	920.59	945.73	927.57	920.59	936.52	921.0	929.9	936.2	352
	549.2	918.46	907.79	907.79	903.40	929.26	913.93	903.40	918.46	904.0	911.7	917.8	134
	608.0	888.21	884.01	900.23	889.62	924.34	886.48	889.62	888.21	895.1	904.2	909.8	13
639.4	772.90	777.37	810.43	790.98	837.01	771.65	790.98	772.90	801.7	815.3	821.0	2	
10	0.0												1800
	68.0	835.54	861.01	871.01	871.32	825.07	787.87	871.32	835.54	874.84	865.43	843.34	1649
	131.8	828.60	846.96	856.62	853.46	825.54	785.79	853.46	828.60	856.84	854.23	840.48	1521
	209.0	824.52	935.65	844.68	838.76	829.98	786.23	838.76	824.52	841.84	845.32	840.87	1322
	272.1	823.77	828.87	835.79	829.29	831.73	791.43	829.29	823.77	831.71	838.01	838.93	1140
	347.4	822.13	823.12	828.46	822.09	832.12	796.54	822.09	822.13	823.98	831.46	836.07	918
	416.4	818.71	816.71	821.65	815.18	831.46	799.84	815.18	818.71	816.96	825.09	832.48	718
	486.4	813.82	809.93	815.29	808.54	829.93	801.23	808.54	813.82	810.51	818.96	828.43	506
	556.3	807.62	802.59	808.43	801.59	827.37	800.98	801.59	807.62	803.76	812.15	823.34	298
	626.1	801.96	796.93	802.65	796.15	823.76	799.18	796.15	801.96	798.34	806.21	817.73	103
660.3	799.90	795.18	799.87	794.37	819.26	797.96	794.37	799.90	796.26	803.01	813.51	1.8	

<sup>a</sup> As provided in J. M. Scaglione, *Three Mile Island Unit 1 Radiochemical Assay Comparisons to SAS2H Calculations*, Yucca Mountain Project Report, CAL-UDC-NU-000011, Rev. A (April 2002).

**Table 4.4 Fuel temperature and concentration of soluble boron in moderator for TMI-1 samples from assembly NJ070G**

Cycle #	Sample ID	O1S1	O1S2	O1S3	O12S4	O12S5	O12S6	O13S7	O13S8	Boron <sup>a</sup> (ppm)
	Time (days)	Temp. <sup>a</sup> (K)								
10	0.0									1800
	68.0	960.29	1119.5	1083.7	960.29	1119.5	1083.7	960.29	1119.51	1649
	131.8	960.71	1084.8	1067.3	960.71	1084.8	1067.3	960.71	1084.79	1521
	209.0	958.68	1043.2	1043.5	958.68	1043.2	1043.5	958.68	1043.23	1322
	272.1	954.18	1007.1	1016.4	954.18	1007.1	1016.4	954.18	1007.09	1140
	347.4	946.12	978.57	991.65	946.12	978.57	991.65	946.12	978.57	918
	416.4	937.15	951.57	967.21	937.15	951.57	967.21	937.15	951.57	718
	486.4	926.04	929.82	945.98	926.04	929.82	945.98	926.04	929.82	506
	556.3	914.37	912.15	928.04	914.37	912.15	928.04	914.37	912.15	298
	626.1	904.09	896.84	912.12	904.09	896.84	912.12	904.09	896.84	103
660.3	897.82	886.54	899.73	897.82	886.54	899.73	897.82	886.54	1.8	

<sup>a</sup> As provided in J. M. Scaglione, *Three Mile Island Unit 1 Radiochemical Assay Comparisons to SAS2H Calculations*, Yucca Mountain Project Report, CAL-UDC-NU-000011, Rev. A (April 2002).

**Table 4.5 Cooling time at measurement date for TMI-1 samples**

Sample ID	Cooling time <sup>a</sup> (days)
A2, B2, C1, C3, D2	1103
O1S1, O1S3, O12S4, O12S6	1298
O1S2, O12S5, O13S7, O13S8	1529
A1B, B1B, B3J, C2B, D1A2, D1A4	1711

<sup>a</sup> As provided in J. M. Scaglione, *Three Mile Island Unit 1 Radiochemical Assay Comparisons to SAS2H Calculations*, Yucca Mountain Project Report, CAL-UDC-NU-000011, Rev. A (April 2002).



<b>NW</b>	<b>N</b>	<b>NE</b>
Batch 12C Enrich = 4.65%	Batch 11C Enrich = 4%	Batch 12E Enrich = 4.75%
<b>W</b>	<b>NJ070G</b>	<b>E</b>
Batch 11A Enrich = 3.63%	Batch 12C Enrich = 4.65%	Batch 12A Enrich = 4%
<b>SW</b>	<b>S</b>	<b>SE</b>
Batch 12B Enrich = 4.65%	Batch 11C Enrich = 4%	Batch 12D Enrich = 4.75%

**Figure 4.3 Assemblies surrounding assembly NJ070G**

## 4.2 CALVERT CLIFFS SAMPLES

The Calvert Cliffs measurements considered in this report were carried out on three samples from the fuel rod MKP-109 belonging to the CE  $14 \times 14$  fuel assembly D047. The samples are identified as 87-81, 87-72, and 87-63. The rod was present in the reactor core for four consecutive cycles, from cycle 2 to cycle 5. The assembly had 176 fuel rods and five guide tubes, as illustrated in Figure 4.4. There were no burnable poison rods or gadolinia-bearing rods in the assembly during any of the irradiation cycles. The location of the rod from which the samples were selected is also shown in the figure.

The geometry data are presented in Table 4.6 and the burnup history data and soluble boron concentration in moderator are presented in Table 4.7. The fuel temperature, moderator temperature and density, and cooling times for each of the three samples are given in Table 4.8. All these data were taken from Refs. 11 and 15.

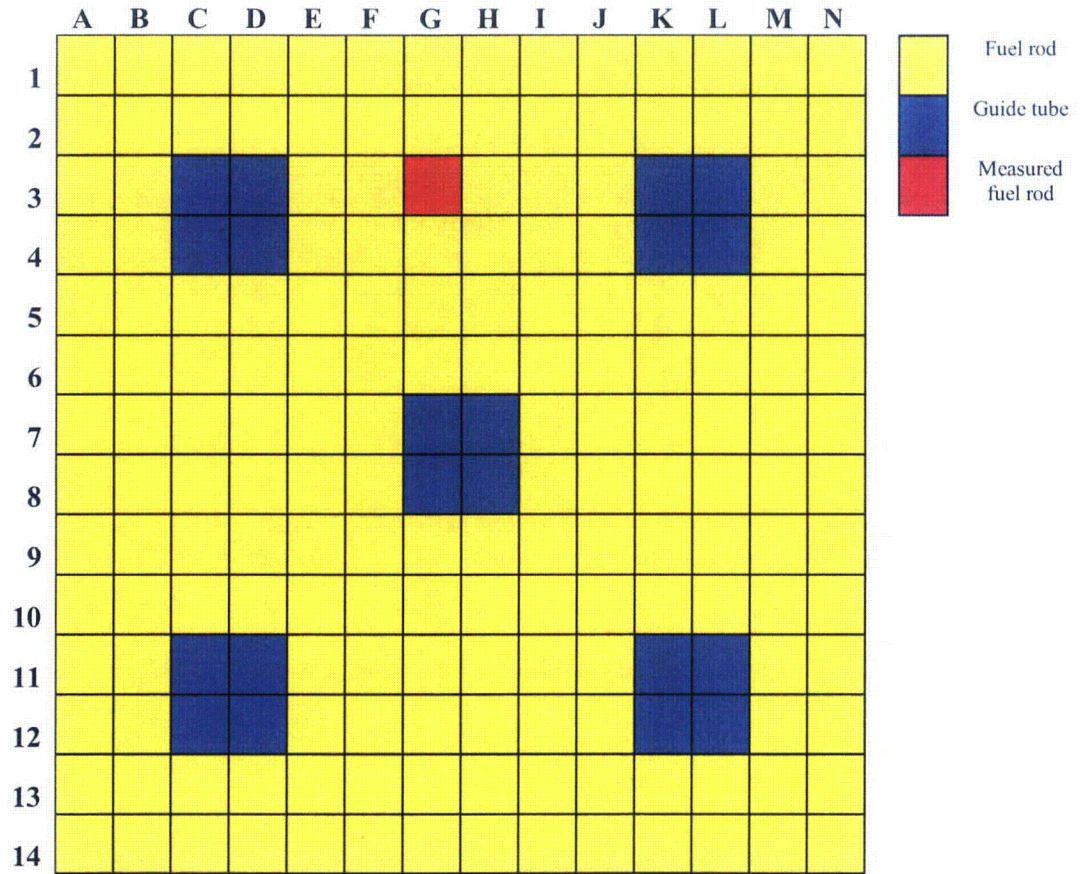


Figure 4.4 Assembly layout for Calvert Cliffs samples

**Table 4.6 Assembly design data for Calvert Cliffs samples**

Parameter	Data
<b>Assembly and reactor data<sup>a</sup></b>	
Reactor	Calvert Cliffs 1
Lattice geometry	14 × 14
Assembly design	CE
Rod pitch (cm)	1.4732
Number of fuel rods	176
Number of water rods	5
Assembly pitch (cm)	20.78
<b>Fuel rod data<sup>a</sup></b>	
Fuel material type	UO <sub>2</sub>
Fuel density (g/cm <sup>3</sup> )	10.045
Fuel pellet diameter (cm)	0.9563
Clad material	Zircaloy-4
Fuel temperature (K)	see Table 4.8
Clad inner diameter (cm)	0.9855
Clad outer diameter (cm)	1.1176
Average clad temperature <sup>b</sup> (K)	620
U isotopic composition <sup>c</sup> (wt %)	
<sup>234</sup> U	0.027
<sup>235</sup> U	3.038
<sup>236</sup> U	0.014
<sup>238</sup> U	96.921
<b>Moderator data<sup>a</sup></b>	
Moderator density (g/cm <sup>3</sup> )	see Table 4.8
Moderator temperature (K)	see Table 4.8
Soluble boron content (ppm)	see Table 4.7
<b>Guide tube data<sup>a</sup></b>	
Guide tube material	Zircaloy-4
Inner radius (cm)	1.314
Outer radius (cm)	1.416

<sup>a</sup> As provided in O. W. Herman, S. M. Bowman, M. C. Brady, and C. V. Parks, *Validation of the SCALE System for PWR Spent Fuel Isotopic Composition Analyses*, ORNL/TM-12667, Oak Ridge National Laboratory, Oak Ridge, Tennessee (March 1995).

<sup>b</sup> Assumed value.

<sup>c</sup> Initial values.

**Table 4.7 Burnup history data for Calvert Cliffs samples**

Cycle #	Start date	End date	Duration (days)	Down (days)	Cycle average boron <sup>a</sup> (ppm)	Burnup <sup>a,b</sup> (GWd/MTU)		
						87-81	87-72	87-63
2	3/22/77	1/22/78	306.0	71.0	330.8	5.28	7.56	9.52
3	4/3/78	4/20/79	381.7	81.3	469.4	12.69	17.78	21.93
4	7/10/79	10/18/80	466.0	85.0	503.7	20.63	28.42	34.14
5	1/11/81	4/17/82	461.1		492.1	27.35	37.12	44.34

<sup>a</sup> As provided in O. W. Herman, S. M. Bowman, M. C. Brady, and C. V. Parks, *Validation of the SCALE System for PWR Spent Fuel Isotopic Composition Analyses*, ORNL/TM-12667, Oak Ridge National Laboratory, Oak Ridge, Tennessee (March 1995).

<sup>b</sup> Cumulative value.

**Table 4.8 Moderator, fuel temperature, and cooling time data for Calvert Cliffs samples**

Parameter	87-81		87-72		87-63	
Moderator temperature <sup>a</sup> (K)	557		558		570	
Moderator density <sup>a</sup> (g/cm <sup>3</sup> )	0.7575		0.7569		0.7332	
Fuel temperature <sup>a</sup> (K)	790		841		873	
Cooling time <sup>b</sup> (days)	1870	4171 <sup>c</sup>	1870	4656 <sup>c</sup>	1870	4656 <sup>c</sup>

<sup>a</sup> As provided in O. W. Herman, S. M. Bowman, M. C. Brady, and C. V. Parks, *Validation of the SCALE System for PWR Spent Fuel Isotopic Composition Analyses*, ORNL/TM-12667, Oak Ridge National Laboratory, Oak Ridge, Tennessee (March 1995).

<sup>b</sup> At time of measurement; values correspond to PNNL and KRI measurement dates, respectively.

<sup>c</sup> Values obtained from PNNL private communication.

### 4.3 TAKAHAMA-3 SAMPLES

Radiochemical analyses were performed at JAERI on 16 samples from three fuel rods identified as SF95, SF96, and SF97.<sup>6,13,17</sup> Rods SF95 and SF97 were standard fuel rods with 4.11 wt % <sup>235</sup>U initial enrichment; whereas SF96 was a fuel rod with gadolinia poison that had a fuel initial enrichment of 2.6 wt % <sup>235</sup>U and a Gd<sub>2</sub>O<sub>3</sub> content of 6%. Rods SF95 and SF96 were from assembly NT3G23 and rod SF97 was from assembly NT3G24. Each of these two assemblies had a 17 × 17 configuration, with 264 fuel rods (14 of these containing gadolinia<sup>17</sup>) and 25 water-filled guide tubes. They resided in the reactor core for two (assembly NT3G23) or three (assembly NT3G24) consecutive cycles, starting from cycle 5. The configuration of the assembly, including the location of the measured rods, is illustrated in Figure 4.5. Assembly parameters are listed in Table 4.9.

Burnup values, sample axial location along the fuel rod, moderator density and temperature, and cycle power for each sample are listed in Table 4.10. Operation history data and soluble boron concentration are presented in Tables 4.11 and 4.12, respectively. The moderator density was determined by interpolating on temperature vs. pressure data,<sup>1</sup> using the available moderator temperature data<sup>17</sup> and a pressure value<sup>19</sup> of 157 kg/cm<sup>2</sup>. The cycle power for each sample was obtained by averaging the power data given in Ref. 17. The measured nuclide concentrations were reported at discharge time with the exception of those for samarium isotopes in samples from rod SF97 that were reported at 3.96 years after discharge.

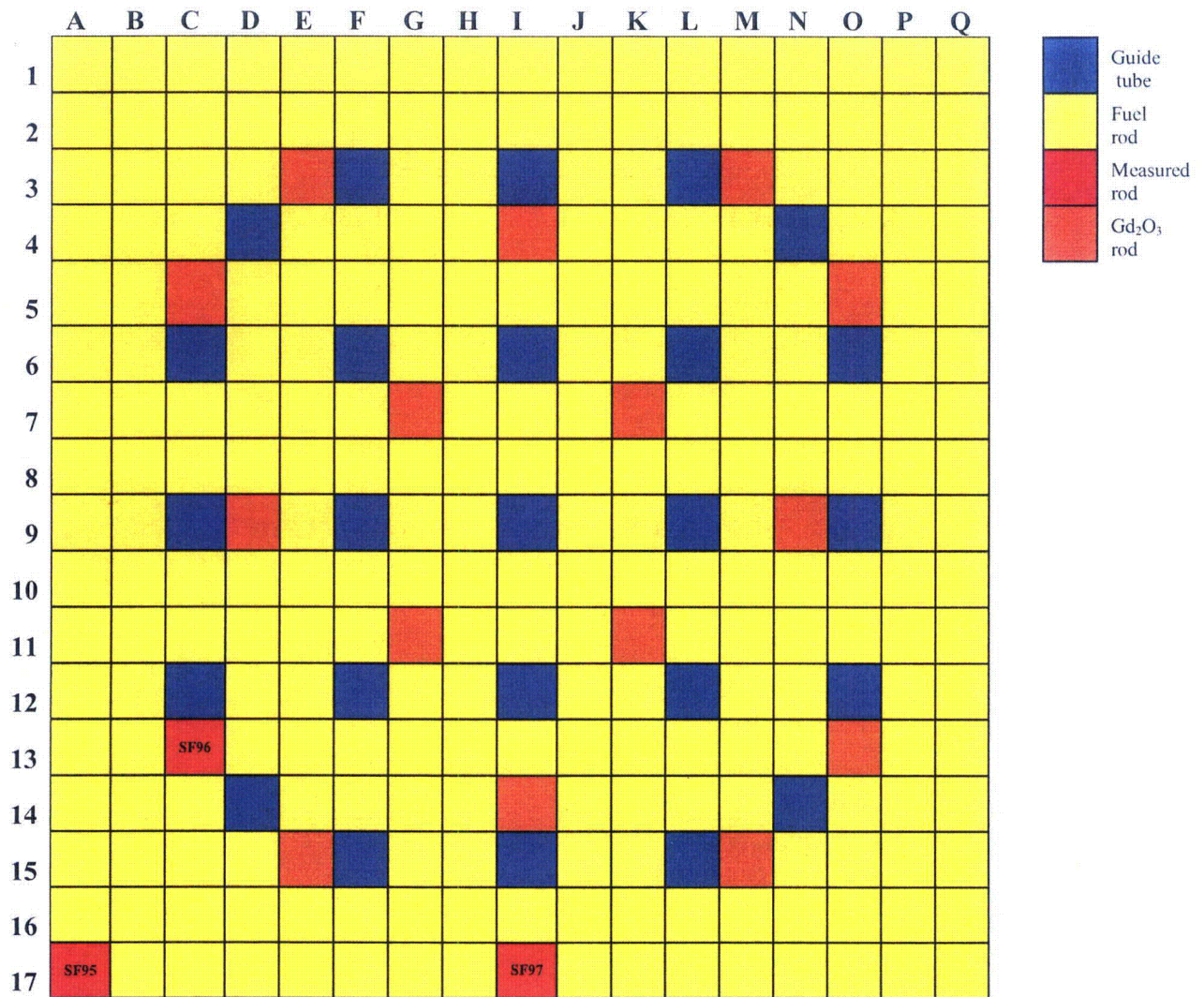


Figure 4.5 Assembly layout for Takahama-3 samples

**Table 4.9 Assembly design data for Takahama-3 samples**

<b>Parameter</b>	<b>Data</b>
<b>Assembly and reactor data<sup>a</sup></b>	
Reactor	Takahama-3
Lattice geometry	17 × 17
Rod pitch (cm)	1.259
Number of fuel rods	264
Number of guide tubes	25
Assembly pitch (cm)	21.4
<b>Fuel rod data<sup>a</sup></b>	
Fuel material type	UO <sub>2</sub>
Fuel pellet density (% TD)	95
Enrichment (wt % <sup>235</sup> U)	4.11 (2.63) <sup>a</sup>
Fuel pellet diameter (cm)	0.805
Average fuel temperature (K)	900
Clad material	Zircaloy-4
Clad inner diameter (cm)	0.822
Clad outer diameter (cm)	0.95
Average clad temperature (K)	600
Number of rods with Gd <sub>2</sub> O <sub>3</sub>	14
Gd <sub>2</sub> O <sub>3</sub> content (wt %)	6.0
U isotopic composition <sup>b</sup> (wt %)	
<sup>234</sup> U	0.04 (0.02) <sup>c</sup>
<sup>235</sup> U	4.11 (2.63)
<sup>238</sup> U	95.85 (97.25)
<b>Moderator data<sup>a</sup></b>	
Moderator density (g/cm <sup>3</sup> )	see Table 4.10
Moderator temperature (K)	see Table 4.10
Soluble boron (ppm)	see Table 4.12
<b>Guide tube data<sup>a</sup></b>	
Guide tube material	Zircaloy-4
Inner radius (cm)	0.5715
Outer radius (cm)	0.6121

<sup>a</sup> As given in Y. Nakahara, Y. Suyama, and T. Suzaki, *Technical Development on Burnup Credit for Spent LWR Fuels*, JAERI-Tech 2000-071 (ORNL/TR-2001/01), English Translation, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2002).

<sup>b</sup> At beginning of life.

<sup>c</sup> Values in parentheses correspond to gadolinia-bearing fuel rods.

**Table 4.10 Burnup, power, sample location, and moderator data for Takahama-3 samples**

Assembly	Rod ID	Sample ID	Burnup <sup>a</sup> (GWd/MTU)	Power <sup>b</sup> cycle 5 (MW/MTU)	Power <sup>b</sup> cycle 6 (MW/MTU)	Power <sup>b</sup> cycle 7 (MW/MTU)	Sample <sup>c</sup> location (cm)	Moderator <sup>a</sup> temperature (K)	Moderator density (g/cm <sup>3</sup> )
NT323G	SF95	SF95-1	14.30	19.21	17.17		20.1	593.04	0.6803
		SF95-2	24.35	32.72	29.25		36.1	592.75	0.6810
		SF95-3	35.52	47.59	42.54		88.1	589.37	0.6898
		SF95-4	36.69	49.30	44.06		216.1	570.40	0.7324
		SF95-5	30.40	40.85	36.51		356.1	554.19	0.7628
	SF96	SF96-1	7.79	8.01	11.72		17.6	593.05	0.6803
		SF96-2	16.44	16.90	24.71		33.6	592.82	0.6809
		SF96-3	28.20	28.99	42.40		85.6	589.62	0.6892
		SF96-4	28.91	29.71	43.46		213.6	570.82	0.7316
		SF96-5	24.19	24.87	36.37		353.6	554.28	0.7627
NT324G	SF97	SF97-1	17.69	14.76	15.74	13.97	16.3	593.05	0.6803
		SF97-2	30.73	25.65	27.36	24.28	35.0	592.78	0.6810
		SF97-3	42.16	35.19	37.53	33.31	62.7	591.48	0.6843
		SF97-4	47.03	39.26	41.87	37.16	183.9	575.83	0.7211
		SF97-5	47.25	39.44	42.06	37.33	292.6	559.14	0.7540
		SF97-6	40.79	34.05	36.31	32.23	355.6	554.21	0.7628

<sup>a</sup> As given in Y. Nakahara, Y. Suyama, and T. Suzuki, *Technical Development on Burnup Credit for Spent LWR Fuels*, JAERI-Tech 2000-071 (ORNL/TR-2001/01), English Translation, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2002).

<sup>b</sup> Cycle-averaged power calculated based on data provided in Y. Nakahara, Y. Suyama, and T. Suzuki, *Technical Development on Burnup Credit for Spent LWR Fuels*, JAERI-Tech 2000-071 (ORNL/TR-2001/01), English Translation, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2002).

<sup>c</sup> Distance measured from top of fuel.

**Table 4.11 Operation history data for Takahama-3 samples**

Cycle #	Start date	End date	Duration (days)	Down (days)
5	1990/01/26	1991/02/15	385	88
6	1991/02/15	1991/05/14	402	62
7	1991/05/14	1992/06/19	406	

**Table 4.12 Soluble boron concentration in moderator for Takahama-3 samples**

Cycle #	Cumulative time <sup>a</sup> (days)	Boron content (ppm)
5	0	1154
	106	894
	205	651
	306	404
	385	210
6	473	1132
	592	864
	704	613
	817	358
	875	228
7	937	1154
	996	1001
	1048	867
	1100	732
	1152	598
	1204	463
	1256	329
	1308	195
1342	104	

<sup>a</sup> Measured from beginning of cycle 5.



## 5 COMPUTATIONAL MODELS

### 5.1 COMPUTATIONAL TOOLS

The computational analysis of the measurements was carried out by using the 2-D depletion sequence TRITON in the SCALE computer code system.<sup>1</sup> This sequence couples the 2-D arbitrary polygonal mesh, discrete ordinates transport code NEWT with the depletion and decay code ORIGEN-S in order to perform the burnup simulation. At each depletion step, the transport flux solution from NEWT is used to generate the cross sections for the ORIGEN-S calculation; the isotopic composition data resulting from ORIGEN-S is employed in the subsequent transport calculation to obtain cross sections for the next depletion step in an iterative manner throughout the irradiation history.

TRITON has the capability of individually simulating the depletion of multiple mixtures in a fuel assembly model. This is a very useful and powerful feature in a nuclide inventory analysis, as it allows a more appropriate representation of the local flux distribution and environmental effects on a specific measured fuel rod in the assembly. The flux normalization in a TRITON calculation can be performed using as a basis the power in a specified mixture, the total power corresponding to multiple mixtures, or the assembly power. The first of the above-mentioned options permits the burnup (power) in the measured sample, usually inferred from experimental measurements of burnup indicators (such as <sup>148</sup>Nd), to be specified.

Individual TRITON models were developed for each of the 38 sample measurements discussed in the previous sections. In all cases, the calculations were carried out by normalizing the power to reproduce the measured concentration of <sup>148</sup>Nd in the sample within the experimental uncertainty. All TRITON calculations employed the SCALE 44-group cross-section library based on ENDF/B-V data and NITAWL as processor for the pin-cell cross-section treatment. Default values were used for the convergence parameters in the NEWT transport calculation. Selected TRITON input files are provided in Appendix B.

TRITON provides the user the option to control the number of nuclides in the depleted mixtures for which the cross sections used in the ORIGEN-S depletion calculation are updated at each depletion step based on the flux solution from the transport calculation with NEWT. The user should specify the control parameter "parm=(addnux=N)" on the first line of the TRITON input file, where N identifies the set of nuclides included in the transport calculation. The nuclides in the selected set that are not present in the initial fuel composition are set to trace concentrations (i.e.,  $10^{-20}$  atoms/b-cm). The calculation in the present report used the option "addnux=3" for which the set of nuclides considered in the transport calculation, and for which, therefore, the NEWT flux solution is used to update the cross sections for ORIGEN-S, contains 232 isotopes.

### 5.2 TMI-1 SAMPLES

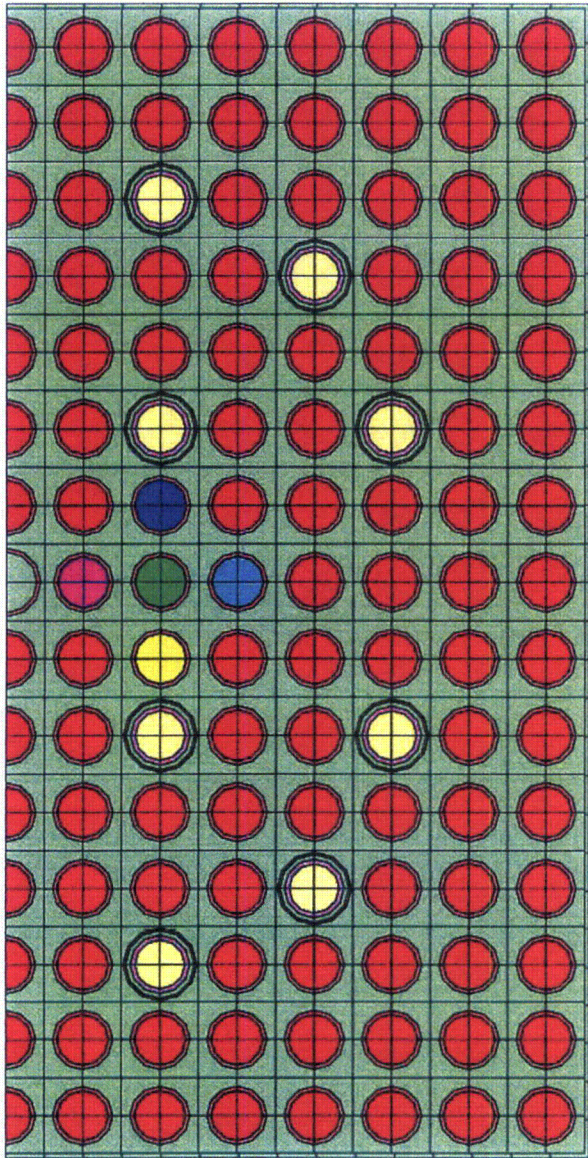
Assembly NJ05YU that hosted the fuel rod H6 (see Figure 4.1), from which 11 samples were selected, was irradiated in two consecutive cycles, cycle 9 and cycle 10. The BPRs present during cycle 9 were removed in cycle 10. Separate TRITON models were developed to accurately represent this change in the assembly geometry, as illustrated in Figure 5.1. Given the symmetry and the location of rod H6 in assembly NJ05YU, the models for the analysis of samples selected from this rod represent only half of the assembly geometry, with a reflective boundary condition on the left side of the configuration and white boundary conditions on the other three bounding surfaces. The geometry and material data were used as given in Table 4.1, and the power data as provided in Table 4.2. Six fuel mixtures were specified: one corresponding to the measured rod, four to the nearest neighbor fuel rods, and one to the rest of the fuel

rods in the assembly. At the end of the depletion simulation for cycle 9, the isotopic composition for each of these six fuel mixtures was extracted and used as input data in the model corresponding to cycle 10 (with no BPR present). A total of 232 nuclides, representing the main light elements, actinides, and fission products, were included to represent the fuel composition at the start of cycle 10. The variation of the soluble boron content in the coolant and of the temperature in fuel during irradiation, as given in Table 4.3, was modeled through the use of the TIMETABLE input block in TRITON; ten burnup steps per cycle were used.

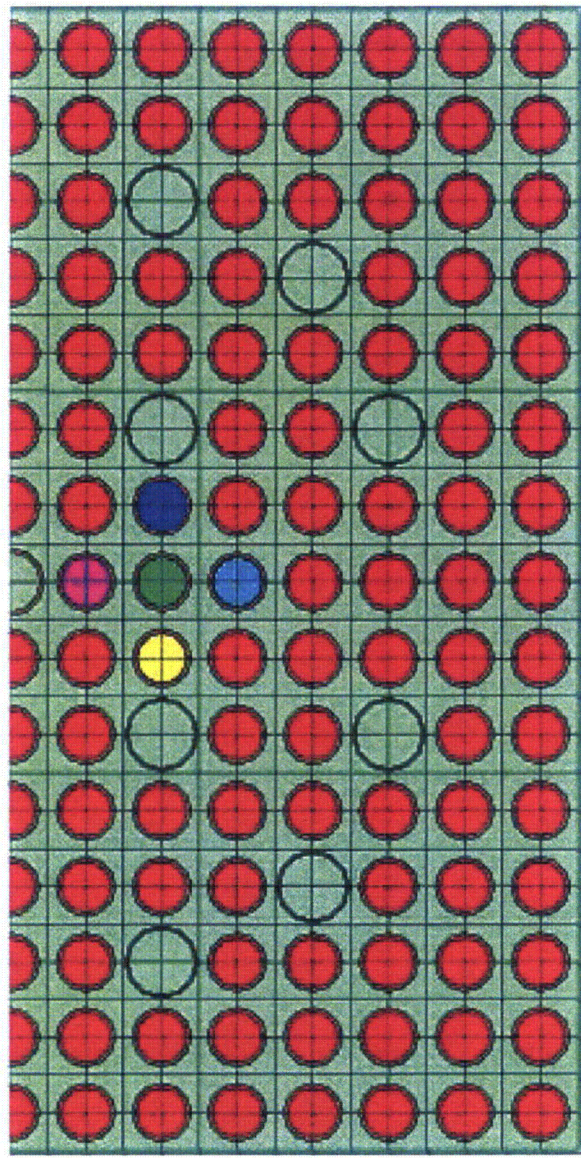
As data became available on the assemblies surrounding the assembly NJ05YU, the TRITON geometry model was extended to include this information. However, as rod H6 is located toward the center of the assembly, it is not expected to be subject to significant edge effects due to the assembly surroundings. These effects will be discussed in detail in Appendix A.

All three rods in assembly NJ070G, from which samples were selected for measurement, were edge rods located along one side of the assembly, with one of these rods placed at the corner of the assembly. The computational models used for the analysis of these samples include information on the assembly surroundings. As is shown in Appendix A, neglecting this type of detail could significantly affect the calculation of the nuclide content in the sample. The models for rods O12 and O13 are similar and include a quarter of assembly NJ070G and a quarter of the assembly surrounding it on the side on which the samples are located, as illustrated for rod O12 in Figure 5.2. As observed in this figure, in order to better approximate the local environment, given the close proximity of the measured rod to the assembly boundary, the nearest neighboring rods were represented by using different mixtures; one of these neighboring rods is located in a different assembly. In the case of the corner rod O1, the TRITON model included a quarter of assembly NJ070G and a quarter of each of the three surrounding assemblies that share the same corner point with assembly NJ070G. This model is illustrated in Figure 5.3. Note that in this model the average burnup at the beginning of cycle 10 for one of the adjacent assemblies (batch 11C in Figure 4.3) was not available; this assembly was assumed to be fresh fuel.

The power was adjusted by less than 1.5%, depending on the sample, in order to obtain a calculated  $^{148}\text{Nd}$  concentration, which is a direct measure of the integral number of fissions (burnup), in agreement with the experimental value.



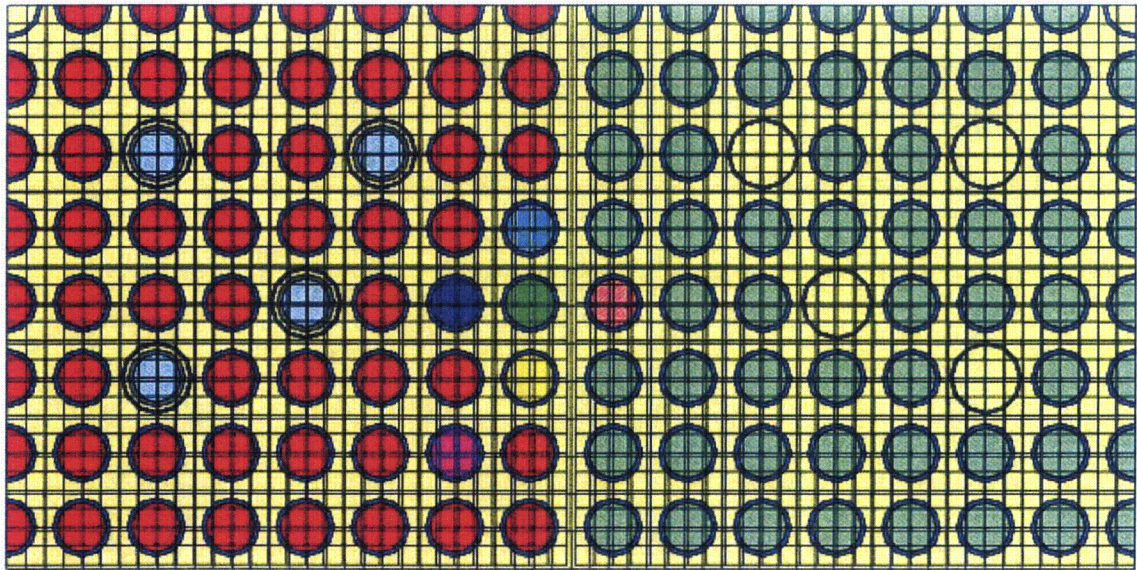
Cycle 9



Cycle 10

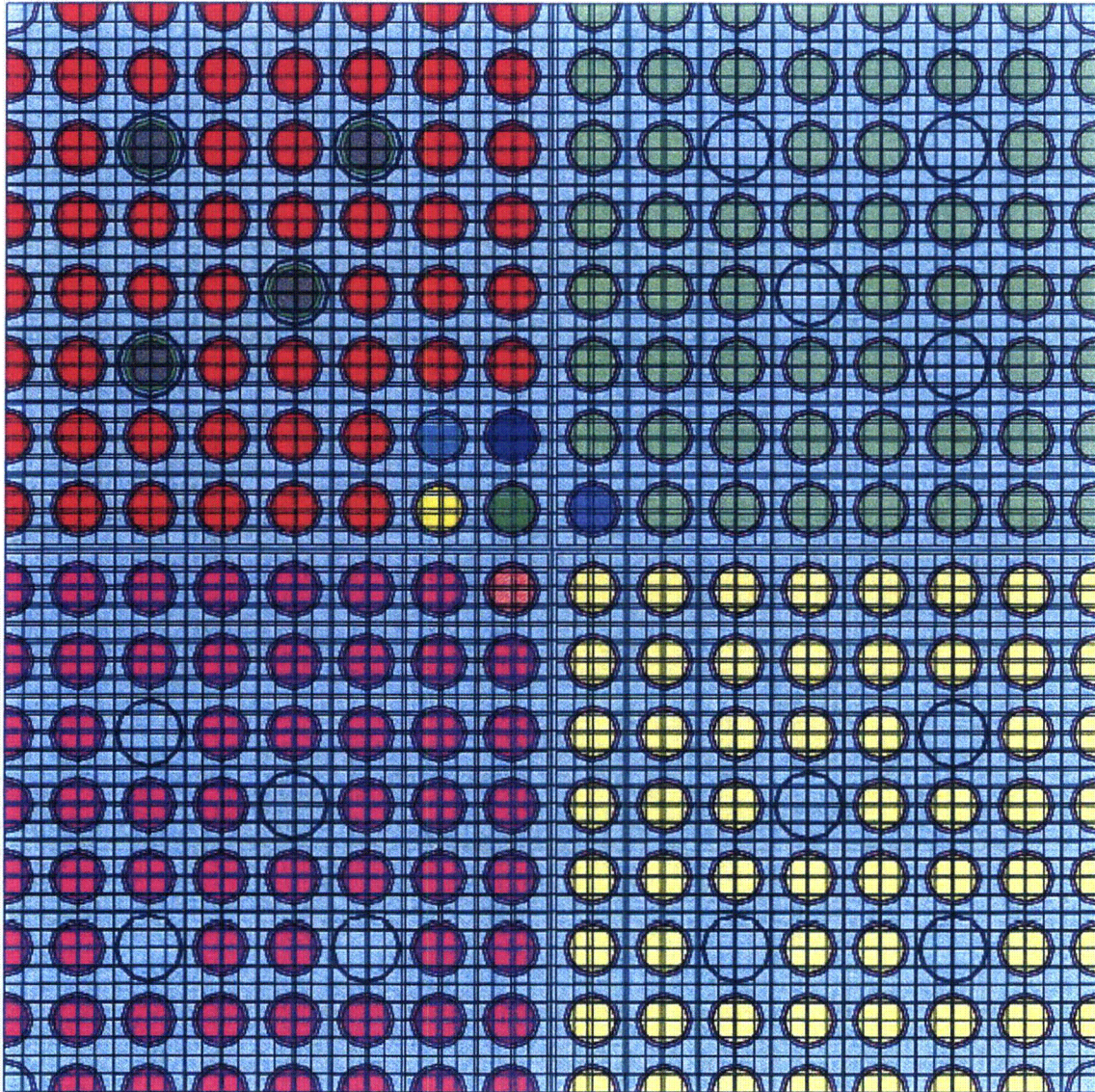
■ regular fuel pin   
 ■ measured fuel pin H6   
 ■ ■ ■ ■ neighbors of measured fuel pin  
■ BPR absorber   
 ■ BPR clad

**Figure 5.1 TRITON assembly model for TMI-1 samples in assembly NJ05YU**



■ measured fuel pin O12    ■ ■ ■ nearest neighbors of measured pin  
■ regular fuel pins in assembly NJ070G    ■ gadolinia fuel pin    ■ fuel pins in neighboring assembly  
■ moderator    ■ BPR absorber

**Figure 5.2 TRITON assembly model for TMI-1 samples in rod O12 of assembly NJ070G**



■ measured fuel pin O1 ■ ■ ■ ■ nearest neighbors of measured pin ■ gadolinia fuel pin  
 ■ BPR absorber ■ regular fuel pins in assembly NJ070G ■ ■ fuel pins in surrounding  
 assemblies ■ moderator

**Figure 5.3 TRITON assembly model for TMI-1 samples in rod O1 of assembly NJ070G**

### 5.3 CALVERT CLIFFS SAMPLES

Half of the Calvert Cliffs D047 assembly was modeled for the analysis of the three measured fuel samples from fuel rod MKP-109, as illustrated in Figure 5.4. Geometry, material composition, temperature, coolant density, and soluble boron in moderator data as specified in Tables 4.6 to 4.8 were used.

The power (burnup) values given in Table 4.7 were adjusted by less than 1.6%, depending on the sample, such that the calculated  $^{148}\text{Nd}$  concentration was consistent with the corresponding measured value, within one standard deviation of the measurement.

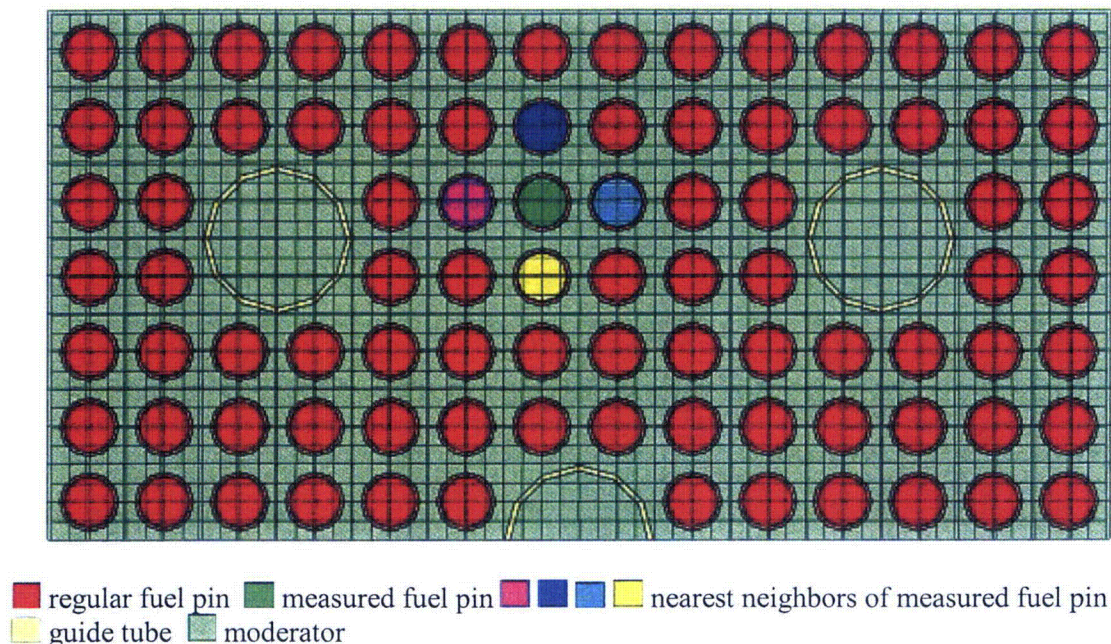
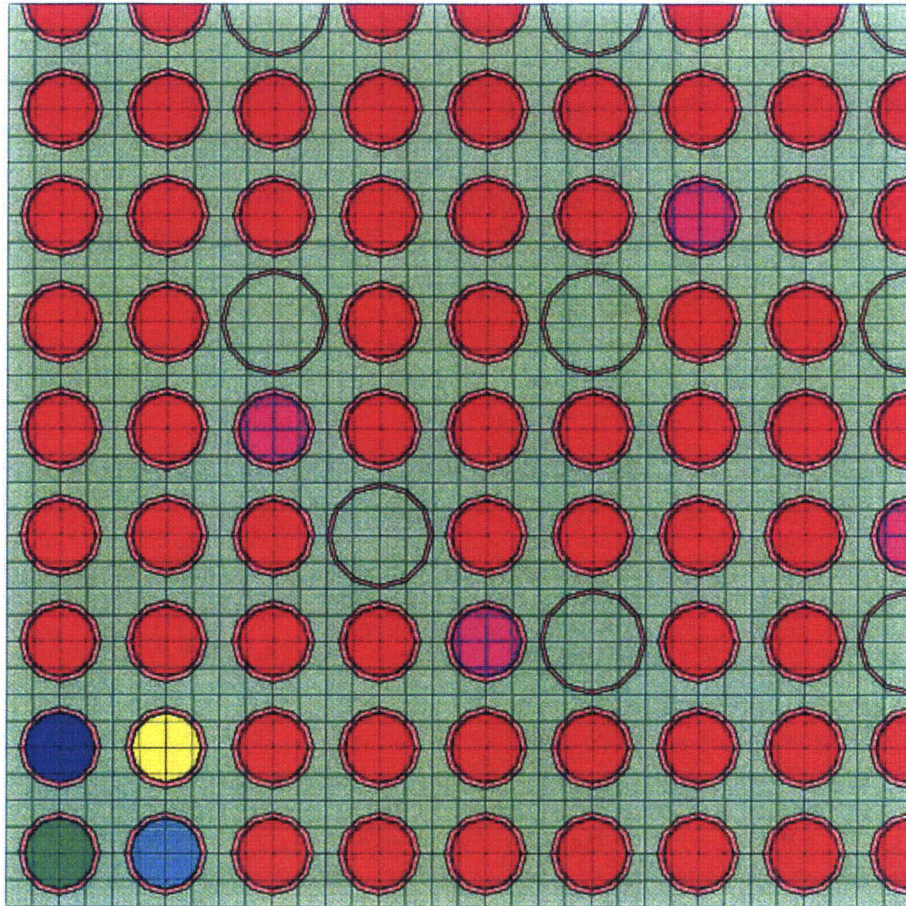


Figure 5.4 TRITON assembly model for Calvert Cliffs samples

## 5.4 TAKAHAMA-3 SAMPLES

Fuel rod SF97, residing in assembly NT3G24, was simulated using a one-half assembly geometry model because the rod was located on a quarter-assembly symmetry axis. The models for fuel rods SF95 and SF96 from assembly NT3G23 used a one-quarter assembly model. The three models used for each rod are illustrated in Figures 5.5 to 5.7. In each model, the measured fuel rod, as well as the fuel rods adjacent to it, was individually depleted. The variation of the soluble boron in the moderator as given in Table 4.12, and the variation in moderator density and temperature provided in Table 4.10 were simulated through the use of the TIMETABLE input block in the TRITON input. Note that fuel rods SF95 and SF97 are located on the edge of the assembly and therefore possibly subjected to edge effects. However, as no information was available on the surrounding assemblies, these assemblies were not included in the model.

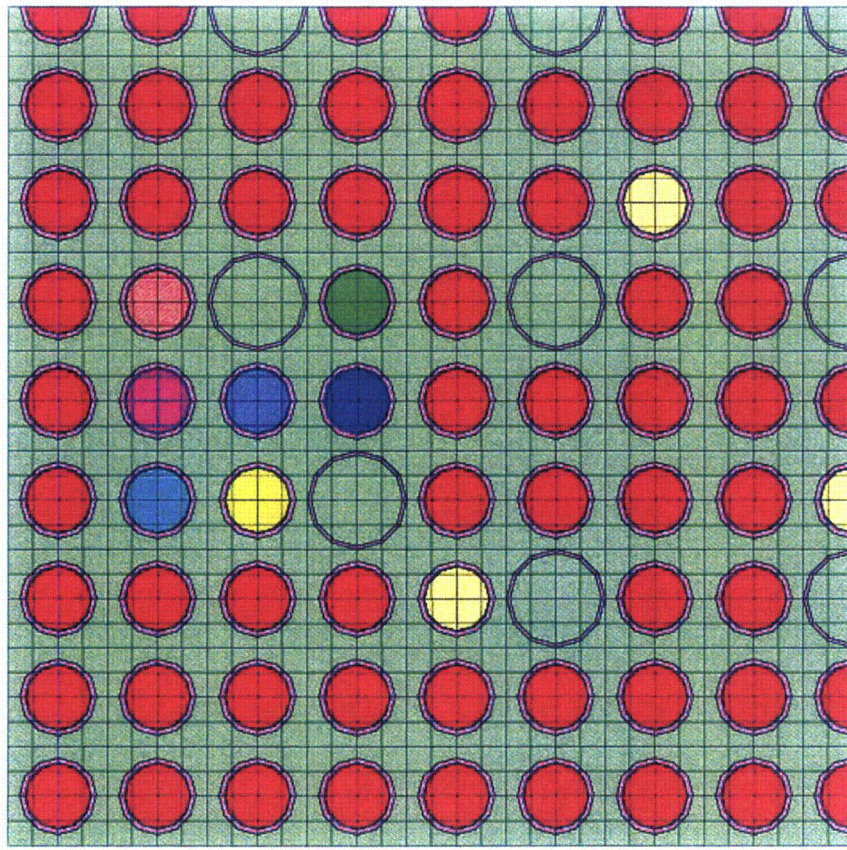
The cycle power data given in Table 4.10 was used for simulating the depletion for fuel samples SF95 and SF97, as these values yielded predicted  $^{148}\text{Nd}$  concentrations that were in agreement with the measurements, within the experimental uncertainty. However, in the case of the samples from rod SF96, the simulation using the sample power (and burnup) in Table 4.10 yielded a calculated  $^{148}\text{Nd}$  concentration that was with 4 to 10% less than the measured value, depending on the sample. This difference is much larger than the maximum 3% error in burnup specified in the JAERI report.<sup>17</sup> The sample burnup determination by JAERI was made using the ASTM E 321-79 standard method that estimates the burnup (in GWd/MTU units) by multiplying the value of the burnup rate (%FIMA = Fission per Initial Metal Atom in percent value that is based on the measured  $^{148}\text{Nd}$  content) by a factor of  $9.6 \pm 0.3$ .<sup>20</sup> However, derivation of this factor is based on a recoverable energy per fission (MeV/fission) value obtained for a system that is near critical (i.e., the number of fissions is equal to the number of non-fission absorptions). While this assumption is valid for a large-scale reactor system, it may not apply on a local level. For the case of a gadolinia-bearing rod or other poison rod the absorption rate may significantly exceed the fission rate. The capture reactions in gadolinium contribute prompt capture gamma-ray energy to the system that is not accounted for in the ASTM method, but may be accounted for in modern depletion computer codes (such as ORIGEN-S). The applicability of simplified methods for burnup determination needs to be carefully considered, particularly when applied to nonstandard type fuel. The cycle power values listed in Table 4.10 for rod SF96 were therefore increased to account for the discrepancy in burnup.



■ regular fuel pin   
 ■ measured fuel pin   
 ■ ■ ■ neighbors of measured fuel pin  
■ gadolinia fuel pin   
 ■ moderator

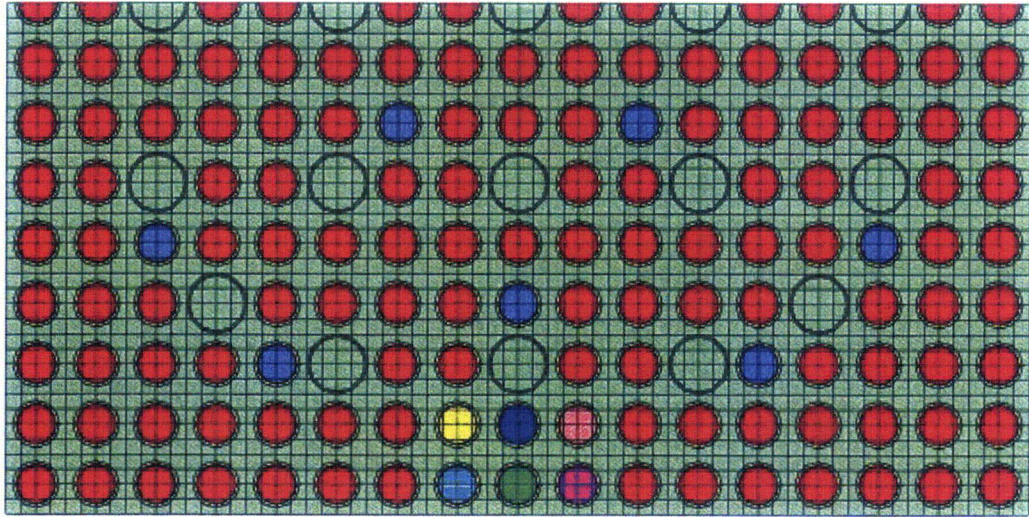
**Figure 5.5 TRITON assembly model for Takahama-3 SF95 samples**





- regular fuel pin
- measured fuel pin
- neighbors of measured fuel pin
- gadolinia fuel pin
- moderator

**Figure 5.6 TRITON assembly model for Takahama-3 SF96 samples**



■ regular fuel pin   
 ■ measured fuel pin   
 ■ gadolinia fuel pin   
 ■ neighbors of measured fuel pin   
 ■ neighbors of measured fuel pin   
 ■ moderator

**Figure 5.7 TRITON assembly model for Takahama-3 SF97 samples**

## 6 RESULTS

### 6.1 TMI-1 SAMPLES

Results of the simulation analysis for the TMI-1 samples from assembly NJ070G that were measured at GE-VNC are illustrated in Figures 6.1-6.4; results for the samples from assembly NJ05YU that were measured at ANL are shown in Figures 6.5-6.8. Tables 6.1 and 6.2 list the calculated-to-experimental (C/E) ratio in percentage and the corresponding average, maximum, and minimum difference, for each of the measured nuclides. The results for samples in assembly NJ070G as shown in Table 6.1 correspond to the computational models illustrated in Figures 5.2 and 5.3. The sensitivity of the results to the level of details used in the computational model is discussed in Appendix A.

The calculations for the samples from assembly NJ070G show an average overestimation of the main actinides  $^{235}\text{U}$  and  $^{239}\text{Pu}$  by 3.5% and 2.0%, respectively. In the case of the minor actinides, the calculated values are on average within 30% of the experimental values. Some of the largest errors in plutonium nuclides and minor actinides are seen for the samples from corner rod O1. A good agreement is observed for neodymium nuclides, with average overestimations of less than 2% for all measured isotopes except for  $^{143}\text{Nd}$ , for which it is 2.5%.

The results for the samples from assembly NJ05YU show a larger overestimation for  $^{235}\text{U}$  and  $^{239}\text{Pu}$ , of 4.7% and 14.9% on average, respectively. The average overestimation in the case of the neodymium isotopes is 0.5%, 4.5% and 8.2% for  $^{148}\text{Nd}$ ,  $^{145}\text{Nd}$ , and  $^{143}\text{Nd}$ , respectively. The average deviation for the minor actinides is less than 30%, but the spread of the values around the mean is quite large.

In addressing the significance of the comparison between the calculated and the experimental results one should take into consideration the magnitude of the measurement uncertainties. In the case of the samples from assembly NJ05YU measured at ANL, the reported experimental uncertainties are relatively large (see Table 3.1). The total measurement uncertainties (RSD) are between about 4% and 6% for uranium nuclides and in the 5% to 8% range for plutonium nuclides. As reported for the other measured fission products, relatively large experimental errors were seen for neodymium nuclides, in the 5% to 7% range. The total measurement uncertainty for  $^{148}\text{Nd}$ , used to estimate the sample burnup, is very large. The large uncertainty in the burnup value used for calculations will consequently propagate into additional uncertainty in calculated nuclide concentrations and comparisons with measurements.

As previously mentioned, assemblies NJ070G and NJ05YU were removed from the core at the end of cycle 10 to investigate fuel failures that occurred during that cycle. As a result, the fuel condition may not be well known. As the large deviations between calculation and measurement observed for samples from assembly NJ05YU were not observed for samples from assembly NJ070G, the large differences may be related more to the measurement methods and accuracies than to the unknown fuel condition due to fuel failure.

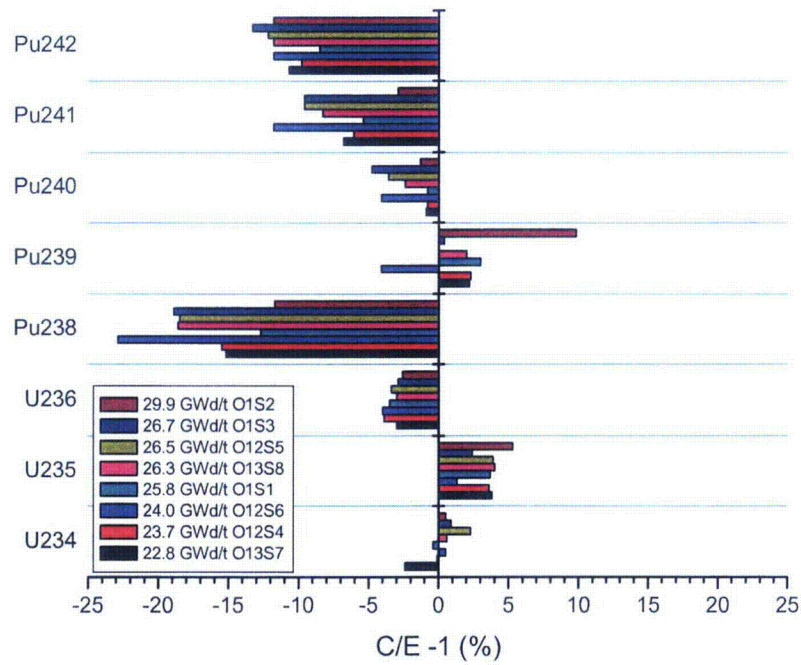


Figure 6.1 TMI-1 samples from assembly NJ070G—major actinides

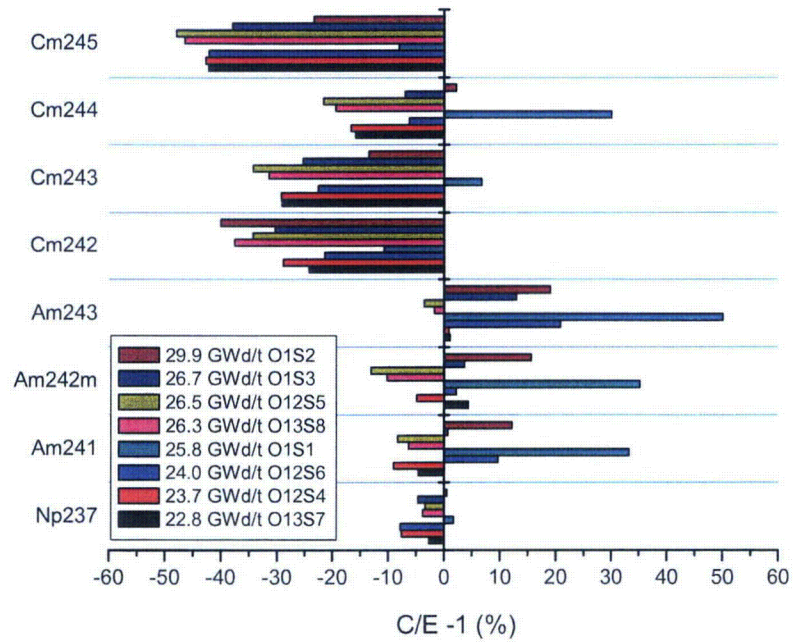


Figure 6.2 TMI-1 samples from assembly NJ070G—minor actinides

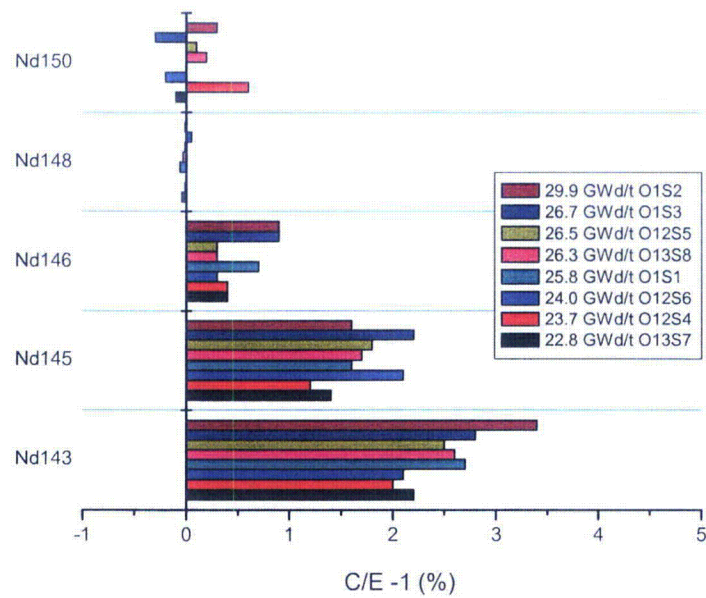


Figure 6.3 TMI-1 samples from assembly NJ070G—fission products (Nd)

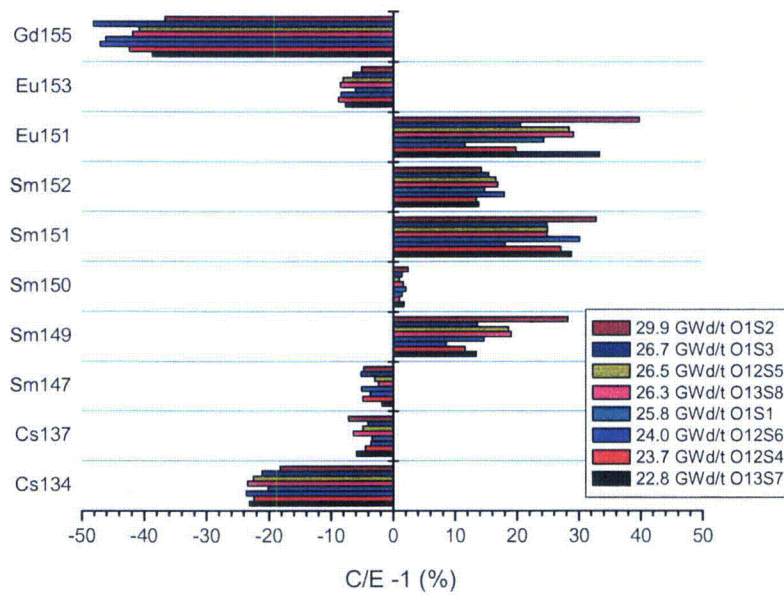


Figure 6.4 TMI-1 samples from assembly NJ070G—fission products (Cs, Sm, Eu, Gd)

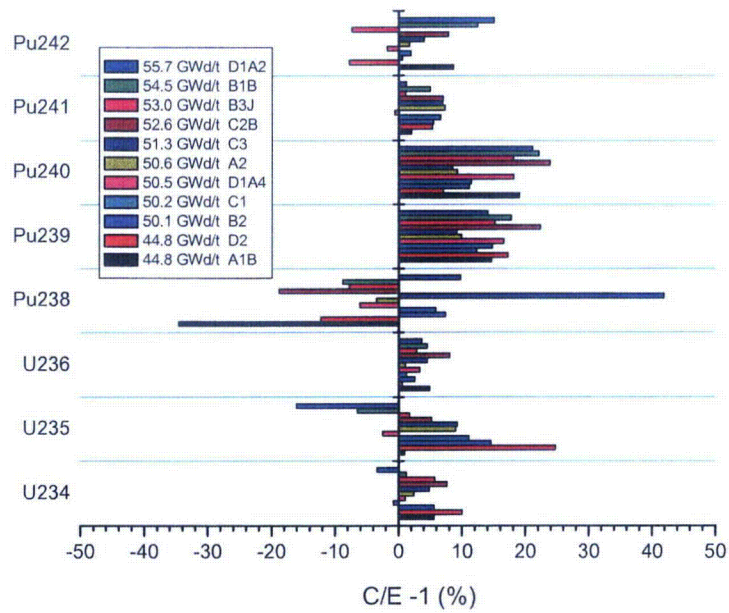


Figure 6.5 TMI-1 samples from assembly NJ05YU—major actinides

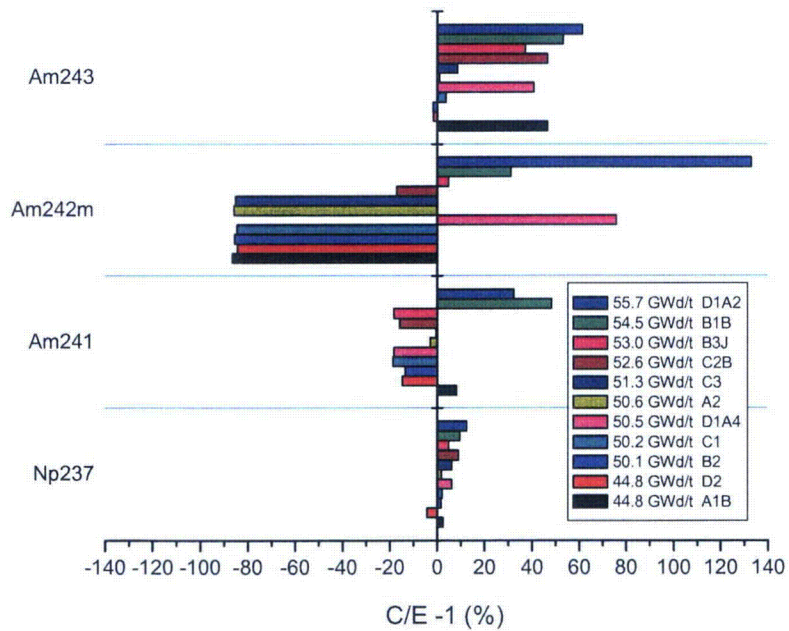


Figure 6.6 TMI-1 samples from assembly NJ05YU—minor actinides

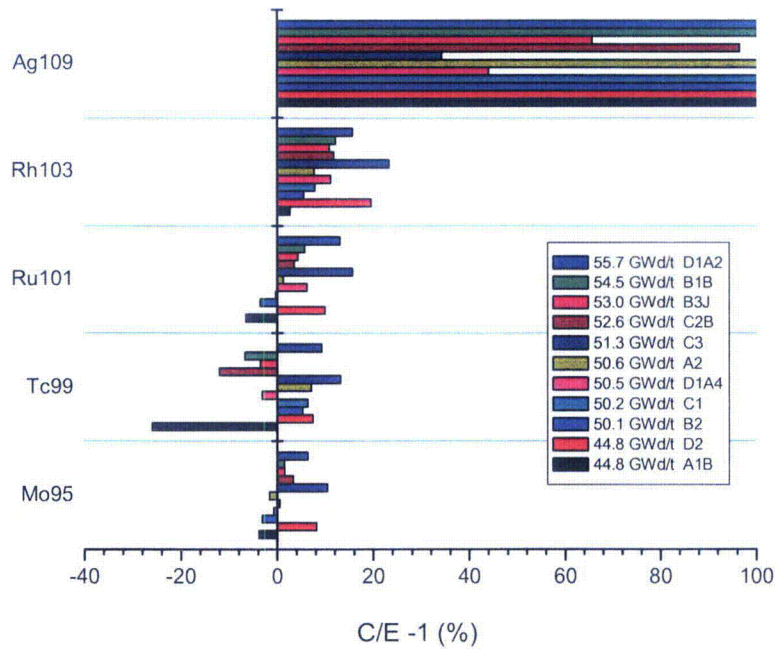


Figure 6.7 TMI-1 samples from assembly NJ05YU—fission products (metallics)

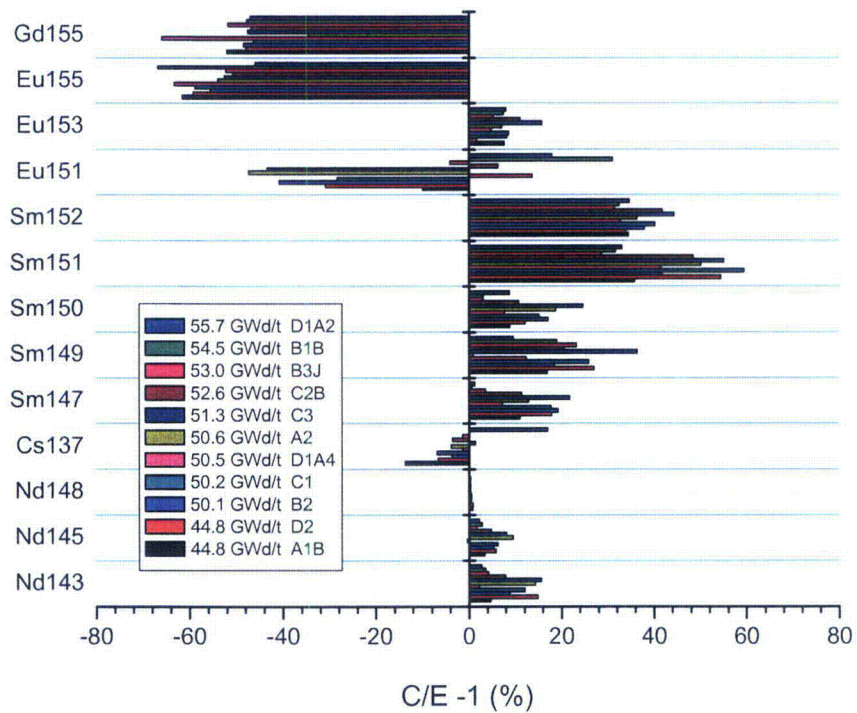


Figure 6.8 TMI-1 samples from assembly NJ05YU—fission products (Nd, Cs, Sm, Eu, Gd)

Table 6.1 C/E-1 (%) for TMI-1 samples from assembly NJ070G

Sample ID	O13S7	O12S4	O12S6	O1S1	O13S8	O12S5	O1S3	O1S2			
Burnup <sup>a</sup> (GWd/MTU)	22.8	23.7	24.0	25.8	26.3	26.5	26.7	29.9			
									Avg	Max	Min
U-234	-2.4	-0.1	0.5	-0.4	0.6	2.3	0.9	0.5	0.2	2.3	-2.4
U-235	3.8	3.6	1.3	3.7	4.0	3.9	2.4	5.3	3.5	5.3	1.3
U-236	-3.0	-3.9	-4.0	-3.5	-3.0	-3.4	-2.9	-2.6	-3.3	-2.6	-4.0
Pu-238	-15.2	-15.5	-22.9	-12.7	-18.6	-18.5	-18.9	-11.7	-16.8	-11.7	-22.9
Pu-239	2.2	2.3	-4.1	3.0	2.0	0.0	0.4	9.8	2.0	9.8	-4.1
Pu-240	-0.9	-0.8	-4.1	-0.8	-2.4	-3.6	-4.8	-1.3	-2.3	-0.8	-4.8
Pu-241	-6.8	-6.1	-11.8	-5.4	-8.3	-9.6	-9.6	-2.9	-7.6	-2.9	-11.8
Pu-242	-10.7	-9.8	-11.8	-8.5	-11.8	-12.2	-13.3	-11.8	-11.2	-8.5	-13.3
Np-237	-2.7	-7.6	-7.8	1.7	-3.8	-3.4	-4.7	0.5	-3.5	1.7	-7.8
Am-241	-4.6	-9.0	9.7	33.2	-6.3	-8.3	0.7	12.2	3.5	33.2	-9.0
Am-242m	4.4	-4.9	2.2	35.2	-10.2	-13.1	3.7	15.7	4.1	35.2	-13.1
Am-243	1.1	0.9	20.9	50.1	-1.7	-3.6	13.0	19.1	12.5	50.1	-3.6
Cm-242	-24.2	-28.9	-21.4	-10.7	-37.5	-34.2	-30.3	-40.0	-28.4	-10.7	-40.0
Cm-243	-29.1	-29.2	-22.5	6.8	-31.4	-34.2	-25.3	-13.5	-22.3	6.8	-34.2
Cm-244	-15.9	-16.7	-6.2	30.1	-19.4	-21.6	-7.0	2.2	-6.8	30.1	-21.6
Cm-245	-42.2	-42.7	-42.1	-8.1	-46.4	-47.9	-37.9	-23.3	-36.3	-8.1	-47.9
Nd-143	2.2	2.0	2.1	2.7	2.6	2.5	2.8	3.4	2.5	3.4	2.0
Nd-145	1.4	1.2	2.1	1.6	1.7	1.8	2.2	1.6	1.7	2.2	1.2
Nd-146	0.4	0.4	0.3	0.7	0.3	0.3	0.9	0.9	0.5	0.9	0.3
Nd-148	0.0	0.0	0.0	-0.1	0.0	0.0	0.0	0.0	0.0	0.0	-0.1
Nd-150	-0.1	0.6	-0.2	0.0	0.2	0.1	-0.3	0.3	0.1	0.6	-0.3
Cs-134	-23.1	-22.4	-23.6	-20.1	-23.4	-22.5	-21.1	-18.2	-21.8	-18.2	-23.6
Cs-137	-5.9	-4.5	-3.6	-3.4	-6.4	-4.9	-4.1	-7.2	-5.0	-3.4	-7.2
Sm-147	-1.8	-4.9	-3.7	-5.1	-2.4	-3.0	-5.2	-4.7	-3.9	-1.8	-5.2
Sm-149	13.4	11.6	8.5	14.6	19.0	18.6	13.6	28.2	15.9	28.2	8.5
Sm-150	1.7	1.0	1.4	2.0	1.6	1.0	1.4	2.4	1.6	2.4	1.0
Sm-151	28.8	27.1	18.0	30.1	24.8	24.9	24.8	32.8	26.4	32.8	18.0
Sm-152	13.8	13.4	17.9	14.7	16.9	16.6	15.4	14.2	15.4	17.9	13.4
Eu-151	33.3	19.8	11.6	24.3	29.1	28.4	20.5	39.8	25.9	39.8	11.6
Eu-153	-7.7	-8.8	-8.4	-6.1	-8.5	-8.1	-6.5	-5.1	-7.4	-5.1	-8.8
Gd-155	-38.7	-42.4	-47.1	-46.2	-41.9	-40.9	-48.2	-36.7	-42.8	-36.7	-48.2

<sup>a</sup> As reported in J. M. Scaglione, *Three Mile Island Unit 1 Radiochemical Assay Comparisons to SAS2H Calculations*, Yucca Mountain Project Report, CAL-UDC-NU-000011, Rev. A (April 2002).



Table 6.2 C/E-1 (%) for TMI-1 samples from assembly NJ05YU

Sample ID	A1B	D2	B2	C1	D1A4	A2	C3	C2B	B3J	B1B	D1A2			
Burnup <sup>a</sup> (GWd/MTU)	44.8	44.8	50.1	50.2	50.5	50.6	51.3	52.6	53.0	54.5	55.7			
												Avg	Max	Min
U-234	5.6	10.0	5.6	-0.8	1.0	2.4	4.8	7.6	5.7	1.2	-3.4	3.6	10.0	-3.4
U-235	0.9	24.7	14.5	11.0	-2.5	9.0	9.2	5.2	1.7	-6.5	-16.1	4.7	24.7	-16.1
U-236	4.9	0.5	2.5	1.2	3.3	1.0	4.5	8.0	2.8	4.5	3.6	3.4	8.0	0.5
Pu-238	-34.6	-12.3	7.4	5.8	-6.1	-3.5	41.9	-18.8	-7.8	-8.8	9.7	-2.5	41.9	-34.6
Pu-239	14.6	17.2	12.3	14.7	16.5	9.9	9.1	22.3	15.1	17.7	14.0	14.9	22.3	9.1
Pu-240	19.0	7.0	11.1	11.4	18.1	9.2	8.5	23.9	18.0	22.1	21.1	15.4	23.9	7.0
Pu-241	2.0	5.3	5.5	6.6	-0.6	7.3	6.9	7.0	1.1	5.0	1.2	4.3	7.3	-0.6
Pu-242	8.6	-7.8	0.6	1.9	-1.8	1.7	4.0	7.8	-7.4	12.4	15.0	3.2	15.0	-7.8
Np-237	2.5	-4.3	1.7	2.0	6.2	1.8	6.1	9.0	4.8	9.6	12.5	4.7	12.5	-4.3
Am-241	8.2	-14.8	-13.6	-18.7	-18.3	-3.0	-0.5	-15.9	-18.4	48.4	32.4	-1.3	48.4	-18.7
Am-242m	-86.3	-84.2	-85.4	-84.4	75.8	-85.7	-85.1	-17.1	4.7	31.0	133.0	-25.8	133.0	-86.3
Am-243	46.6	-1.7	-1.8	3.7	40.7	1.0	8.6	46.6	37.1	53.2	61.4	26.9	61.4	-1.8
Nd-143	4.6	14.9	8.8	12.0	2.2	14.3	15.6	7.9	4.2	3.5	2.7	8.2	15.6	2.2
Nd-145	3.4	5.8	5.3	6.2	-0.4	9.5	8.1	4.8	1.6	2.8	2.2	4.5	9.5	-0.4
Nd-148	0.8	0.9	0.4	0.5	0.5	0.3	0.3	0.3	0.2	0.3	-0.1	0.4	0.9	-0.1
Cs-137	-13.7	-6.7	-3.7	-6.9	-1.3	-3.8	1.3	-3.6	-1.3	0.1	17.0	-2.1	17.0	-13.7
Sm-147	11.0	17.8	19.2	17.7	7.2	12.8	21.7	11.4	3.5	0.6	1.2	11.3	21.7	0.6
Sm-149	16.9	27.0	18.5	25.8	12.3	0.9	36.3	20.6	23.2	18.9	9.5	19.1	36.3	0.9
Sm-150	8.8	12.1	17.1	15.1	7.6	18.7	24.6	10.7	3.0	3.0	8.7	11.8	24.6	3.0
Sm-151	35.8	54.4	41.7	59.4	41.5	50.1	55.0	48.5	28.6	31.6	33.0	43.6	59.4	28.6
Sm-152	34.5	33.8	37.9	40.2	32.7	36.3	44.3	41.8	31.4	32.5	34.7	36.4	44.3	31.4
Eu-151	1.5	-30.8	-40.8	-28.2	13.7	-47.3	-43.3	6.3	-4.0	31.0	17.9	-11.3	31.0	-47.3
Eu-153	7.6	1.7	8.2	8.6	4.8	7.1	15.8	11.1	5.3	7.5	8.0	7.8	15.8	1.7
Eu-155	-61.5	-59.2	-55.5	-58.8	-63.2	-53.9	-52.5	-50.7	-52.2	-66.7	-45.9	-56.4	-45.9	-66.7

**Table 6.2 C/E-1 (%) for TMI-1 samples from assembly NJ05YU (continued)**

Sample ID	A1B	D2	B2	C1	D1A4	A2	C3	C2B	B3J	B1B	D1A2			
<b>Burnup<sup>a</sup> (GWd/MTU)</b>	<b>33.8</b>	<b>44.8</b>	<b>50.1</b>	<b>50.2</b>	<b>50.5</b>	<b>50.6</b>	<b>51.3</b>	<b>52.6</b>	<b>53.0</b>	<b>54.5</b>	<b>55.7</b>			
Gd-155	-52.0	-47.9	-48.4	-46.3	-65.9	-34.5	-47.5	-46.8	-51.8	-47.7	-46.9	Avg -48.7	Max -34.5	Min -65.9
Mo-95	-3.9	8.2	-3.2	-0.8	0.5	-1.6	10.4	3.3	1.5	1.4	6.3	2.0	10.4	-3.9
Tc-99	-26.0	7.4	5.3	6.3	-3.2	7.1	13.1	-12.1	-3.5	-6.7	9.2	-0.3	13.1	-26.0
Ru-101	-6.5	9.9	-3.6	-0.4	6.1	1.2	15.6	3.5	4.3	5.7	13.0	4.4	15.6	-6.5
Rh-103	2.6	19.5	5.5	7.8	11.1	7.7	23.2	11.8	10.8	12.1	15.6	11.6	23.2	2.6
Ag-109	100.7	123.4	127.2	125.3	44.0	103.2	34.2	96.5	65.6	205.4	200.1	111.4	205.4	34.2

<sup>a</sup> As reported in J. M. Scaglione, *Three Mile Island Unit 1 Radiochemical Assay Comparisons to SAS2H Calculations*, Yucca Mountain Project Report, CAL-UDC-NU-000011, Rev. A (April 2002).

## 6.2 CALVERT CLIFFS SAMPLES

TRITON depletion simulations were carried out for each sample by slightly adjusting, by about 1%, the power (burnup) data, as given in Table 4.7, in order to obtain a calculated  $^{148}\text{Nd}$  concentration in agreement with the measured value. Calculated results are illustrated in Figures 6.9-6.11 and listed in Table 6.3. The measured results that were used for comparison to calculation are those provided in Table 3.14.

Figure 6.9 shows good agreement between calculation and measurement for actinides. Computed concentrations for all uranium and plutonium nuclides, except for  $^{238}\text{Pu}$ , are within 6% of the measured values. The  $^{238}\text{Pu}$  and  $^{241}\text{Am}$  nuclides, both important contributors for decay heat applications, are each underestimated by about 8% on average. As observed in Figure 6.10, all cesium isotopes (except  $^{134}\text{Cs}$ ) are predicted within about 6% of the experimental values;  $^{133}\text{Cs}$  and  $^{137}\text{Cs}$  are predicted to within 1.9% and 0.7%, respectively, on average. The nuclide  $^{134}\text{Cs}$  is underestimated by about 14% on average; this underprediction is consistent with results of previous analyses with SCALE.<sup>15</sup> Very good predictions were obtained for neodymium: all neodymium isotopes except for  $^{150}\text{Nd}$  were estimated on average within about 1% of the experimental values. The comparison for other measured fission products is illustrated in Figure 6.11. As seen,  $^{90}\text{Sr}$  and  $^{99}\text{Tc}$ , important in decay heat and burnup credit applications, respectively, are well predicted, being overestimated by 2% and 9% on average.

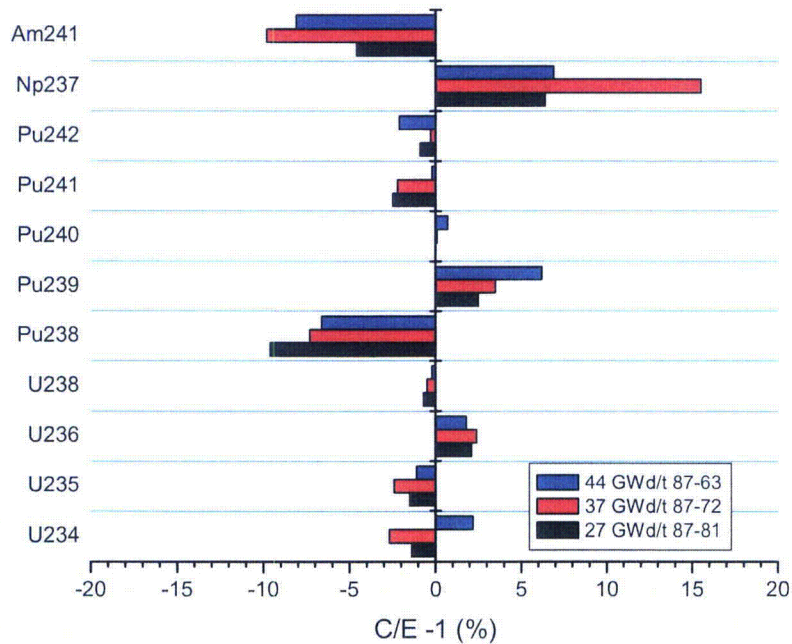


Figure 6.9 Calvert Cliffs samples—actinides

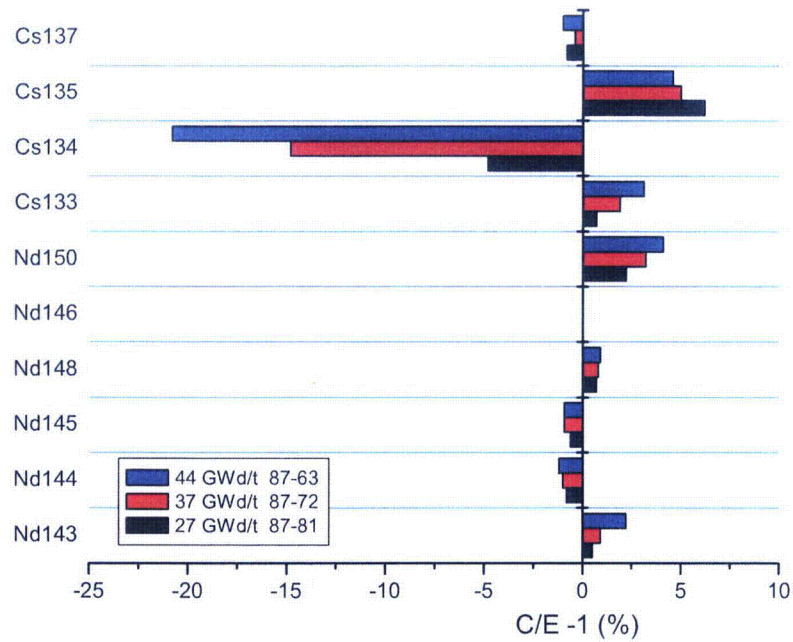


Figure 6.10 Calvert Cliffs samples—fission products (Nd, Cs)

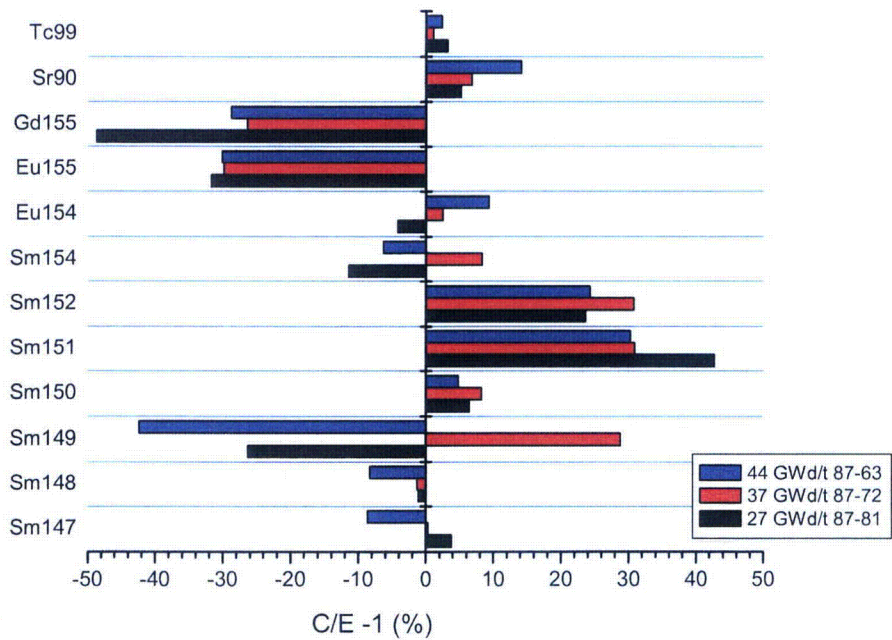


Figure 6.11 Calvert Cliffs samples—fission products (Sm, Eu, Gd, Sr, Tc)

Table 6.3 C/E-1 (%) for Calvert Cliffs samples

Sample ID	87-81	87-72	87-63			
Burnup <sup>a</sup> (GWd/MTU)	27.35	37.12	44.34	Avg <sup>b</sup>	Max <sup>b</sup>	Min <sup>b</sup>
U-234	-1.4	-2.7	2.2	-0.6	2.2	-2.7
U-235	-1.5	-2.4	-1.1	-1.7	-1.1	-2.4
U-236	2.1	2.4	1.8	2.1	2.4	1.8
U-238	-0.7	-0.5	-0.2	-0.4	-0.2	-0.7
Pu-238	-9.6	-7.3	-6.6	-7.8	-6.6	-9.6
Pu-239	2.5	3.5	6.2	4.1	6.2	2.5
Pu-240	0.0	0.1	0.7	0.3	0.7	0.0
Pu-241	-2.5	-2.2	-0.2	-1.6	-0.2	-2.5
Pu-242	-0.9	-0.3	-2.1	-1.1	-0.3	-2.1
Np-237	6.4	15.5	6.9	9.6	15.5	6.4
Am-241	-4.6	-9.8	-8.1	-7.5	-4.6	-9.8
Cs-133	0.7	1.9	3.1	1.9	3.1	0.7
Cs-134	-4.8	-14.8	-20.8	-13.5	-4.8	-20.8
Cs-135	6.2	5.0	4.6	5.3	6.2	4.6
Cs-137	-0.8	-0.4	-1.0	-0.7	-0.4	-1.0
Nd-143	0.5	0.9	2.2	1.2	2.2	0.5
Nd-144	-0.8	-1.0	-1.2	-1.0	-0.8	-1.2
Nd-145	-0.6	-0.9	-0.9	-0.8	-0.6	-0.9
Nd-146	0.7	0.8	0.9	0.8	0.9	0.7
Nd-148	0.0	0.0	0.0	0.0	0.0	0.0
Nd-150	2.2	3.2	4.1	3.2	4.1	2.2
Sm-147	3.8	0.3	-8.6	-1.5	3.8	-8.6
Sm-148	-1.1	-1.3	-8.3	-3.5	1.1	-8.3
Sm-149	-26.3	28.8	-42.4	-13.3	28.8	-42.4
Sm-150	6.4	8.2	4.8	6.5	8.2	4.8
Sm-151	42.7	30.9	30.3	34.6	42.7	30.3
Sm-152	23.61	30.8	24.3	26.2	30.8	23.6
Sm-154	-11.4	8.3	-6.3	-3.1	8.3	-11.4
Eu-151	-43.4	23.5	-57.4	-20.8	23.5	-57.4
Eu-152	-69.0	-48.4	-93.8	-70.4	-48.4	-93.8
Eu-153	3.2	3.0	3.4	3.2	3.6	3.0
Eu-154	-4.2	2.5	9.3	2.5	9.3	-4.2
Eu-155	-31.7	-29.9	-30.1	-30.6	-29.9	-31.7
Gd-154	-20.7	32.3	32.7	14.8	32.7	-20.7
Gd-155	-48.7	-26.4	-28.8	-34.6	-26.4	-48.7
Gd-156	-24.9	37.2	64.6	25.7	64.6	-24.9
Gd-158	-19.1	-99.4	-99.4	-72.6	-18.7	-99.4
Gd-160	-48.6					
Tc-99	5.2	6.8	14.1	8.7	14.1	5.2
Sr-90	3.2	1.1	2.4	2.2	3.2	1.1

<sup>a</sup> As provided in O. W. Herman, S. M. Bowman, M. C. Brady, and C. V. Parks, *Validation of the SCALE System for PWR Spent Fuel Isotopic Composition Analyses*, ORNL/TM-12667, Oak Ridge National Laboratory, Oak Ridge, Tennessee (March 1995).

<sup>b</sup> Shown only for isotopes measured in all three samples.

### 6.3 TAKAHAMA-3 SAMPLES

The results of the simulations are presented in Table 6.4 as calculated-to-experimental concentration ratios in percent and illustrated in Figures 6.12-6.19. The uranium isotopes are well predicted except for  $^{234}\text{U}$ , for which there is a large spread of the errors (see Figure 6.12); this could be attributed to possible uncertainties in the initial  $^{234}\text{U}$  concentration in the fuel. Predictions for  $^{235}\text{U}$  and  $^{236}\text{U}$  are on average within 2% and 1%, respectively, of the experimental values.

As seen from Figures 6.13 to 6.15, there is a systematically large overprediction of plutonium and some higher actinides (americium, curium) in the case of samples (SF97-1, SF96-1, and SF95-1) located near the end of the active fuel length as compared to samples not subjected to possible rod end effects. The three above-mentioned samples were cut from axial locations at 16.3 cm, 17.6 cm, and 20.1 cm, respectively, from the top of the rod, corresponding to about 4 mm, 17 mm, and 41 mm distance from the end of the active fuel length. Large deviations have also been observed in previous analyses of these samples with the HELIOS code.<sup>6</sup> The effect is most pronounced for samples SF97-1 and SF96-1, located at a shorter distance from the end of the active fuel region than SF95-1. For example, the overestimation of  $^{239}\text{Pu}$  is 32%, 22%, and 13% for samples SF97-1, SF96-1, and SF95-1, respectively. These values are very large as compared to the average overestimation corresponding to the other 14 samples, which is about 4%. All these three samples are located in a region of the fuel characterized by high leakage and large flux gradients. Although results for these samples are shown here, they would likely be excluded from code validation studies and uncertainty evaluation analyses that are usually carried out using a consistent set of experimental data typical of the average fuel behavior. However, analyses of these samples are valuable as they provide useful information on fuel characteristics for fuel regions in the proximity of the lower burnup assembly ends, regions of importance in burnup credit applications. A more appropriate representation of these samples would require a three-dimensional model; this is not possible with TRITON/NEWT, which is limited to 2-D geometry.

The results for the fission product group consisting of neodymium, cesium, cerium, and samarium isotopes as well as two metallic ruthenium and antimony nuclides of importance to burnup credit are illustrated in Figures 6.16 to 6.19. With the exception of  $^{142}\text{Nd}$ , which was measured only in the SF95 samples, the other neodymium nuclides (see Figure 6.16) are well predicted, with an average overestimation about 1% for  $^{145,146,148,150}\text{Nd}$  nuclides and an average underestimation of about 1% and 3% for  $^{143}\text{Nd}$  and  $^{144}\text{Nd}$ , respectively. Most of samarium nuclides (see Figure 6.19) are well predicted, within 5% on average, except for  $^{150}\text{Sm}$  and  $^{151}\text{Sm}$ , for which there is a systematic overestimation in the 30% range. Cesium isotopes (see Figure 6.17) are underestimated by about 10% and 3% in the case of  $^{134}\text{Cs}$  and  $^{137}\text{Cs}$ , respectively. The nuclides  $^{144}\text{Ce}$  and  $^{154}\text{Eu}$  are well predicted, within 1% and 4% of the measurement, on average. Note that the average deviations shown in Table 6.4 include the results corresponding to the gadolinia fuel rod SF96.

Table 6.4 C/E-1 (%) for Takahama-3 samples

Sample ID	SF95-1	SF95-2	SF95-3	SF95-4	SF95-5	SF97-1	SF97-2	SF97-3	SF97-4	SF97-5	SF97-6	SF96-1	SF96-2	SF96-3	SF96-4	SF96-5			
Burnup <sup>a</sup> (Gwd/MTU)	14.3	24.4	35.4	36.7	30.4	17.69	30.7	42.16	47.03	47.25	40.79	8.55	17.38	29.58	30.35	25.35			
																	Avg	Max	Min
U-234	9.4	-1.4	26.4	25.1	-8.2	6.4	9.6	6.8	-6.6	7.2	8.4	-7.6	-5.9	-7.6	-7.9	-6.9	3.8	26.4	-8.2
U-235	0.9	2.7	3.1	3.9	2.1	3.3	0.7	1.4	1.9	0.6	2.0	1.9	1.9	3.3	1.5	1.9	2.1	3.9	0.6
U-236	0.6	-1.7	-0.1	-0.3	-1.0	1.2	-0.2	-0.3	-0.4	-0.3	-0.7	-2.0	-1.6	-0.4	-0.8	-0.4	-0.5	1.2	-2.0
Pu-238	8.9	-3.7	4.9	4.4	2.0	31.7	-5.5	-7.6	-10.4	-12.6	-7.0	20.4	-1.4	-1.2	-6.8	1.1	1.1	31.7	-12.6
Pu-239	12.8	8.0	8.7	7.9	8.3	31.7	4.0	4.1	3.3	0.8	4.9	22.0	3.8	1.7	0.5	2.2	7.8	31.7	0.5
Pu-240	7.0	3.4	5.9	6.2	6.2	14.9	7.0	7.6	6.3	5.8	7.3	13.2	7.4	7.3	5.5	9.0	7.5	14.9	3.4
Pu-241	11.4	0.6	1.0	1.6	2.3	30.4	-2.6	-2.5	-3.0	-5.4	-1.4	26.4	1.9	1.2	-2.5	2.3	3.9	30.4	-5.4
Pu-242	13.6	0.0	-0.8	-0.1	3.1	23.3	1.0	-1.1	-2.4	-2.9	-0.8	21.9	5.6	3.9	0.7	7.9	4.6	23.3	-2.9
Np-237						24.5	1.8	3.8	1.2	-1.9	-0.6	36.5	45.1	65.9	58.5	52.6	26.1	65.9	-1.9
Am-241	-6.5	23.4	23.9	70.3	18.7	74.5	29.2	27.9	15.4	10.4	31.9	67.6	45.0	29.1	9.7	47.2	32.4	74.5	-6.5
Am-242m	22.5	17.5	17.3	19.7	22.5	111.4	25.8	18.0	6.7	1.7	18.9	31.0	9.0	23.5	2.6	10.8	22.4	111.4	1.7
Am-243	35.8	22.2	21.7	23.8	23.8	77.0	15.3	13.6	10.9	9.0	15.4	65.4	25.8	24.2	16.5	29.5	26.9	77.0	9.0
Cm-242	-16.0	-30.5	-37.5	-45.5	-18.1	19.6	-4.4	1.9	6.9	12.6	2.2	0.3	-18.6	-17.8	-22.8	-14.4	-11.4	19.6	-45.5
Cm-243	-6.3	-19.2	-10.5	-13.5	-20.9	29.9	-18.5	-17.4	-17.9	-20.6	-17.8						-12.1	29.9	-20.9
Cm-244	30.3	-0.3	8.1	5.8	13.0	86.6	-2.3	-4.0	-6.8	-9.3	-1.1	51.8	7.3	6.7	-0.9	13.1	12.4	86.6	-9.3
Cm-245	13.9	-21.5	-13.9	-19.7	-14.1	79.9	-28.4	-30.2	-33.1	-36.3	-26.2						-11.8	79.9	-36.3
Cm-246	-45.1	-66.1	-21.2	-23.8	25.0	48.2	-93.2	-34.0	-38.2	-40.7	-33.5						-29.3	48.2	-93.2
Cm-247							-31.5	-32.1	-35.9	-38.4	-36.0						-34.8	-31.5	-38.4
Nd-142	-19.0	-7.3	-15.3	-13.1	-5.4												-12.0	-5.4	-19.0
Nd-143	-2.0	-2.0	-1.9	-1.0	-1.4	0.4	0.2	0.2	0.7	-0.2	0.3	-4.2	-2.6	-1.9	-1.8	-3.0	-1.3	0.7	-4.2
Nd-144	0.0	-1.6	-1.0	-4.7	-1.2	3.3	1.4	-2.1	-3.9	-4.3	-2.3	-6.8	-6.0	-10.3	-8.0	-7.1	-3.4	3.3	-10.3
Nd-145	0.3	-0.3	-0.5	-0.1	0.2	0.4	1.3	0.9	1.1	1.1	0.8	-1.2	0.3	0.4	1.0	0.0	0.4	1.3	-1.2
Nd-146	2.8	1.8	1.7	1.6	2.3	2.4	1.5	0.8	0.7	0.6	1.0	-1.0	0.1	0.3	0.5	0.1	1.1	2.8	-1.0
Nd-148	1.0	-0.3	-0.5	-0.7	-0.1	1.7	0.9	0.2	0.0	0.0	0.4	-0.2	0.0	-0.1	-0.1	0.0	0.1	1.7	-0.7
Nd-150	-0.2	0.4	-0.4	-0.3	1.1	4.3	1.9	1.6	1.3	1.4	2.1	0.7	0.7	1.3	1.0	1.7	1.2	4.3	-0.4
Cs-134	-8.6	-13.9	-12.5	-12.7	-12.8	-5.4	-19.7	-17.6	-14.9	-15.4	-16.2	1.1	0.9	1.0	0.9	1.0	-9.1	1.1	-19.7
Cs-137	-1.6	-3.0	-2.3	-2.7	-1.6	-2.1	-2.3	-2.6	-1.8	-2.0	-2.6	5.2	-8.0	-4.8	-6.0	-3.9	-2.6	5.2	-8.0

**Table 6.4 C/E-1 (%) for Takahama-3 samples (continued)**

Sample ID	SF95-1	SF95-2	SF95-3	SF95-4	SF95-5	SF97-1	SF97-2	SF97-3	SF97-4	SF97-5	SF97-6	SF96-1	SF96-2	SF96-3	SF96-4	SF96-5			
Burnup <sup>a</sup> (GWd/ MTU)	14.3	24.4	35.4	36.7	30.4	17.69	30.7	42.16	47.03	47.25	40.79	8.55	17.38	29.58	30.35	25.35			
																	Avg	Max	Min
Ce-144	-2.1	-2.0	-5.0	4.2	-1.7	-17.7	-10.2	-2.7	6.0	6.7	-4.8	-0.3	5.1	15.5	15.4	7.9	0.9	15.5	-17.7
Eu-154	7.3	0.8	5.1	1.8	3.2	21.4	-2.7	1.3	1.9	0.3	2.4	5.0	-2.3	7.9	5.3	7.6	4.1	21.4	-2.7
Ru-106	2.8	20.5	29.2	30.4	12.5	-6.5	-4.7	-2.2	8.3	80.4	-15.0	27.5	53.0	36.3	50.5	12.7	21.0	80.4	-15.0
Sb-125	94.9	86.3	126.3	175.9	112.8	31.4	22.5	84.4	70.6	38.6	91.3	30.5	52.8	118.7	75.2	79.6	80.7	175.9	22.5
Sm-147						-2.3	0.6	-1.7	-2.9	-2.3	-0.9						-1.6	0.6	-2.9
Sm-148						17.8	-4.2	-9.6	-12.7	-13.6	-8.1						-5.1	17.8	-13.6
Sm-149						3.2	-8.5	-2.5	6.1	6.3	-3.0						0.3	6.3	-8.5
Sm-150						5.4	4.9	5.1	5.0	4.4	6.4						5.2	6.4	4.4
Sm-151						51.4	30.0	34.3	33.3	28.0	33.9						35.2	51.4	28.0
Sm-152						7.2	23.1	29.1	30.8	30.3	26.3						24.5	30.8	7.2
Sm-154						3.5	0.2	0.3	-0.2	-1.1	1.0						0.6	3.5	-1.1

<sup>a</sup> As stated in Y. Nakahara, Y. Suyama, and T. Suzuki, *Technical Development on Burnup Credit for Spent LWR Fuels*, JAERI-Tech 2000-071 (ORNL/TR-2001/01), English Translation, Oak Ridge National Laboratory, Oak Ridge, Tennessee (2002).



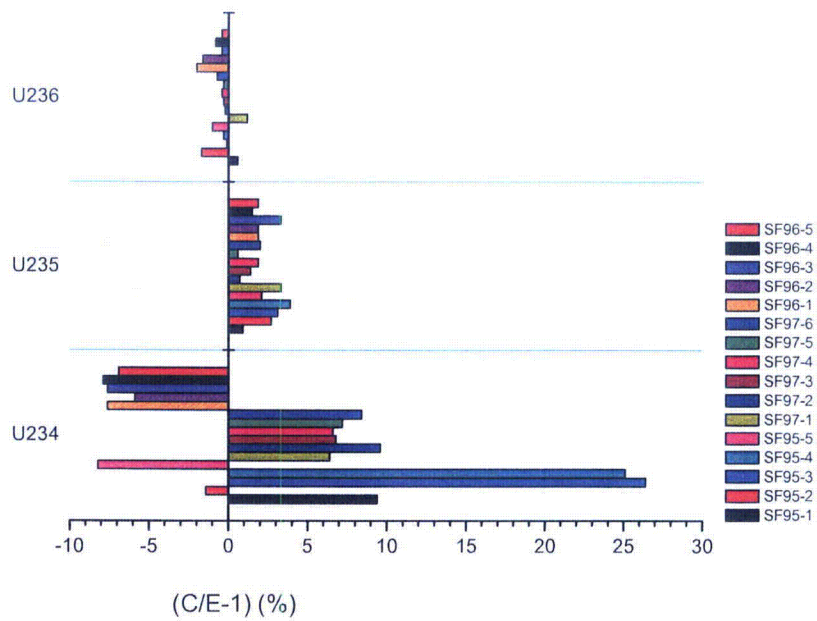


Figure 6.12 Takahama-3 samples—uranium nuclides

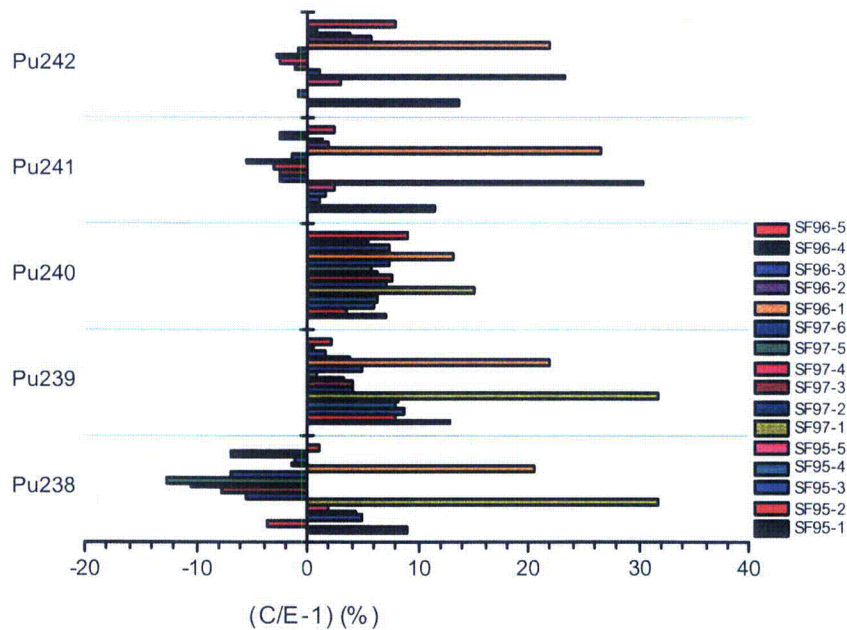


Figure 6.13 Takahama-3 samples—plutonium nuclides

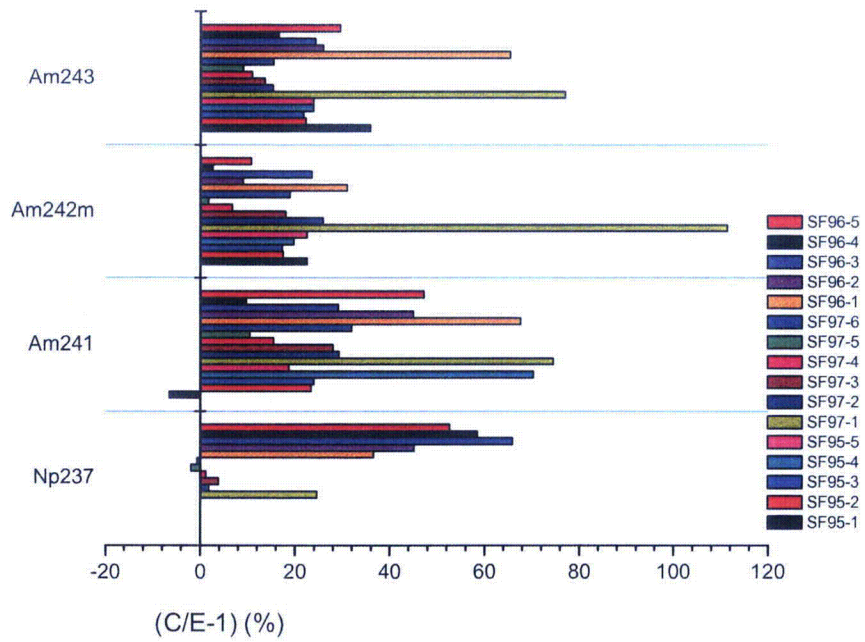


Figure 6.14 Takahama-3 samples—minor actinides (Np, Am)

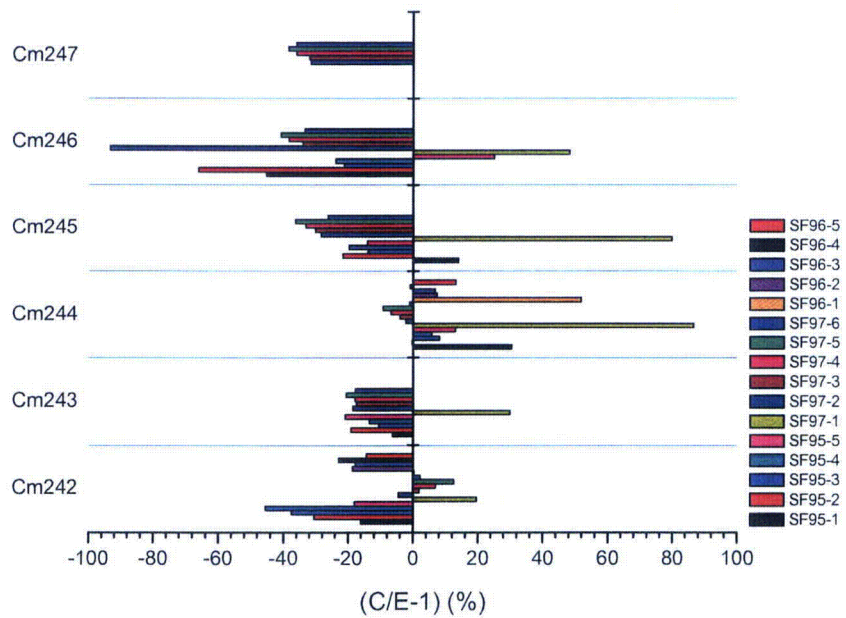


Figure 6.15 Takahama-3 samples—minor actinides (Cm)

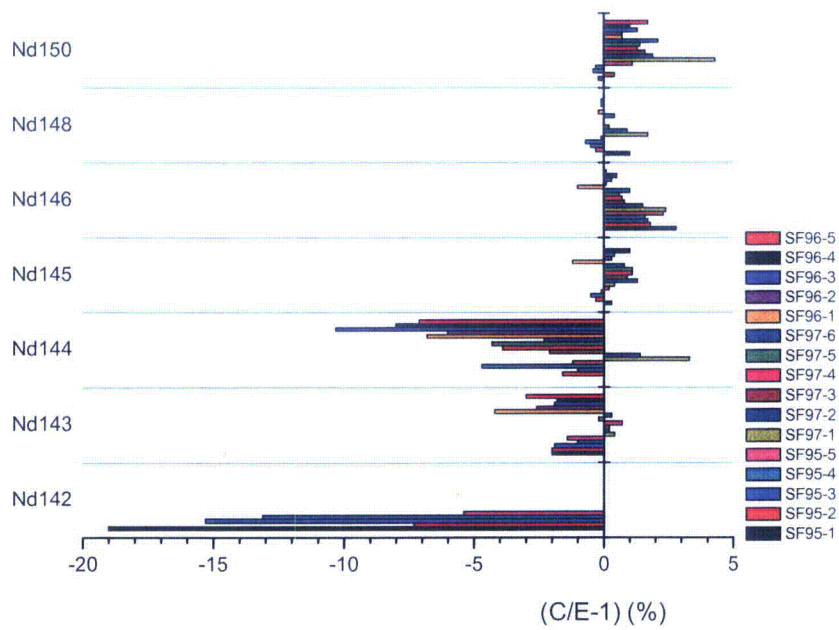


Figure 6.16 Takahama-3 samples—fission products (Nd)

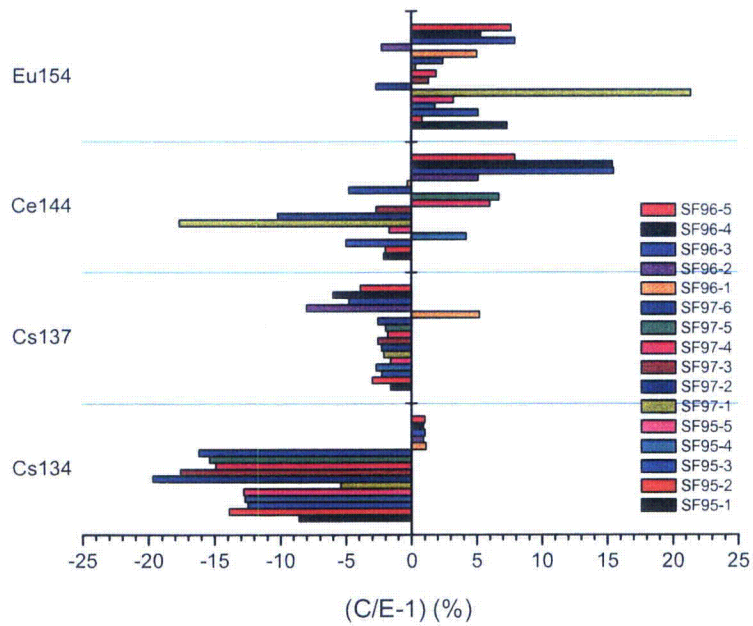


Figure 6.17 Takahama-3 samples—fission products (Cs, Ce, Eu)

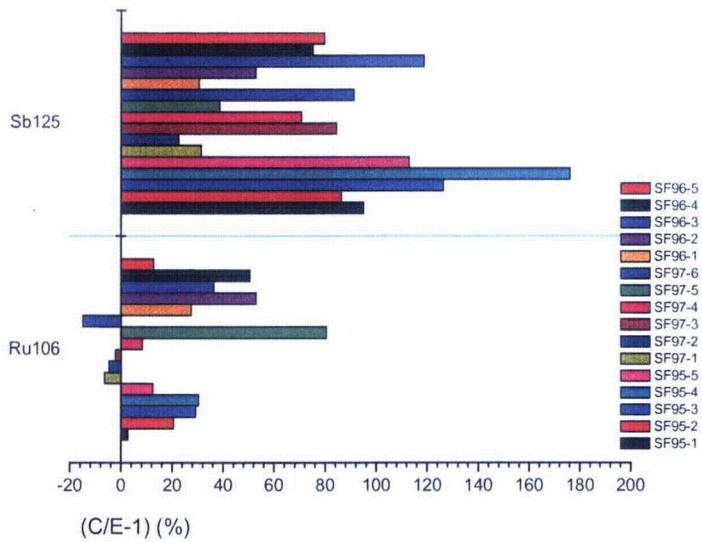


Figure 6.18 Takahama-3 samples—fission products (metallics)

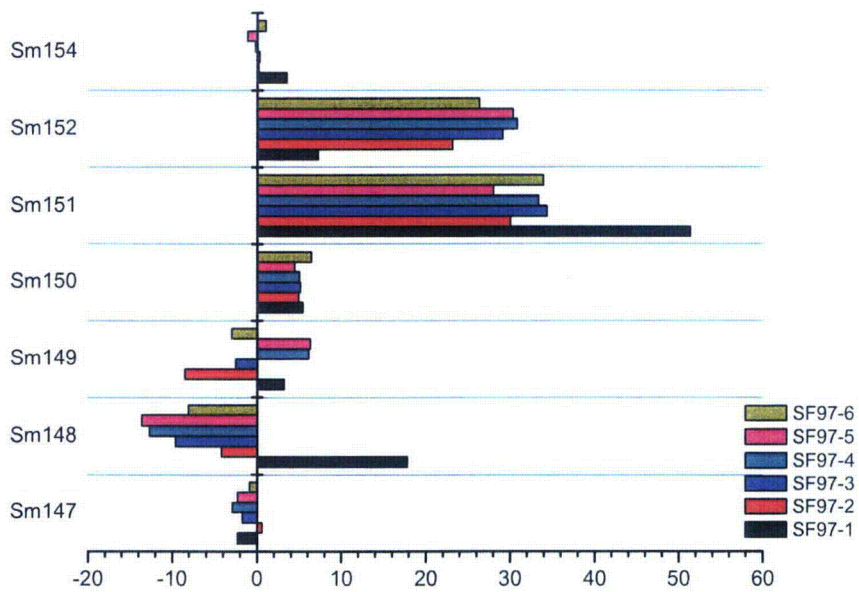


Figure 6.19 Takahama-3 samples—fission products (Sm)

## 7 SUMMARY

The purpose of the work described in this report was to evaluate available isotopic measurements involving high burnup fuel and to analyze the data using the ORNL SCALE computer code system. This information is needed to assess and quantify the uncertainties associated with the high burnup fuel characteristics of importance for spent fuel storage applications involving decay heat, radiation sources, criticality with burnup credit, and for reactor safety studies. Previously available experimental data for low- and medium-range burnup fuel was also considered so that the set of data used for uncertainty evaluations would cover a large burnup range, which would allow possible trends with high burnup to be evaluated.

The measurements analyzed in this report include 38 spent fuel samples from fuel irradiated in three PWRs operated in the United States and Japan. The samples cover a large burnup range, from 14 to 56 GWd/MTU, and an initial fuel enrichment domain from 2.6 to 4.7 wt %  $^{235}\text{U}$ . Twenty-two of the 38 samples considered are of domestic origin (TMI-1 and Calvert Cliffs-1 reactors) and 16 are from experiments carried out in Japan (Takahama-3 reactor). Information is presented on the fuel assembly geometry, irradiation history, and sample burnup. This information is necessary for developing a computational model to simulate the irradiation and decay of the samples under consideration. The data are presented in sufficient detail to allow an independent analysis to be performed.

The analysis of the measurements in this report was carried out by employing the two-dimensional depletion sequence of the TRITON module in the SCALE computer code system. Individual TRITON models were developed for each of the samples considered, including as many geometry and irradiation history details as available. The results of the simulations reported here were obtained using the fuel sample burnup that reproduced, within the experimental uncertainty margins, the measured concentration of the fission product burnup indicator  $^{148}\text{Nd}$ .

Some of the key modeling issues in isotopic assay data analysis are discussed in Appendix A in relation to the analysis of TMI-1 samples. The effect on predicted nuclide concentrations of modeling details, such as information on nearest assemblies (enrichment, burnup) or poison rod location was assessed and shown to be significant for samples selected from edge rods.



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**APPENDIX A**

**EFFECT OF MODELING DETAILS ON PREDICTED NUCLIDES  
FOR TMI-1 SAMPLES**



## A.1 Assembly NJ05YU

The transport calculation for a fuel assembly in TRITON usually assumes a reflective boundary condition, given the unavailability in most cases of detailed information on the assembly surroundings. This is expected to be a reasonable approximation for assemblies located in a generally uniform core and to not significantly influence the depletion of fuel rods located far from the assembly edge. As the H6 fuel rod, from which the samples were selected, was located toward the center of the assembly, and therefore far from the assembly edge, a more accurate representation of the assembly environment (i.e., more rigorous boundary condition) is expected to have less influence on the flux in the samples under consideration. However, the magnitude of the effect would depend on the characteristics (burnup, fuel enrichment, etc.) of the assemblies surrounding the NJ05YU assembly. The effect of using a more rigorous boundary condition in the depletion simulation on the predicted nuclide concentrations for this type of assembly is analyzed in this Appendix.

Data were available from Ref. 18 on the assemblies surrounding assembly NJ05YU during cycles 9 and 10, as illustrated in Figures A.1 and A.2, respectively. During cycle 9, all the first-order neighboring assemblies (at N, S, E and W locations) were from batch 10B with an initial fuel enrichment of 3.63%; these assemblies were irradiated since cycle 8 and did not contain BPRs or gadolinia fuel rods. The assembly located at the NW position was also from batch 10B; whereas, the assembly at the NE position was from batch 11B and had BPRs with a load of 1.1 wt % B<sub>4</sub>C. Assemblies at SW and SE were from batch 11C and had BPRs with 2.1 wt % B<sub>4</sub>C. The burnup of the assemblies from batch 10B at the beginning of cycle 9 was not known. As shown in Figure A.2, the arrangement of the assemblies surrounding NJ05YU is symmetric. During cycle 10, the first-order neighbors of NJ05YU at N, S, E, and W were fresh fuel assemblies with 4.65 wt % <sup>235</sup>U initial enrichment and containing BPRs with 2.1% B<sub>4</sub>C load. The assemblies located at NW, NE, SW, and SE were all from batch 11, with 4.0 wt % <sup>235</sup>U initial enrichment and no BPRs present.

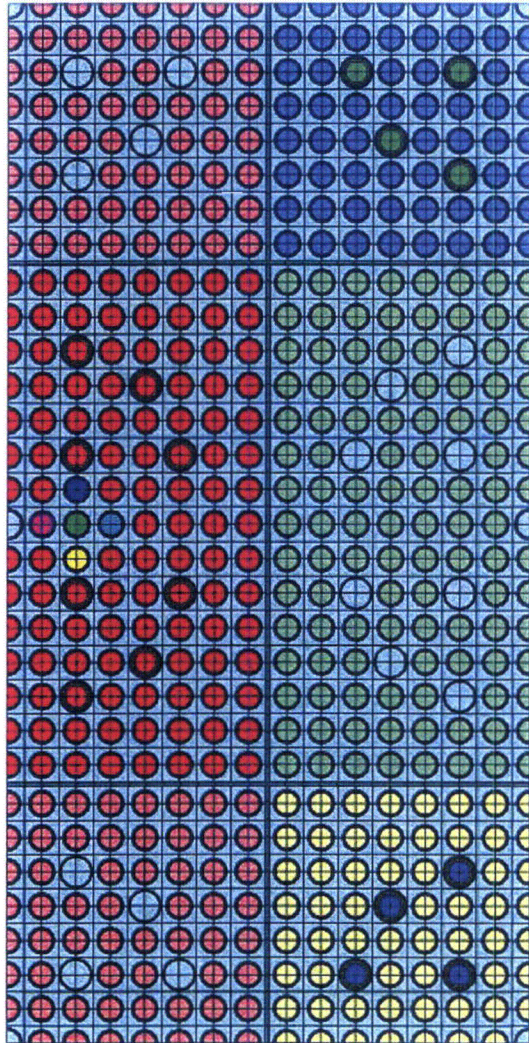
The first computational model (called "model #1") represents a half assembly, as illustrated in Figure 5.1. The second TRITON model (called "model #2") represents half of the test assembly NJ05YU and surrounding assemblies, taking advantage of the configuration symmetry as shown in Figures A.1 and A.2. The TRITON model in this case is illustrated in Figure A.3.

<b>NW</b>	<b>N</b>	<b>NE</b>
Batch 10B Enrich = 3.63%	Batch 10B Enrich = 3.63%	Batch 11B Enrich = 4% BP load = 1.1%
<b>W</b>	<b>NJ05YU</b>	<b>E</b>
Batch 10B Enrich = 3.63%	Batch 11C Enrich = 4% BP load = 1.7%	Batch 10B Enrich = 3.63%
<b>SW</b>	<b>S</b>	<b>SE</b>
Batch 11C Enrich = 4% BP load = 2.1%	Batch 10B Enrich = 3.63%	Batch 11C Enrich = 4% BP load = 2.1%

**Figure A.1 Assemblies surrounding NJ05YU during cycle 9**

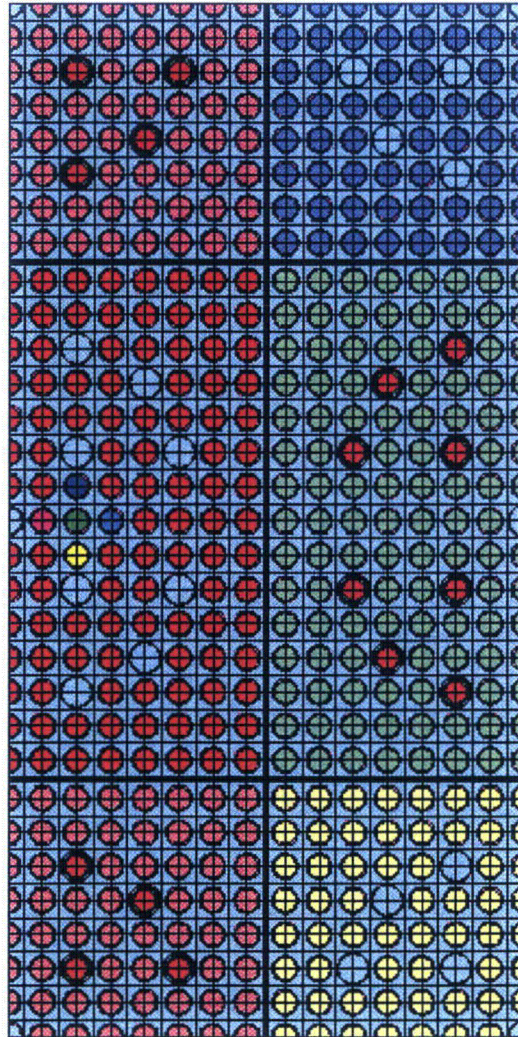
<b>NW</b>	<b>N</b>	<b>NE</b>
Batch 11C Enrich = 4%	Batch 12B Enrich = 4.65% BP load = 2.1%	Batch 11A Enrich = 4%
<b>W</b>	<b>NJ05YU</b>	<b>E</b>
Batch 12B Enrich = 4.65% BP load = 2.1%	Batch 11C Enrich = 4%	Batch 12B Enrich = 4.65% BP load = 2.1%
<b>SW</b>	<b>S</b>	<b>SE</b>
Batch 11A Enrich = 4%	Batch 12B Enrich = 4.65% BP load = 2.1%	Batch 11C Enrich = 4%

**Figure A.2 Assemblies surrounding NJ05YU during cycle 10**



- regular fuel pin in test assembly
- test fuel pin
- ■ ■ ■ neighbors of test pin
- pins in N and S assembly
- pins in E assembly
- pins in SE assembly
- pins in NE assembly
- BPR absorber in test assembly
- BPR absorber in NE assembly
- BPR absorber in SE assembly

(a) cycle 9



- regular fuel pin in test assembly
- test fuel pin
- ■ ■ ■ neighbors of test pin
- pins in N and S assembly
- pins in E assembly
- pins in SE assembly
- pins in NE assembly
- BPR absorber in N, S, E assembly

(b) cycle 10

**Figure A.3 TRITON model #2 for TMI-1 samples in assembly NJ05YU**

The two modeling approaches described above were used to assess the effect of modeling the assembly surroundings on the calculated nuclide inventory. All calculations reported here used the sample burnup as provided in Ref. 4, with no power (burnup) adjustment done to match the measured concentration of  $^{148}\text{Nd}$  because the calculated value for this nuclide was within one standard deviation reported for the measurement. A comparison of the C/E average and standard deviation over all 11 samples obtained with each of the two computational models is presented in Table A.1 and illustrated in Figure A.4 for uranium and plutonium nuclides. Results for all samples and both modeling approaches are shown in Tables A.2 and A.3.

For the considered samples, the effect of modeling the assemblies surrounding the assembly NJ05YU has small, but not a major impact. In the case of uranium isotopes, for example, the average overprediction decreases from 4.7% to 3.9% for  $^{235}\text{U}$ , and remains practically unchanged for  $^{234}\text{U}$  and  $^{236}\text{U}$  when going from model #1 to model #2. For plutonium nuclides, the change is less than 0.5% for all measured nuclides except for  $^{239}\text{Pu}$  for which there is a 1.3% decrease in the average overestimation, from 14.9% to 13.6%. The change in fission products average C/E does not exceed 1.4%. Note though that part of the differences observed may be due to the modeling of the assemblies from batch 10B during cycle 9 as fresh fuel, as their burnup was not known.

**Table A.1 Effect of modeling assumptions on C/E-1 (%)  
for samples from assembly NJ05YU**

Nuclide ID	Model #1 <sup>a</sup>				Model #2 <sup>b</sup>			
	Avg	$\sigma$	Max	Min	Avg	$\sigma$	Max	Min
U-234	<b>3.6</b>	3.9	10.0	-3.4	<b>3.5</b>	3.9	10.0	-3.5
U-235	<b>4.7</b>	11.0	24.7	-16.1	<b>3.9</b>	11.0	24.0	-16.9
U-236	<b>3.4</b>	2.2	8.0	0.5	<b>3.4</b>	2.2	8.2	0.6
Pu-238	<b>-2.5</b>	19.4	41.9	-34.6	<b>-2.6</b>	19.3	41.6	-34.7
Pu-239	<b>14.9</b>	3.7	22.3	9.1	<b>13.6</b>	3.7	20.9	7.9
Pu-240	<b>15.4</b>	6.1	23.9	7.0	<b>15.0</b>	6.0	23.5	6.8
Pu-241	<b>4.3</b>	2.8	7.3	-0.6	<b>3.9</b>	2.8	6.9	-1.0
Pu242	<b>3.2</b>	7.4	15.0	-7.8	<b>3.7</b>	7.4	15.7	-7.4
Nd-143	<b>8.2</b>	5.2	15.6	2.2	<b>7.9</b>	5.2	15.2	1.9
Nd-145	<b>4.5</b>	2.9	9.5	-0.4	<b>4.4</b>	2.9	9.4	-0.5
Nd-148	<b>0.4</b>	0.3	0.9	-0.1	<b>0.3</b>	0.3	0.8	-0.1
Cs-137	<b>-2.1</b>	7.5	17.0	-13.7	<b>-2.1</b>	7.5	16.9	-13.7
Eu-151	<b>-11.3</b>	27.3	31.0	-47.3	<b>-13.2</b>	27.0	29.3	-47.8
Eu-153	<b>7.8</b>	3.6	15.8	1.7	<b>7.7</b>	3.6	15.8	1.6
Eu-155	<b>-56.4</b>	6.1	-45.9	-66.7	<b>-56.5</b>	6.1	-46.1	-66.8
Sm-147	<b>11.3</b>	7.4	21.7	0.6	<b>11.1</b>	7.5	21.5	0.2
Sm-149	<b>19.1</b>	9.5	36.3	0.9	<b>18.2</b>	9.4	35.3	0.2
Sm-150	<b>11.8</b>	6.6	24.6	3.0	<b>11.7</b>	6.7	24.5	2.8
Sm-151	<b>43.6</b>	10.6	59.4	28.6	<b>42.2</b>	10.5	57.9	27.3
Sm-152	<b>36.4</b>	4.2	44.3	31.4	<b>36.2</b>	4.2	44.2	31.3
Gd-155	<b>-48.7</b>	7.3	-34.5	-65.9	<b>-48.9</b>	7.3	-34.7	-66.0
Am-241	<b>-1.3</b>	22.6	48.4	-18.7	<b>-1.8</b>	22.4	47.3	-19.1
Am-242m	<b>-25.8</b>	78.1	133.0	-86.3	<b>-26.6</b>	77.1	130.3	-86.4
Am-243	<b>26.9</b>	24.8	61.4	-1.8	<b>27.5</b>	24.9	62.3	-1.3
Np-237	<b>4.7</b>	4.7	12.5	-4.3	<b>4.0</b>	4.6	11.7	-4.9
Mo-95	<b>2.0</b>	4.6	10.4	-3.9	<b>2.0</b>	4.6	10.4	-3.9
Tc-99	<b>-0.3</b>	11.5	13.1	-26.0	<b>-0.4</b>	11.5	13.0	-26.1
Ru-101	<b>4.4</b>	6.7	15.6	-6.5	<b>4.4</b>	6.7	15.5	-6.5
Rh-103	<b>11.6</b>	6.0	23.2	2.6	<b>11.3</b>	6.0	22.8	2.4
Ag-109	<b>111.4</b>	55.1	205.4	34.2	<b>111.4</b>	55.0	204.9	34.2

<sup>a</sup> As illustrated in Figure 5.1.

<sup>b</sup> As illustrated in Figure A.3.

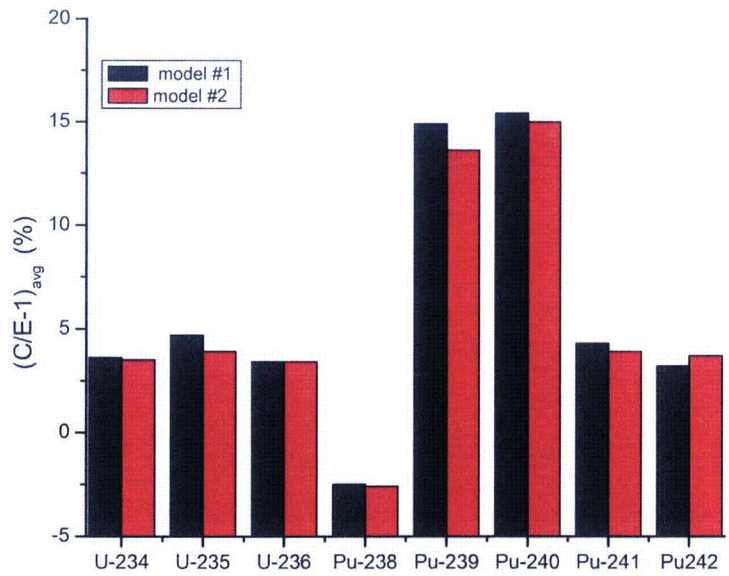


Figure A.4 Effect of modeling assumptions on U and Pu—assembly NJ05YU



**Table A.2 C/E-1 (%) for samples in assembly NJ05YU – computational model #1**

Sample ID	A1B	D2	B2	C1	D1A4	A2	C3	C2B	B3J	B1B	D1A2				
<b>Burnup (GWd/MTU)</b>	<b>44.8</b>	<b>44.8</b>	<b>50.1</b>	<b>50.2</b>	<b>50.5</b>	<b>50.6</b>	<b>51.3</b>	<b>52.6</b>	<b>53.0</b>	<b>54.5</b>	<b>55.7</b>	Avg	Max	Min	$\sigma$
U-234	5.6	10.0	5.6	-0.8	1.0	2.4	4.8	7.6	5.7	1.2	-3.4	3.6	10.0	-3.4	3.9
U-235	0.9	24.7	14.5	11.0	-2.5	9.0	9.2	5.2	1.7	-6.5	-16.1	4.7	24.7	-16.1	11.0
U-236	4.9	0.5	2.5	1.2	3.3	1.0	4.5	8.0	2.8	4.5	3.6	3.4	8.0	0.5	2.2
Pu-238	-34.6	-12.3	7.4	5.8	-6.1	-3.5	41.9	-18.8	-7.8	-8.8	9.7	-2.5	41.9	-34.6	19.4
Pu-239	14.6	17.2	12.3	14.7	16.5	9.9	9.1	22.3	15.1	17.7	14.0	14.9	22.3	9.1	3.7
Pu-240	19.0	7.0	11.1	11.4	18.1	9.2	8.5	23.9	18.0	22.1	21.1	15.4	23.9	7.0	6.1
Pu-241	2.0	5.3	5.5	6.6	-0.6	7.3	6.9	7.0	1.1	5.0	1.2	4.3	7.3	-0.6	2.8
Pu242	8.6	-7.8	0.6	1.9	-1.8	1.7	4.0	7.8	-7.4	12.4	15.0	3.2	15.0	-7.8	7.4
Nd-143	4.6	14.9	8.8	12.0	2.2	14.3	15.6	7.9	4.2	3.5	2.7	8.2	15.6	2.2	5.2
Nd-145	3.4	5.8	5.3	6.2	-0.4	9.5	8.1	4.8	1.6	2.8	2.2	4.5	9.5	-0.4	2.9
Nd-148	0.8	0.9	0.4	0.5	0.5	0.3	0.3	0.3	0.2	0.3	-0.1	0.4	0.9	-0.1	0.3
Cs-137	-13.7	-6.7	-3.7	-6.9	-1.3	-3.8	1.3	-3.6	-1.3	0.1	17.0	-2.1	17.0	-13.7	7.5
Eu-151	1.5	-30.8	-40.8	-28.2	13.7	-47.3	-43.3	6.3	-4.0	31.0	17.9	-11.3	31.0	-47.3	27.7
Eu-153	7.6	1.7	8.2	8.6	4.8	7.1	15.8	11.1	5.3	7.5	8.0	7.8	15.8	1.7	3.6
Eu-155	-61.5	-59.2	-55.5	-58.8	-63.2	-53.9	-52.5	-50.7	-52.2	-66.7	-45.9	-56.4	-45.9	-66.7	6.1
Sm-147	11.0	17.8	19.2	17.7	7.2	12.8	21.7	11.4	3.5	0.6	1.2	11.3	21.7	0.6	7.4
Sm-149	16.9	27.0	18.5	25.8	12.3	0.9	36.3	20.6	23.2	18.9	9.5	19.1	36.3	0.9	9.5
Sm-150	8.8	12.1	17.1	15.1	7.6	18.7	24.6	10.7	3.0	3.0	8.7	11.8	24.6	3.0	6.6
Sm-151	35.8	54.4	41.7	59.4	41.5	50.1	55.0	48.5	28.6	31.6	33.0	43.6	59.4	28.6	10.6
Sm-152	34.5	33.8	37.9	40.2	32.7	36.3	44.3	41.8	31.4	32.5	34.7	36.4	44.3	31.4	4.2
Gd-155	-52.0	-47.9	-48.4	-46.3	-65.9	-34.5	-47.5	-46.8	-51.8	-47.7	-46.9	-48.7	-34.5	-65.9	7.3
Am-241	8.2	-14.8	-13.6	-18.7	-18.3	-3.0	-0.5	-15.9	-18.4	48.4	32.4	-1.3	48.4	-18.7	22.6
Am-242m	-86.3	-84.2	-85.4	-84.4	75.8	-85.7	-85.1	-17.1	4.7	31.0	133.0	-25.8	133.0	-86.3	78.1
Am-243	46.6	-1.7	-1.8	3.7	40.7	1.0	8.6	46.6	37.1	53.2	61.4	26.9	61.4	-1.8	24.8
Np-237	2.5	-4.3	1.7	2.0	6.2	1.8	6.1	9.0	4.8	9.6	12.5	4.7	12.5	-4.3	4.7
Mo-95	-3.9	8.2	-3.2	-0.8	0.5	-1.6	10.4	3.3	1.5	1.4	6.3	2.0	10.4	-3.9	4.6
Tc-99	-26.0	7.4	5.3	6.3	-3.2	7.1	13.1	-12.1	-3.5	-6.7	9.2	-0.3	13.1	-26.0	11.5
Ru-101	-6.5	9.9	-3.6	-0.4	6.1	1.2	15.6	3.5	4.3	5.7	13.0	4.4	15.6	-6.5	6.7
Rh-103	2.6	19.5	5.5	7.8	11.1	7.7	23.2	11.8	10.8	12.1	15.6	11.6	23.2	2.6	6.0
Ag-109	100.7	123.4	127.2	125.3	44.0	103.2	34.2	96.5	65.6	205.4	200.1	111.4	205.4	34.2	55.1

Table A.3 C/E-1 (%) for samples in assembly NJ05YU – computational model #2

Sample ID	A1B	D2	B2	C1	D1A4	A2	C3	C2B	B3J	B1B	D1A2						
Burnup (GWd/MTU)	44.8	44.8	50.1	50.2	50.5	50.6	51.3	52.6	53.0	54.5	55.7						
U-234	5.5	10.0	5.5	-0.9	0.9	2.3	4.7	7.5	5.6	0.9	-3.5	Avg	3.5	10.0	-3.5	σ	3.9
U-235	0.4	24.0	13.7	10.2	-3.3	8.3	8.4	4.4	0.8	-7.5	-16.9	3.9	24.0	-16.9	11.0		
U-236	5.0	0.6	2.6	1.3	3.4	1.1	4.6	8.2	2.9	4.4	3.7	3.4	8.2	0.6	2.2		
Pu-238	-34.7	-12.5	7.2	5.6	-6.2	-3.7	41.6	-18.9	-7.9	-9.1	9.5	-2.6	41.6	-34.7	19.3		
Pu-239	13.6	16.2	11.0	13.5	15.3	8.7	7.9	20.9	13.8	16.1	12.6	13.6	20.9	7.9	3.7		
Pu-240	18.7	6.8	10.7	11.1	17.7	8.9	8.1	23.5	17.5	21.4	20.6	15.0	23.5	6.8	6.0		
Pu-241	1.7	5.1	5.1	6.3	-1.0	6.9	6.4	6.6	0.6	4.4	0.7	3.9	6.9	-1.0	2.8		
Pu242	9.1	-7.4	1.1	2.5	-1.2	2.2	4.5	8.4	-6.9	12.8	15.7	3.7	15.7	-7.4	7.4		
Nd-143	4.5	14.6	8.4	11.8	1.9	13.9	15.2	7.5	3.8	3.0	2.4	7.9	15.2	1.9	5.2		
Nd-145	3.3	5.7	5.2	6.1	-0.5	9.4	8.0	4.7	1.5	2.5	2.1	4.4	9.4	-0.5	2.9		
Nd-148	0.7	0.8	0.4	0.5	0.4	0.2	0.3	0.3	0.1	0.0	-0.1	0.3	0.8	-0.1	0.3		
Cs-137	-13.7	-6.7	-3.8	-7.0	-1.4	-3.8	1.3	-3.6	-1.4	-0.1	16.9	-2.1	16.9	-13.7	7.5		
Eu-151	0.6	-31.4	-41.4	-29.0	12.6	-47.8	-43.9	5.2	-5.0	29.3	16.6	-12.2	29.3	-47.8	27.3		
Eu-153	7.5	1.6	8.1	8.6	4.8	7.1	15.8	11.1	5.3	7.2	7.9	7.7	15.8	1.6	3.6		
Eu-155	-61.6	-59.3	-55.6	-59.0	-63.3	-54.0	-52.6	-50.9	-52.4	-66.8	-46.1	-56.5	-46.1	-66.8	6.1		
Sm-147	10.9	17.7	19.0	17.5	7.0	12.7	21.5	11.2	3.2	0.2	0.9	11.1	21.5	0.2	7.5		
Sm-149	16.1	26.1	17.7	25.0	11.5	0.2	35.3	19.7	22.3	17.8	8.7	18.2	35.3	0.2	9.4		
Sm-150	8.7	12.1	17.1	15.1	7.5	18.6	24.5	10.7	3.0	2.8	8.6	11.7	24.5	2.8	6.7		
Sm-151	34.6	53.1	40.3	57.9	40.1	48.7	53.4	47.1	27.3	30.0	31.6	42.2	57.9	27.3	10.5		
Sm-152	34.4	33.7	37.7	40.0	32.7	36.2	44.2	41.7	31.3	32.1	34.6	36.2	44.2	31.3	4.2		
Gd-155	-52.2	-48.1	-48.6	-46.5	-66.0	-34.7	-47.7	-47.0	-51.9	-48.0	-47.0	-48.9	-34.7	-66.0	7.3		
Am-241	7.8	-15.1	-14.0	-19.1	-18.6	-3.4	-1.0	-16.3	-18.9	47.3	31.7	-1.8	47.3	-19.1	22.4		
Am-242m	-86.4	-84.3	-85.6	-84.6	74.1	-85.8	-85.3	-18.0	3.5	29.3	130.3	-26.6	130.3	-86.4	77.1		
Am-243	47.2	-1.3	-1.3	4.2	41.4	1.5	9.2	47.4	37.9	53.8	62.3	27.5	62.3	-1.3	24.9		
Np-237	1.9	-4.9	1.0	1.3	5.6	1.2	5.4	8.2	4.0	8.7	11.7	4.0	11.7	-4.9	4.6		
Mo-95	-3.9	8.2	-3.2	-0.7	0.5	-1.5	10.4	3.2	1.5	1.2	6.3	2.0	10.4	-3.9	4.6		
Tc-99	-26.1	7.4	5.3	6.2	-3.3	7.1	13.0	-12.1	-3.6	-7.0	9.1	-0.4	13.0	-26.1	11.5		
Ru-101	-6.5	10.0	-3.6	-0.4	6.0	1.2	15.5	3.4	4.2	5.5	12.9	4.4	15.5	-6.5	6.7		
Rh-103	2.4	19.2	5.2	7.5	10.7	7.4	22.8	11.5	10.5	11.5	15.2	11.3	22.8	2.4	6.0		
Ag-109	100.7	123.5	127.2	125.5	44.0	103.3	34.2	96.6	65.6	204.9	200.0	111.4	204.9	34.2	55.0		

## A.2 Assembly NJ070G

The initial model for assembly NJ070G, built based on the information available at the time, did not include any details on the assembly surroundings. It also assumed the location for the gadolinia fuel rods, as shown in Figure A.5, and assumed that the assembly pitch was 15 times larger than the rod pitch (i.e., no extra water between adjacent assemblies). The initial TRITON model (called here model #1) is shown in Figure A.6 for samples in corner rod O1.

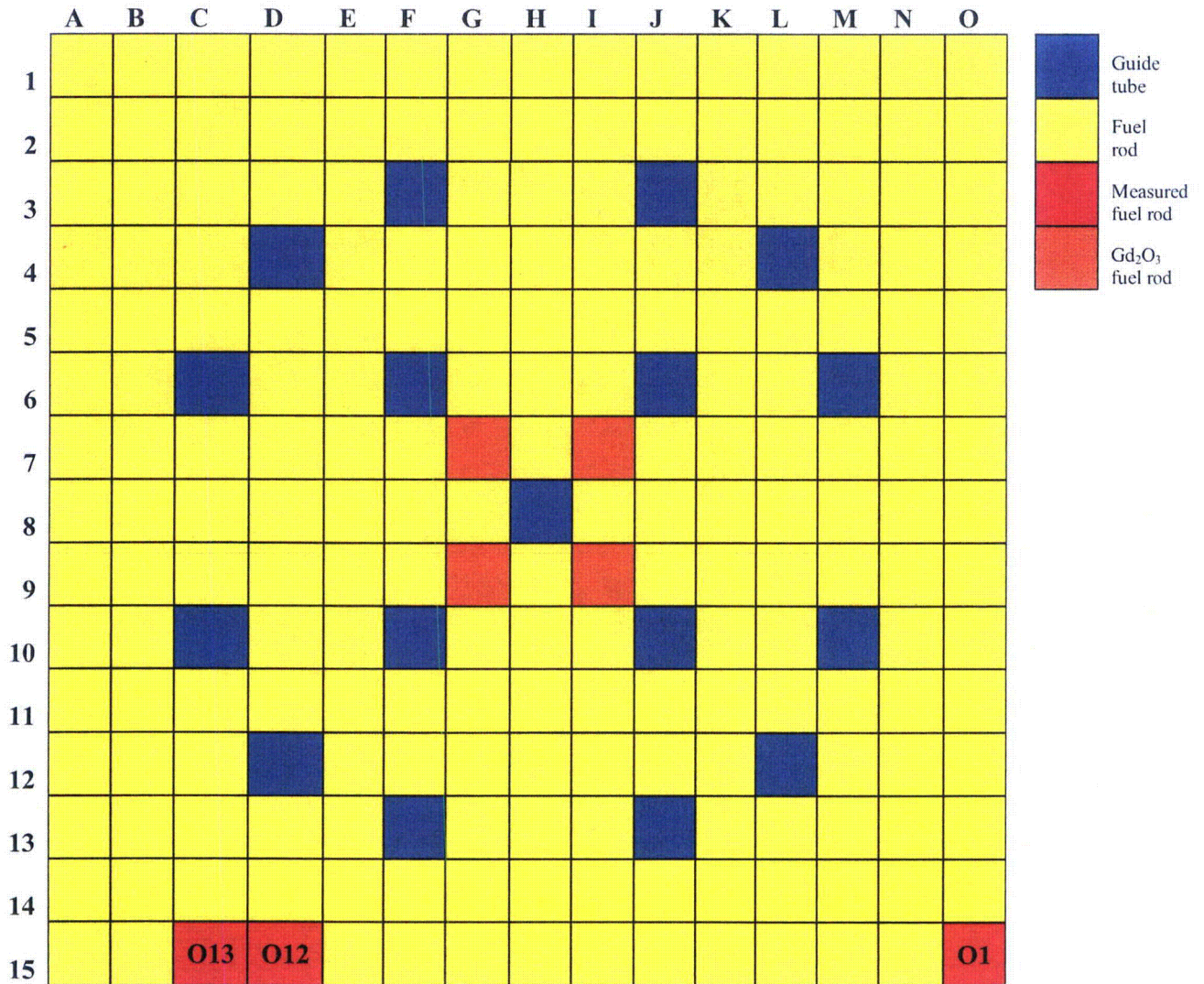
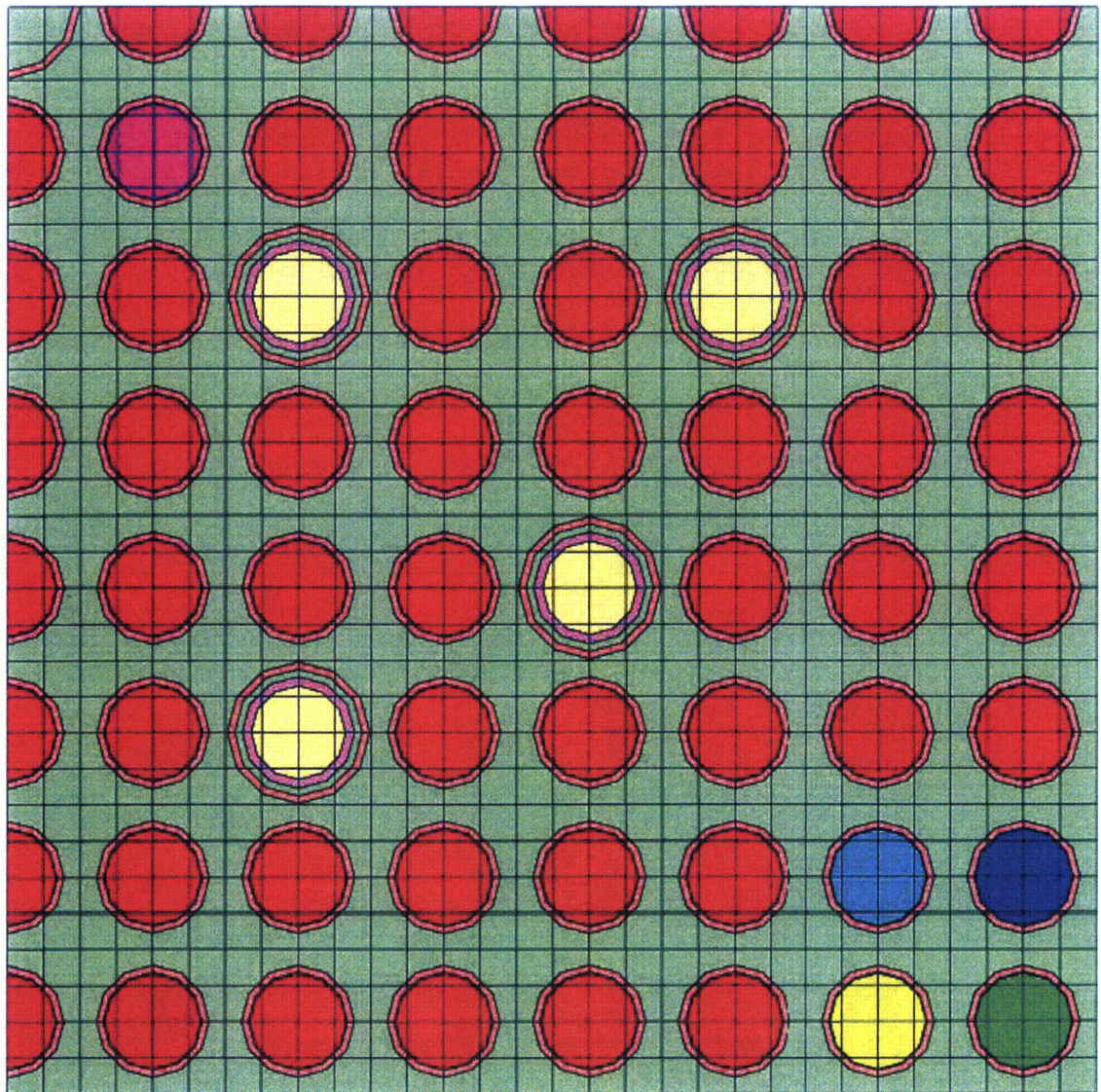


Figure A.5 Initial layout—assembly NJ070G



■ regular fuel pin  
 ■ test fuel pin  
 ■ ■ neighbors of test pin  
 ■ gadolinia fuel pin  
 ■ clad  
■ moderator  
 ■ BPR absorber  
 ■ BPR clad

**Figure A.6 Initial TRITON model for samples in corner rod O1 of assembly NJ070G**

As additional information (Ref. 18) on the assemblies surrounding the NJ070G assembly, or data related to assembly geometry became available, new computational models were developed to include this information and therefore assess the effect on the calculated isotopic inventory. All of the three rods measured were located at the edge of the assembly; therefore, the boundary condition is expected to influence the flux spectrum in the samples under consideration.

Important information on the location of the gadolinia fuel rods was obtained from AREVA. These rods were actually located at B2, B14, N2, and N14 with respect to the layout illustrated in Figure A.5, therefore being close to the rods from which samples were selected. Assembly pitch also became available (Ref. 18); the initial model considered the assembly pitch to be the product of the rod pitch and the number of fuel rods in a row of the assembly lattice. Consideration of the actual assembly pitch value is expected to slightly increase the moderation for the measured rod near the edge of the assembly. Another change was for the dimensions of the guide and instrument tubes – the actual dimensions were smaller than the initially assumed values. This led to an increase in the moderator volume in the assembly by 0.7%. Data on the assemblies surrounding assembly NJ070G are illustrated in Figure 4.3. All the available data was included to build a more detailed TRITON model (called model #2) as discussed in Section 5.1 and illustrated in Figures 5.2 and 5.3.

Both modeling approaches described above were used in simulations to assess the effect of including more detailed information on the assembly configuration (i.e. assembly pitch, gadolinia rod location), as well as more accurately modeling the assembly surroundings, on the calculated nuclide inventory. It was found that the use of a more detailed model has a significant effect on the calculated concentration for some of the main actinides, as illustrated in Figure A.7 for  $^{235}\text{U}$  and  $^{239}\text{Pu}$ . The data shown in the figure correspond to a calculation that used the sample burnup as provided in Ref. 4. The calculated concentration of  $^{148}\text{Nd}$ , in this case, was within the experimental uncertainty of 1.5% for most of the samples considered. The more accurate model led to a decrease of the  $^{235}\text{U}$  and  $^{239}\text{Pu}$  average overestimation from 4.7% and 10.4%, respectively, to 3.3% and 1.8%. The comparison for all other nuclides is presented in Table A.4.

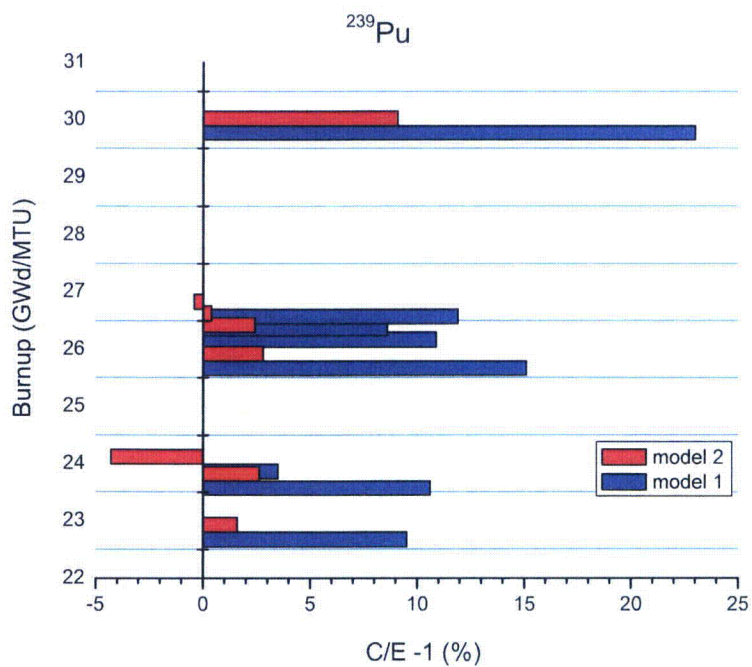
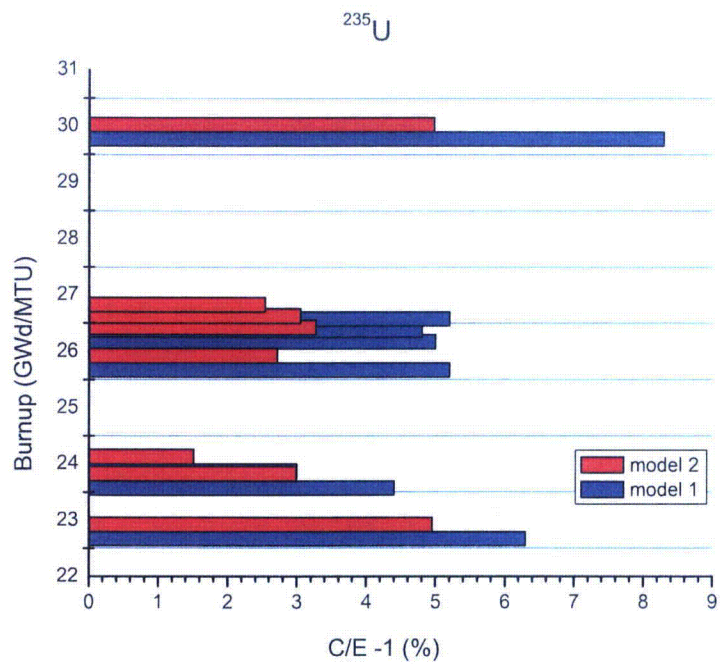


Figure A.7 Effect of modeling assumptions on  $^{235}\text{U}$  and  $^{239}\text{Pu}$ —assembly NJ070G

Table A.4 C/E -1 (%) for samples in assembly NJ070G – computational models # 1 and #2

SampleID	O13S7		O12S4		O12S6		O1S1		O13S8		O12S5		O1S3		O1S2		Avg	
Burnup (Gwd/MTU)	22.8		23.7		24.0		25.8		26.3		26.5		26.7		29.9			
Nuclide ID	mod1 <sup>a</sup>	mod2 <sup>b</sup>	mod1	mod2	mod1	mod2	mod1	mod2	mod1	mod2	mod1	mod2	mod1	mod2	mod1	mod2	mod1	mod2
U-234	-2.6	-1.9	-1.1	-0.3	-0.2	0.6	-1.8	-0.7	-0.5	0.3	1.0	1.9	0.1	1.2	-0.6	0.6	-0.6	0.2
U-235	6.3	4.9	4.4	3.0	3.0	1.5	5.2	2.7	5.0	3.3	4.8	3.0	5.2	2.5	8.3	5.0	4.7	3.3
U-236	-3.8	-4.1	-3.0	-3.4	-3.8	-4.2	-2.4	-2.7	-2.1	-2.3	-2.3	-2.7	-2.9	-3.3	-2.3	-2.6	-2.5	-3.1
Pu-238	-11.1	-18.4	-6.0	-13.7	-16.6	-23.4	1.0	-10.6	-9.5	-16.7	-9.2	-16.3	-10.2	-20.3	-1.2	-12.0	-7.0	-16.4
Pu-239	9.5	1.6	10.6	2.6	3.5	-4.3	15.1	2.8	10.9	2.4	8.6	0.4	11.9	-0.4	23.0	9.1	10.4	1.8
Pu-240	-0.8	-2.9	2.6	0.3	-2.2	-4.4	3.6	0.5	0.7	-1.3	0.0	-2.3	-2.5	-5.4	1.8	-1.2	0.4	-2.1
Pu-241	-2.5	-9.0	2.1	-5.0	-5.8	-12.2	5.9	-4.4	-0.4	-7.0	-1.5	-8.2	-1.5	-10.9	6.8	-3.5	0.3	-7.5
Pu242	-12.5	-14.5	-5.2	-7.8	-10.3	-12.5	-2.9	-5.9	-8.1	-9.5	-7.8	-9.7	-12.5	-14.5	-10.1	-11.8	-7.7	-10.8
Nd-143	1.1	0.9	2.9	2.7	2.0	1.8	4.1	3.7	3.6	3.4	3.6	3.4	2.8	2.4	4.2	3.5	2.7	2.7
Nd-145	-0.5	-0.1	1.5	2.0	1.4	1.9	2.0	2.7	2.2	2.6	2.3	2.8	1.2	1.9	1.1	1.8	1.2	2.0
Nd-146	-1.0	-1.2	1.5	1.3	0.3	0.0	2.3	2.0	1.6	1.4	1.7	1.5	0.8	0.4	1.5	1.1	1.0	0.8
Nd-148	-1.5	-1.6	1.0	0.8	-0.2	-0.3	1.4	1.2	1.1	1.0	1.2	1.1	-0.2	-0.4	0.4	0.2	0.4	0.2
Nd-150	-1.1	-1.8	2.3	1.6	0.2	-0.5	2.4	1.3	2.0	1.2	2.1	1.3	0.3	-0.8	1.5	0.4	1.1	0.4
Cs-134	-22.5	-25.5	-18.2	-21.2	-21.2	-24.1	-14.2	-18.6	-19.1	-22.0	-18.0	-20.9	-18.1	-22.2	-14.4	-18.4	-16.2	-21.6
Cs-137	-7.4	-7.4	-3.7	-3.7	-3.8	-3.8	-2.2	-2.2	-5.5	-5.5	-3.8	-3.8	-4.4	-4.5	-7.0	-7.0	-4.2	-4.8
Eu-151	41.7	32.6	28.4	20.1	19.5	11.5	38.2	24.2	39.4	29.5	38.5	28.9	33.6	19.6	56.1	39.0	32.8	25.7
Eu-153	-8.6	-9.8	-6.5	-7.7	-7.7	-8.8	-2.9	-4.6	-6.1	-7.2	-5.5	-6.7	-5.7	-7.2	-3.6	-5.0	-5.2	-7.1
Sm-147	-4.1	-2.8	-5.8	-4.5	-5.2	-3.8	-6.2	-4.3	-3.2	-1.8	-3.7	-2.3	-7.1	-5.2	-6.4	-4.4	-4.6	-3.6
Sm-149	20.1	12.5	19.4	12.1	16.0	8.4	26.1	14.7	28.2	19.6	27.5	19.3	24.4	12.5	40.6	27.4	22.5	15.8
Sm-150	0.3	-0.2	2.5	2.0	1.5	1.1	4.2	3.4	3.2	2.7	12.1	11.6	1.4	0.8	3.2	2.5	3.2	3.0
Sm-151	36.7	28.0	36.2	27.5	26.1	17.8	44.4	30.1	34.7	25.3	34.7	25.5	38.1	23.9	48.1	32.1	33.2	26.3
Sm-152	11.1	12.0	13.4	14.3	16.6	17.6	14.7	16.2	16.9	18.0	16.8	17.8	13.6	15.1	13.1	14.6	12.9	15.7
Gd-155	-39.1	-40.2	-40.5	-41.6	-46.2	-47.3	-43.7	-45.1	-39.8	-41.0	-38.7	-39.8	-47.2	-48.6	-34.9	-36.6	-36.7	-42.5
Cm-242	-22.0	-27.2	-22.2	-27.4	-16.6	-22.0	0.2	-8.7	-31.9	-36.0	-27.7	-32.5	-25.3	-31.6	-34.7	-40.3	-20.0	-28.2
Cm-243	-25.1	-33.1	-17.7	-26.9	-13.7	-23.3	30.0	10.3	-21.0	-29.0	-23.4	-31.6	-14.9	-27.3	0.0	-14.1	-9.5	-21.9
Cm-244	-11.7	-22.3	-0.7	-13.2	5.2	-7.5	63.7	36.2	-5.1	-15.5	-6.7	-17.4	6.5	-10.3	19.0	1.3	7.8	-6.1
Cm-245	-36.4	-47.5	-26.6	-39.7	-31.1	-43.1	27.3	-3.3	-32.2	-43.2	-33.2	-44.5	-23.1	-40.8	-2.6	-24.3	-17.6	-35.8
Am-241	-0.2	-6.9	-1.0	-7.8	17.2	9.2	49.1	34.5	1.8	-5.0	-0.1	-6.9	9.9	-0.7	23.5	11.5	11.1	3.5
Am-242m	12.5	1.6	7.4	-3.6	13.1	1.7	59.1	36.2	1.1	-8.9	-1.6	-11.7	18.8	1.8	34.3	14.5	16.1	4.0
Am-243	3.3	-4.8	13.6	4.1	29.7	19.6	74.7	55.5	9.3	1.8	8.2	0.3	22.5	10.2	30.8	18.6	21.4	13.2
Np-237	0.8	-5.0	-1.0	-6.5	-2.8	-8.1	11.9	3.2	3.1	-2.5	3.6	-1.9	2.1	-5.6	8.4	0.4	2.9	-3.2

<sup>a</sup> Assembly surroundings modeled with a reflective boundary condition.

<sup>b</sup> Assemblies surrounding the test assembly close to the boundary the samples were selected are explicitly modeled.

In order to estimate the relative importance of various assumptions used in the computational model on the calculated nuclide concentrations, separate calculations were carried out for sample O13S7 by changing some of the model parameters one at a time. The following modeling parameters were considered:

- boundary condition on the assembly sides (modeling of surrounding assemblies);
- location of gadolinia fuel rods in the assembly (in some cases no precise information on position is available and therefore it must be assumed); and
- assembly pitch.

The model illustrated in Figure 5.3 was considered as a reference. Three models were developed starting from this reference model, as follows:

1. The assemblies neighboring the assembly NJ070G were not explicitly modeled; a reflective boundary condition was employed on the sides of NJ070G. The TRITON geometry in this case represented a quarter of an assembly.
2. The location of the gadolinia rod in the assembly was assumed, as shown in Figure A.5, farther from its actual location shown in Figure 5.2.
3. The value used for the assembly pitch was assumed as rod pitch times 15 instead of the actual value.

Given the proximity of the measured rod O13 to the assembly boundary and to the gadolinia rod location, each of the three above-mentioned changes are expected to influence the flux spectrum in the measured fuel rod and therefore the calculated nuclide concentrations for samples selected from that rod.

The results of the analysis are shown in Table A.5. One parameter only was changed at a time; the other remained as in the model shown in Figure 5.2. The effect of the assumptions is illustrated in Figure A.8 for three nuclides:  $^{235}\text{U}$ ,  $^{239}\text{Pu}$  and  $^{148}\text{Nd}$ . As expected, the content of the  $^{148}\text{Nd}$  nuclide, which is a burnup indicator, does not change appreciably when changing the model. The effect is, however, significant in case of  $^{239}\text{Pu}$ : the C/E ratio increases by about 2.5% as compared to the reference model when either the gadolinia rod location or the surrounding assemblies are not exactly represented; when the assembly pitch is assumed, the C/E increases to 9.7%, as compared to the reference model for which it is 1.6%. The C/E change for  $^{235}\text{U}$  is not as dramatic as for  $^{239}\text{Pu}$ . It increases by about one half of a percent when the gadolinia rod location or the surrounding assemblies' effect is assumed and about 1.5% when the assembly pitch is assumed.



**Table A.5 Effect of modeling assumptions on C/E-1 (%) for sample O13S7 from assembly NJ070G**

Nuclide ID	Reference model	Surrounding assemblies not modeled explicitly	Assumed location for gadolinia rod	Assumed value for assembly pitch
U-234	-1.9	-2.3	-2.1	-2.7
U-235	4.9	5.5	5.4	6.5
U-236	-4.1	-4.0	-4.1	-3.8
Pu-238	-18.4	-15.6	-16.2	-10.7
Pu-239	1.6	4.3	4.0	9.7
Pu-240	-2.9	-1.7	-2.3	-0.2
Pu-241	-9.0	-6.4	-7.0	-2.0
Pu242	-14.5	-13.1	-14.0	-11.7
Nd-143	0.9	0.9	1.0	1.0
Nd-145	-0.1	-0.2	-0.2	-0.6
Nd-146	-1.2	-1.2	-1.2	-1.1
Nd-148	-1.6	-1.6	-1.6	-1.5
Nd-150	-1.8	-1.5	-1.6	-1.0
Cs-134	-25.5	-24.4	-24.4	-22.6
Cs-137	-7.4	-7.5	-7.4	-7.4
Eu-151	32.6	35.7	35.4	41.9
Eu-153	-9.8	-9.2	-9.3	-8.5
Sm-147	-2.8	-3.3	-3.3	-4.1
Sm-149	12.5	15.0	15.0	20.1
Sm-150	-0.2	0.0	0.0	0.2
Sm-151	28.0	30.9	30.6	36.8
Sm-152	12.0	11.7	11.6	11.2
Gd-155	-40.2	-39.8	-39.8	-39.0
Cm-242	-27.2	-24.7	-25.8	-21.1
Cm-243	-33.1	-29.7	-31.0	-24.0
Cm-244	-22.3	-18.1	-19.5	-10.5
Cm-245	-47.5	-43.1	-44.3	-35.5
Am-241	-6.9	-4.1	-4.8	0.4
Am-242m	1.6	6.3	4.8	13.9
Am-243	-4.8	-1.3	-2.7	4.5
Np-237	-5.0	-2.8	-3.1	1.0

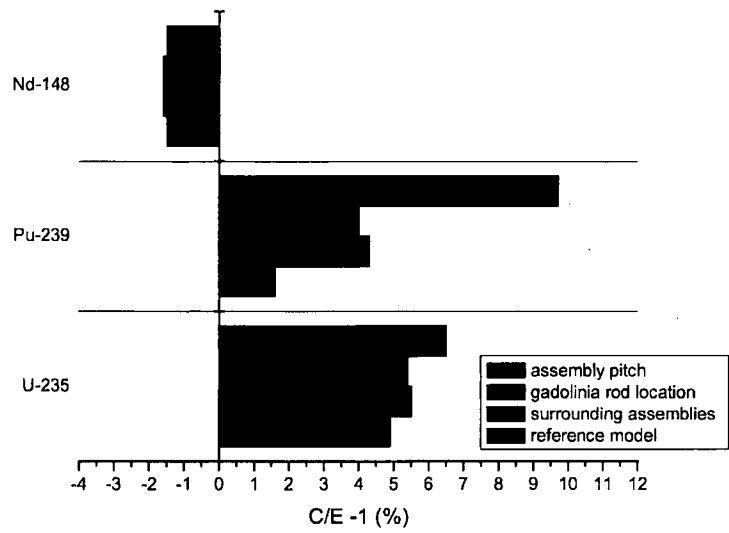
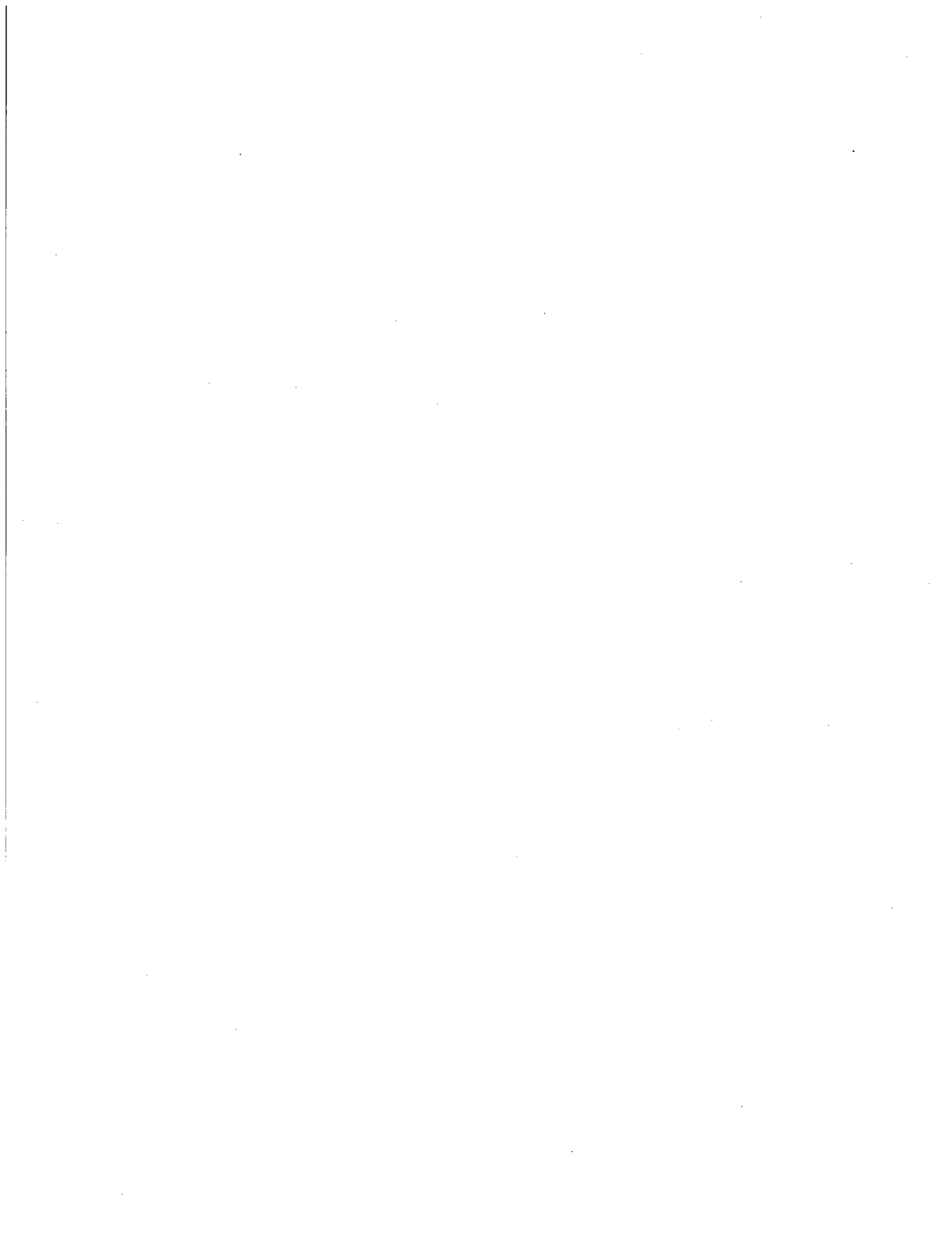


Figure A.8 Effect of modeling assumptions on  $^{235}\text{U}$ ,  $^{239}\text{Pu}$ , and  $^{148}\text{Nd}$  for sample O1S7

**APPENDIX B**

**SELECTED TRITON INPUT FILES**



## B.1 Sample O12S4 from Rod O12 in TMI-1 Assembly NJ070G

```
=t-depl parm=(nitawl,addnux=3)
TMI-1 Assembly NJ070G, rod O12, sample O12S4
44groupndf5
,
read alias
$fuel1 10 11 12 13 14 end
$fuel2 15 end
$fuel3 16 17 end
$clad1 20 21 22 23 24 end
$clad2 25 end
$clad3 26 27 end
$mod1 30 31 32 33 34 end
$mod2 35 end
$mod3 36 37 end
$gap1 40 41 42 43 44 end
$gap2 45 end
$gap3 46 47 end
,
read comp
'fuel
uo2 $fuel1 den=10.217 1 960.29 92234 0.045
92235 4.657
92238 95.298 end
uo2 $fuel2 den=10.217 0.98 960.29 92234 0.037
92235 4.190
92236 0.019
92238 95.754 end
arbm-gd 10.217 2 0 1 0 64000 2 8016 3 $fuel2 0.02 960.29 end
uo2 $fuel3 den=10.412 1 960.29 92234 0.040
92235 4.013
92238 95.947 end

'clad
zirc4 $clad1 1 640 end
zirc4 $clad2 1 640 end
zirc4 $clad3 1 640 end
'moderator
h2o $mod1 den=0.7382 1 582 end
arbm-bormod 0.7382 1 1 0 0 5000 100 $mod1 1800.0-6 582 end
h2o $mod2 den=0.7382 1 582 end
arbm-bormod 0.7382 1 1 0 0 5000 100 $mod2 1800.0-6 582 end
h2o $mod3 den=0.7382 1 582 end
arbm-bormod 0.7382 1 1 0 0 5000 100 $mod3 1800.0-6 582 end
'gap
n $gap1 den=0.00125 1 640 end
n $gap2 den=0.00125 1 640 end
n $gap3 den=0.00125 1 640 end
' BPR Al2O3-B4C
Al 50 0 3.817e-2 582 end
O-16 50 0 5.726e-2 582 end
C 50 0 7.547e-4 582 end
B-10 50 0 6.015e-4 582 end
B-11 50 0 2.421e-3 582 end
```

```

' BPR clad
zirc4 51 1          582  end
'
end comp
'
read celldata
latticecell squarepitch pitch=1.44272 $mod1 fuelr=0.4699 $fuel1
                                         cladr=0.5461 $clad1
                                         gapr=0.47879 $gap1  end
latticecell squarepitch pitch=1.44272 $mod2 fuelr=0.4699 $fuel2
                                         cladr=0.5461 $clad2
                                         gapr=0.47879 $gap2  end
latticecell squarepitch pitch=1.44272 $mod3 fuelr=0.4699 $fuel3
                                         cladr=0.5461 $clad3
                                         gapr=0.47879 $gap3  end

end celldata
'
read depletion
 10 -11 12 13 14 15 16 17 50
end depletion
'
read timetable
' change B in moderator
densmult $mod1 2 5010 5011
0.0 1.0000
68.0 0.9161
131.8 0.8450
209.0 0.7344
272.1 0.6333
347.4 0.5100
416.4 0.3989
486.4 0.2811
556.3 0.1656
626.1 0.0572
660.3 0.0010  end
densmult $mod2 2 5010 5011
0.0 1.0000
68.0 0.9161
131.8 0.8450
209.0 0.7344
272.1 0.6333
347.4 0.5100
416.4 0.3989
486.4 0.2811
556.3 0.1656
626.1 0.0572
660.3 0.0010  end
densmult $mod3 2 5010 5011
0.0 1.0000
68.0 0.9161
131.8 0.8450
209.0 0.7344
272.1 0.6333
347.4 0.5100
416.4 0.3989
486.4 0.2811
556.3 0.1656

```

```

626.1 0.0572
660.3 0.0010 end
' change temperature in fuel
temperature $fuel1
0.0 960.29
68.0 960.29
131.8 960.71
209.0 958.68
272.1 954.18
347.4 946.12
416.4 937.15
486.4 926.04
556.3 914.37
626.1 904.09
660.3 897.82 end
temperature $fuel2
0.0 960.29
68.0 960.29
131.8 960.71
209.0 958.68
272.1 954.18
347.4 946.12
416.4 937.15
486.4 926.04
556.3 914.37
626.1 904.09
660.3 897.82 end
temperature $fuel3
0.0 960.29
68.0 960.29
131.8 960.71
209.0 958.68
272.1 954.18
347.4 946.12
416.4 937.15
486.4 926.04
556.3 914.37
626.1 904.09
660.3 897.82 end
end timetable
'
read burndata
power= 35.893 burn= 68.0 down=0 end
power= 35.893 burn= 63.8 down=0 end
power= 35.893 burn= 77.2 down=0 end
power= 35.893 burn= 63.1 down=0 end
power= 35.893 burn= 75.3 down=0 end
power= 35.893 burn= 69.0 down=0 end
power= 35.893 burn= 70.0 down=0 end
power= 35.893 burn= 69.9 down=0 end
power= 35.893 burn= 69.8 down=0 end
power= 35.893 burn= 34.2 down=1298 end
end burndata
'
read opus
units=grams
symnuc=u-234 u-235 u-236 u-238

```

```

        pu-238 pu-239  pu-240 pu-241 pu-242
        nd-143 nd-145  nd-146 nd-148 nd-150
        cs-134 cs-137
        eu-151 eu-153
        sm-147 sm-149  sm-150 sm-151 sm-152
        gd-155 cm-242  cm-243 cm-244 cm-245
        am-241 am-242m am-243 np-237 end
matl= 10 11 12 13 14 15 end
end opus
'
read model
TMI-1 Assy NJ070G rod 012 sample 012S4
read parm
run=yes drawit=yes fillmix=30 epsinner=-1e-4
cmfd=yes xycmfd=4 echo=yes
end parm
'
read materials
10 2 ! fuel pin ! end
11 2 ! test pin ! end
12 2 ! N neighbor ! end
13 2 ! W neighbor ! end
14 2 ! E neighbor ! end
15 2 ! Gd pin ! end
16 2 ! S neighbor ! end
17 2 ! fuel neighbor assy ! end
20 2 ! clad ! end
30 2 ! moderator! end
40 0 ! gap ! end
50 2 ! BPR abs ! end
51 2 ! BPR clad ! end
end materials
'
read geom
unit 1
com='fuel pin cell'
cylinder 1 0.4699
cylinder 2 0.47879
cylinder 3 0.5461
cuboid 4 4p0.72136
media 10 1 1
media 40 1 2 -1
media 20 1 3 -2
media 30 1 4 -3
boundary 4 4 4
unit 2
com='test pin'
cylinder 1 0.4699
cylinder 2 0.47879
cylinder 3 0.5461
cuboid 4 4p0.72136
media 11 1 1
media 40 1 2 -1
media 20 1 3 -2
media 30 1 4 -3
boundary 4 4 4
unit 3

```



com='N neighbor test pin'

cylinder 1 0.4699  
cylinder 2 0.47879  
cylinder 3 0.5461  
cuboid 4 4p0.72136  
media 12 1 1  
media 40 1 2 -1  
media 20 1 3 -2  
media 30 1 4 -3  
boundary 4 4 4

unit 4

com='E neighbor test pin'

cylinder 1 0.4699  
cylinder 2 0.47879  
cylinder 3 0.5461  
cuboid 4 4p0.72136  
media 13 1 1  
media 40 1 2 -1  
media 20 1 3 -2  
media 30 1 4 -3  
boundary 4 4 4

unit 5

com='W neighbor test pin'

cylinder 1 0.4699  
cylinder 2 0.47879  
cylinder 3 0.5461  
cuboid 4 4p0.72136  
media 14 1 1  
media 40 1 2 -1  
media 20 1 3 -2  
media 30 1 4 -3  
boundary 4 4 4

unit 6

com='Gd fuel pin'

cylinder 1 0.4699  
cylinder 2 0.47879  
cylinder 3 0.5461  
cuboid 4 4p0.72136  
media 15 1 1  
media 40 1 2 -1  
media 20 1 3 -2  
media 30 1 4 -3  
boundary 4 4 4

unit 7

com='BPR'

cylinder 1 0.4572  
cylinder 2 0.5461  
cylinder 3 0.63246  
cylinder 4 0.6731  
cuboid 5 4p0.72136  
media 50 1 1  
media 51 1 2 -1  
media 30 1 3 -2  
media 20 1 4 -3  
media 30 1 5 -4  
boundary 5 4 4

unit 8

```

com='left half fuel pin cell'
cylinder 1 0.4699 chord -x=0
cylinder 2 0.47879 chord -x=0
cylinder 3 0.5461 chord -x=0
cuboid 4 0.0 -0.72136 2p0.72136
media 10 1 1
media 40 1 2 -1
media 20 1 3 -2
media 30 1 4 -3
boundary 4 2 4
unit 9
com='bottom half fuel pin cell'
cylinder 1 0.4699 chord -y=0
cylinder 2 0.47879 chord -y=0
cylinder 3 0.5461 chord -y=0
cuboid 4 2p0.72136 0.0 -0.72136
media 10 1 1
media 40 1 2 -1
media 20 1 3 -2
media 30 1 4 -3
boundary 4 4 2
unit 10
com='quarter left-bottom instrument tube'
cylinder 1 0.56007 chord -x=0 chord -y=0
cylinder 2 0.62611 chord -x=0 chord -y=0
cuboid 3 0.0 -0.72136 0.0 -0.72136
media 30 1 1
media 20 1 2 -1
media 30 1 3 -2
boundary 3 2 2
unit 11
com='S neighbor test pin'
cylinder 1 0.4699
cylinder 2 0.47879
cylinder 3 0.5461
cuboid 4 4p0.72136
media 16 1 1
media 40 1 2 -1
media 20 1 3 -2
media 30 1 4 -3
boundary 4 4 4
unit 12
com='neighbor assy pin'
cylinder 1 0.4699
cylinder 2 0.47879
cylinder 3 0.5461
cuboid 4 4p0.72136
media 17 1 1
media 40 1 2 -1
media 20 1 3 -2
media 30 1 4 -3
boundary 4 4 4
unit 13
com='left half fuel pin cell neigh assy'
cylinder 1 0.4699 chord -x=0
cylinder 2 0.47879 chord -x=0
cylinder 3 0.5461 chord -x=0

```

```

cuboid 4 0.0 -0.72136 2p0.72136
media 17 1 1
media 40 1 2 -1
media 20 1 3 -2
media 30 1 4 -3
boundary 4 2 4
unit 14
com='top half fuel pin cell'
cylinder 1 0.4699 chord +y=0
cylinder 2 0.47879 chord +y=0
cylinder 3 0.5461 chord +y=0
cuboid 4 2p0.72136 0.72136 0.0
media 17 1 1
media 40 1 2 -1
media 20 1 3 -2
media 30 1 4 -3
boundary 4 4 2
unit 15
com='quarter left-top instrument tube'
cylinder 1 0.56007 chord -x=0 chord +y=0
cylinder 2 0.62611 chord -x=0 chord +y=0
cuboid 3 0.0 -0.72136 0.72136 0.0
media 30 1 1
media 20 1 2 -1
media 30 1 3 -2
boundary 3 2 2
unit 16
com='guide tube'
cylinder 3 0.63246
cylinder 4 0.6731
cuboid 5 4p0.72136
media 30 1 3
media 20 1 4 -3
media 30 1 5 -4
boundary 5 4 4
unit 17
com='1/4 of top assembly'
cuboid 10 10.90549 0.0 10.90549 0.0
array 1 10 place 1 1 0.80645 0.80645
media 30 1 10
boundary 10 15 30
unit 18
com='1/4 of bottom assembly'
cuboid 10 10.90549 0.0 10.90549 0.0
array 2 10 place 1 1 0.80645 0.0
media 30 1 10
boundary 10 15 30
global unit 20
cuboid 10 10.90549 0.0 21.81098 0.0
array 3 10 place 1 1 0.0 0.0
media 30 1 10
boundary 10 15 30
end geom
read array
ara=1 nux=8 nuy=8 typ=cuboidal
fill
1 1 4 2 5 1 1 8

```

```

    1  6  1  3  1  1  1  8
    1  1  1  1  1  7  1  8
    1  1  1  7  1  1  1  8
    1  1  1  1  1  1  1  8
    1  1  7  1  1  7  1  8
    1  1  1  1  1  1  1  8
    9  9  9  9  9  9  9 10
end fill
ara=2 nux=8 nuy=8 typ=cuboidal
fill
  14 14 14 14 14 14 14 15
  12 12 12 12 12 12 12 13
  12 12 16 12 12 16 12 13
  12 12 12 12 12 12 12 13
  12 12 12 16 12 12 12 13
  12 12 12 12 12 16 12 13
  12 12 12 12 12 12 12 13
  12 12 12 11 12 12 12 13
end fill
ara=3 nux=1 nuy=2 typ=cuboidal
fill
  18
  17
end fill
end array
read bounds
-x=white +x=ref -y=ref +y=ref
end bounds
end model
end
=shell
cp ft71f001 $RTNDIR/O12S4.den
end

```

## B.2 Sample 87-72 from Rod MKP-109 in Calvert Cliffs Assembly D047

```
=t-depl parm=(nitawl,addnux=3)
Calvert Cliffs Assembly D047 Rod MKP109 Sample 87-72
44groupndf
read alias
  $fuel1 10 11 12 13 14 15 end
  $clad1 20 21 22 23 24 25 end
  $mod1 30 31 32 33 34 35 end
  $gap1 40 41 42 43 44 45 end
end alias
read comp
  uo2  $fuel1 den=10.045 1 841 92234 0.027
      92235 3.038
      92236 0.014
      92238 96.921 end

  zirc4 $clad1 1 620 end
  h2o  $mod1 den=0.7569 1 558 end
  arbmb 0.7569 1 1 0 0 5000 100 $mod1 330.8e-06 558 end
  n  $gap1 den=0.00125 1 620 end
' guide tube
  zirc4 5 1 558 end
end comp
'
read celldata
  latticecell squarepitch pitch=1.4732 $mod1
      fueld=0.9563 $fuel1
      gapd=0.9855 $gap1
      cladd=1.1176 $clad1 end

end celldata
''
read timetable
  density $mod1 2 5010 5011
0.00 1.000
377.00 1.000
377.01 1.419
840.00 1.419
840.01 1.523
1391.00 1.523
1391.01 1.488
1852.10 1.488 end
end timetable
'
read depletion
  10 -11 12 13 14 15 end
end depletion
'
read burndata
  power=24.53 burn=306 nlib=3 down=71 end
  power=26.55 burn=381.7 nlib=3 down=81.3 end
  power=22.66 burn=466 nlib=3 down=85 end
  power=18.72 burn=461.1 nlib=3 down=1870 end
end burndata
'
read opus
```

```

units=grams
symnuc= u-234 u-235 u-236 u-238 pu-238 pu-239 pu-240
        pu-241 pu-242 np-237 am-241 cm-243 cm-244 cs-133
        cs-134 cs-135 cs-137 eu-154 nd-143 nd-144 nd-145
        nd-146 nd-148 nd-150 pm-147 sm-147 sm-148 sm-149
        sm-150 sm-151 sm-152 sm-154 eu-151 eu-153 eu-154
        eu-155 gd-154 gd-155 end
matl= 0 10 11 12 13 14 15 end
end opus

read model
Calvert Cliffs Rod MKP109 Sample mkp109-2
read parm
run=yes drawit=no fillmix=30 echo=yes
cmfd=yes xycmfd=4 epsinner=-1e-4
end parm
read materials
10 1 ! regular pin ! end
11 1 ! test pin ! end
12 1 ! N test pin ! end
13 1 ! S test pin ! end
14 1 ! E test pin ! end
15 1 ! W test pin ! end
20 1 ! clad ! end
30 2 ! moderator ! end
40 0 ! gap ! end
5 1 ! guide tube ! end
end materials
read geom
unit 1
com='regular fuel pin'
cylinder 10 .47815
cylinder 20 .49275
cylinder 30 .5588
cuboid 40 4p0.7366
media 10 1 10
media 40 1 20 -10
media 20 1 30 -20
media 30 1 40 -30
boundary 40 4 4
unit 2
com='test fuel pin'
cylinder 10 .47815
cylinder 20 .49275
cylinder 30 .5588
cuboid 40 4p0.7366
media 11 1 10
media 40 1 20 -10
media 20 1 30 -20
media 30 1 40 -30
boundary 40 4 4
unit 3
com='N test fuel pin'
cylinder 10 .47815
cylinder 20 .49275
cylinder 30 .5588
cuboid 40 4p0.7366

```

```

media 12 1 10
media 40 1 20 -10
media 20 1 30 -20
media 30 1 40 -30
boundary 40 4 4
unit 4
com='S test fuel pin'
cylinder 10 .47815
cylinder 20 .49275
cylinder 30 .5588
cuboid 40 4p0.7366
media 13 1 10
media 40 1 20 -10
media 20 1 30 -20
media 30 1 40 -30
boundary 40 4 4
unit 5
com='E test fuel pin'
cylinder 10 .47815
cylinder 20 .49275
cylinder 30 .5588
cuboid 40 4p0.7366
media 14 1 10
media 40 1 20 -10
media 20 1 30 -20
media 30 1 40 -30
boundary 40 4 4
unit 6
com='W test fuel pin'
cylinder 10 .47815
cylinder 20 .49275
cylinder 30 .5588
cuboid 40 4p0.7366
media 15 1 10
media 40 1 20 -10
media 20 1 30 -20
media 30 1 40 -30
boundary 40 4 4
unit 71
com='guide tube - 1/4 NE'
cylinder 1 1.314 chord +x=0 chord +y=0
cylinder 2 1.416 chord +x=0 chord +y=0
cuboid 3 1.473 0 1.473 0
media 30 1 1
media 5 1 2 -1
media 30 1 3 -2
boundary 3 4 4
unit 72
com='guide tube - 1/4 SE'
cylinder 1 1.314 origin x=0 y=1.473 chord +x=0 chord -y=1.473
cylinder 2 1.416 origin x=0 y=1.473 chord +x=0 chord -y=1.473
cuboid 3 1.473 0 1.473 0
media 30 1 1
media 5 1 2 -1
media 30 1 3 -2
boundary 3 4 4
unit 73

```

```

com='guide tube - 1/4 SW'
cylinder 1 1.314 origin x=1.473 y=1.473 chord -x=1.473 chord -y=1.473
cylinder 2 1.416 origin x=1.473 y=1.473 chord -x=1.473 chord -y=1.473
cuboid 3 1.473 0 1.473 0
media 30 1 1
media 5 1 2 -1
media 30 1 3 -2
boundary 3 4 4
unit 74
com='guide tube - 1/4 NW'
cylinder 1 1.314 origin x=1.473 y=0 chord -x=1.473 chord +y=0
cylinder 2 1.416 origin x=1.473 y=0 chord -x=1.473 chord +y=0
cuboid 3 1.473 0 1.473 0
media 30 1 1
media 5 1 2 -1
media 30 1 3 -2
boundary 3 4 4
global unit 10
cuboid 10 20.78 0.0 10.39 0.0
array 1 10 place 1 1 0.8142 0.7366
media 30 1 10
boundary 10 28 14
end geom
,
read array
ara=1 nux=14 nuy=7
fill
1 1 1 1 1 1 74 71 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 73 72 1 1 4 1 1 1 73 72 1 1
1 1 74 71 1 1 6 2 5 1 1 74 71 1 1
1 1 1 1 1 1 3 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 end fill
end array
read bounds
all=refl
end bounds
end data
end
=shell
cp ft71f001 $RTNDR/87-72.den
end

```



### B.3 Sample SF97-3 from Rod SF97 in Takahama-3 Assembly NT3G23

```
=t-depl parm=(nitawl,addnux=3)
Takahama-3 Rod SF97 Sample SF97-3
44groupndf
read alias
  $fuel1 10 11 12 13 14 15 16 end
  $clad1 20 21 22 23 24 25 26 end
  $mod1 30 31 32 33 34 35 36 end
  $gap1 40 41 42 43 44 45 46 end
  $fuel2 17 end
  $clad2 27 end
  $mod2 37 end
  $gap2 47 end
end alias
read comp
  uo2  $fuel1 den=10.412 1 900 92234 0.04
      92235 4.11
      92238 95.85 end

  zirc4 $clad1 1 600 end
  h2o  $mod1 den=0.6843 1 591.48 end
  arbmb 0.6843 1 1 0 0 5000 100 $mod1 1154e-06 591.48 end
  n  $gap1 den=0.00125 1 600 end
  uo2  $fuel2 den=10.412 0.94 900 92234 0.02
      92235 2.63
      92238 97.35 end

  arbmgd 10.412 2 0 1 0 64000 2 8016 3 $fuel2 0.06 900 end
  zirc4 $clad2 1 600 end
  h2o  $mod2 den=0.6843 1 591.48 end
  arbmb 0.6843 1 1 0 0 5000 100 $mod2 1154e-06 591.48 end
  n  $gap2 den=0.00125 1 600 end
end comp
,
read celldata
  latticecell squarepitch pitch=1.259 $mod1
      fueld=0.805 $fuel1
      gapd=0.822 $gap1
      cladd=0.950 $clad1 end
  latticecell squarepitch pitch=1.259 $mod2
      fueld=0.805 $fuel2
      gapd=0.822 $gap2
      cladd=0.950 $clad2 end

end celldata
,
read depletion
  10 -11 12 13 14 15 16 17 end
end depletion
,
read burndata
  power=35.162 burn=385 nlib=3 down=88 end
  power=37.498 burn=402 nlib=3 down=62 end
  power=33.282 burn=406 nlib=3 down=1446 end
end burndata
,
read opus
```

```

units=grams
symnuc= u-234 u-235 u-236 u-238 np-237 pu-238 pu-239
        pu-240 pu-241 pu-242 am-241 am-242m am-243 cm-242
        cm-243 cm-244 cm-245 cm-246 cm-247 nd-143 nd-144
        nd-145 nd-146 nd-148 nd-150 cs-137 cs-134 eu-154
        ce-144 sb-125 ru-106 sm-147 sm-148 sm-149 sm-150
        sm-151 sm-152 sm-154 end
matl=0 10 11 12 13 14 15 16 17 end
end opus

read timetable
density $mod1 2 5010 5011
0 1.000
106 0.775
205 0.564
306 0.350
385 0.182
473 0.981
592 0.749
704 0.531
817 0.310
875 0.198
937 1.000
996 0.867
1048 0.751
1100 0.634
1152 0.518
1204 0.401
1256 0.285
1308 0.169
1342 0.090 end
density $mod2 2 5010 5011
0 1.000
106 0.775
205 0.564
306 0.350
385 0.182
473 0.981
592 0.749
704 0.531
817 0.310
875 0.198
937 1.000
996 0.867
1048 0.751
1100 0.634
1152 0.518
1204 0.401
1256 0.285
1308 0.169
1342 0.090 end
end timetable

read model
Takahama-3 Rod SF97 Sample SF97-3
read parm
run=yes drawit=no fillmix=30 echo=yes

```

```

cmfd=yes xycmfd=4 epsinner=-1e-4
end parm
read materials
  10 1 ! regular pin ! end
  11 1 ! test pin ! end
  12 1 ! N test pin ! end
  13 1 ! NE test pin ! end
  14 1 ! E test pin ! end
  15 1 ! W test pin ! end
  16 1 ! SW test pin ! end
  17 1 ! gadolinia pin ! end
  20 1 ! clad ! end
  30 2 ! moderator ! end
  40 0 ! gap ! end
end materials
read geom
unit 1
com='regular fuel pin'
cylinder 10 .4025
cylinder 20 .411
cylinder 30 .475
cuboid 40 4p0.6295
media 10 1 10
media 40 1 20 -10
media 20 1 30 -20
media 30 1 40 -30
boundary 40 4 4
unit 2
com='test fuel pin'
cylinder 10 .4025
cylinder 20 .411
cylinder 30 .475
cuboid 40 4p0.6295
media 11 1 10
media 40 1 20 -10
media 20 1 30 -20
media 30 1 40 -30
boundary 40 4 4
unit 3
com='N test fuel pin'
cylinder 10 .4025
cylinder 20 .411
cylinder 30 .475
cuboid 40 4p0.6295
media 12 1 10
media 40 1 20 -10
media 20 1 30 -20
media 30 1 40 -30
boundary 40 4 4
unit 4
com='NE test fuel pin'
cylinder 10 .4025
cylinder 20 .411
cylinder 30 .475
cuboid 40 4p0.6295
media 13 1 10
media 40 1 20 -10

```

```

media 20 1 30 -20
media 30 1 40 -30
boundary 40 4 4
unit 5
com='E test fuel pin'
cylinder 10 .4025
cylinder 20 .411
cylinder 30 .475
cuboid 40 4p0.6295
media 14 1 10
media 40 1 20 -10
media 20 1 30 -20
media 30 1 40 -30
boundary 40 4 4
unit 6
com='Gd203 fuel pin'
cylinder 10 .4025
cylinder 20 .411
cylinder 30 .475
cuboid 40 4p0.6295
media 17 1 10
media 40 1 20 -10
media 20 1 30 -20
media 30 1 40 -30
boundary 40 4 4
unit 7
com='guide tube'
cylinder 10 .5715
cylinder 20 .6121
cuboid 40 4p0.6295
media 30 1 10
media 20 1 20 -10
media 30 1 40 -20
boundary 40 4 4
unit 8
com='W test fuel pin'
cylinder 10 .4025
cylinder 20 .411
cylinder 30 .475
cuboid 40 4p0.6295
media 15 1 10
media 40 1 20 -10
media 20 1 30 -20
media 30 1 40 -30
boundary 40 4 4
unit 9
com='SW test fuel pin'
cylinder 10 .4025
cylinder 20 .411
cylinder 30 .475
cuboid 40 4p0.6295
media 16 1 10
media 40 1 20 -10
media 20 1 30 -20
media 30 1 40 -30
boundary 40 4 4
unit 12

```

```

com='bottom half of regular fuel pin'
cylinder 10 .4025 chord -y=0
cylinder 20 .411 chord -y=0
cylinder 30 .475 chord -y=0
cuboid 40 2p0.6295 0.0 -0.6295
media 10 1 10
media 40 1 20 -10
media 20 1 30 -20
media 30 1 40 -30
boundary 40 4 2
unit 72
com='bottom half of guide tube'
cylinder 10 .5715 chord -y=0
cylinder 20 .6121 chord -y=0
cuboid 40 2p0.6295 0.0 -0.6295
media 30 1 10
media 20 1 20 -10
media 30 1 40 -20
boundary 40 4 2
global unit 10
cuboid 10 21.403 0.0 10.7015 0.0
array 1 10 place 1 1 0.6295 0.6295
media 30 1 10
boundary 10 34 34
end geom
'
read array
ara=1 nux=17 nuy=9
fill
1 1 1 1 1 1 1 5 2 8 1 1 1 1 1 1 1
1 1 1 1 1 1 1 4 3 9 1 1 1 1 1 1 1
1 1 1 1 6 7 1 1 7 1 1 7 6 1 1 1 1
1 1 1 7 1 1 1 1 6 1 1 1 1 7 1 1 1
1 1 6 1 1 1 1 1 1 1 1 1 1 6 1 1
1 1 7 1 1 7 1 1 7 1 1 7 1 1 7 1 1
1 1 1 1 1 1 6 1 1 1 6 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
12 12 72 12 12 72 12 12 72 12 12 72 12 12 72 12 12 end fill
end array
read bounds
all=refl
end bounds
end data
end
=shell
cp ft71f001 $RTNDIR/sf97-3.den
end

```



<b>NRC FORM 335</b> (9-2004) NRCMD 3.7  <p style="text-align: center;"><b>BIBLIOGRAPHIC DATA SHEET</b>  <i>(See instructions on the reverse)</i></p>	<b>U.S. NUCLEAR REGULATORY COMMISSION</b>  <b>1. REPORT NUMBER</b> <i>(Assigned by NRC, Add Vol., Supp., Rev., and Addendum Numbers, if any.)</i>  NUREG/CR-6968 (ORNL/TM-2008/071)				
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<b>10. SUPPLEMENTARY NOTES</b> M. Aissa, NRC Project Manager					
<b>11. ABSTRACT</b> <i>(200 words or less)</i>  This report is part of a report series designed to document benchmark-quality radiochemical isotopic assay data against which computer code accuracy can be quantified to establish the uncertainty and bias associated with the code predictions. The experimental data included in the report series were acquired from domestic and international programs and include spent fuel samples that cover a large burnup range. The measurements analyzed in the current report, for which experimental data is publicly available, include 38 spent fuel samples selected from fuel rods with a 2.6 to 4.7 wt % U-235 initial enrichment that were irradiated in three pressurized water reactors operated in the United States and Japan and achieved burnup values from 14 to 56 GWd/MTU. The analysis of the measurements was performed by employing the two-dimensional depletion sequence TRITON in the SCALE code system.					
<b>12. KEY WORDS/DESCRIPTORS</b> <i>(List words or phrases that will assist researchers in locating the report.)</i>  SCALE, TRITON, ORIGEN-S, spent nuclear fuel, isotopic validation, burnup credit, radiochemical analysis, experimental programs, Calvert Cliffs, Takahama, TMI-1	<b>13. AVAILABILITY STATEMENT</b> unlimited  <b>14. SECURITY CLASSIFICATION</b> <i>(This Page)</i> unclassified  <i>(This Report)</i> unclassified  <b>15. NUMBER OF PAGES</b>  <b>16. PRICE</b>				

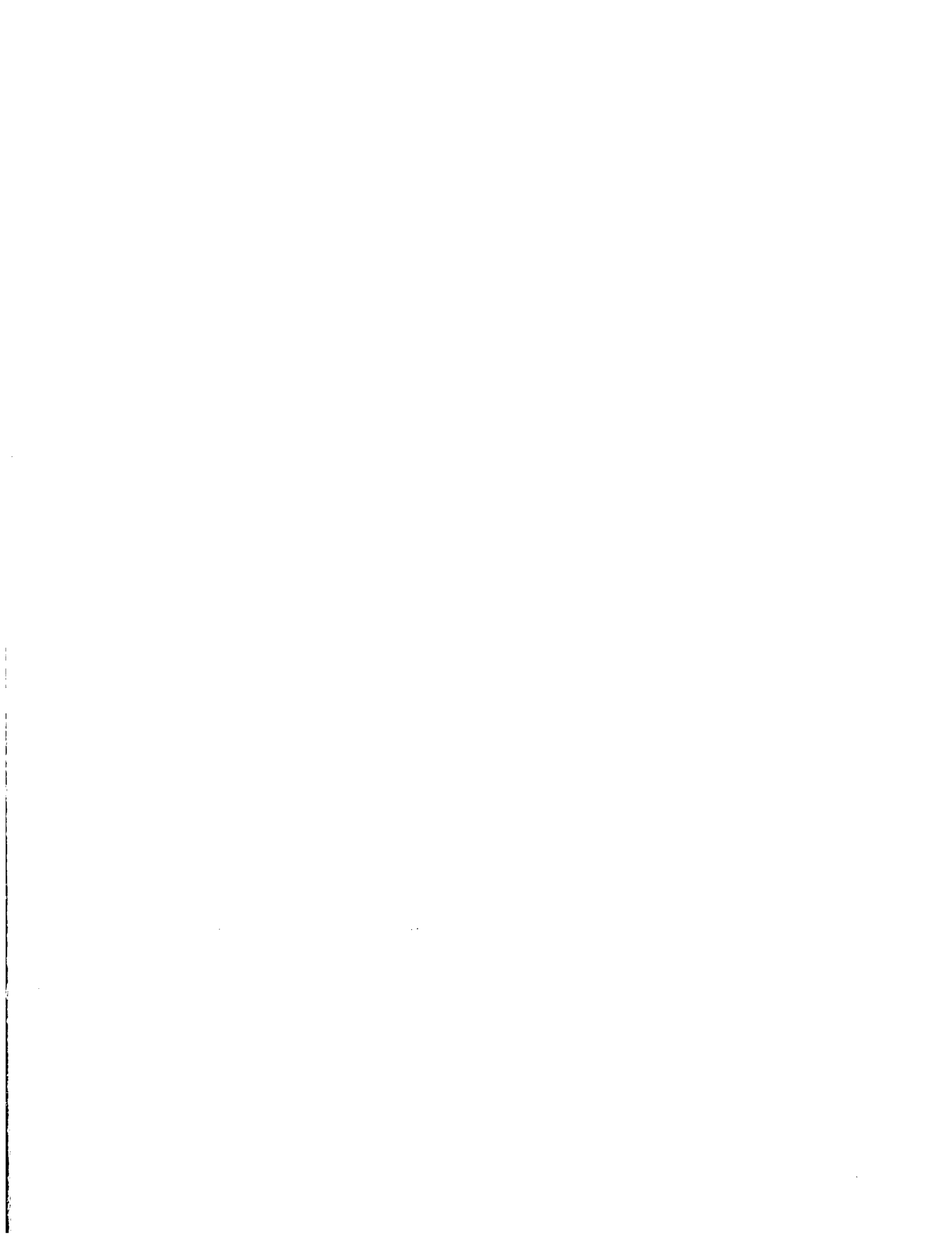


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