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Civilian Radioactive Waste Management System
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Summary Report of SNF Isotopic Comparisons for the Disposal Criticality Analysis Methodology

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1.0 INTRODUCTION

The "Summary Report of SNF Isotopic Comparisons for the Disposal Criticality Analysis Methodology" contains a summary of the analyses that compare SNF measured isotopic concentrations (radiochemical assays) to calculated SNF isotopic concentrations (SAS2H module of Scale 4.3). The results of these analyses are used to support the validation of the isotopic models for spent commercial light water reactor (LWR) fuel.

1.1 Background

The United States Department of Energy (DOE) Office of Civilian Radioactive Waste Management (OCRWM) is developing a methodology for criticality analysis to support disposal of commercial spent nuclear fuel in a geologic repository. A topical report on the disposal criticality analysis methodology is scheduled to be submitted to the United States Nuclear Regulatory Commission (NRC) for formal review in 1998. This technical report in one of a series of reports that provides a summary of the analyses results that support the development of the disposal criticality analysis methodology.

1.2 Objective

The objective of this report is to present a summary of the analysis results for the SNF isotopic comparisons. Results from these analyses will support the development and validation of the isotopic model used for criticality analyses involving commercial LWR spent nuclear fuel (SNF). These models and their validation will be discussed in the Disposal Criticality Analysis Methodology Topical Report.

1.3 Scope

The scope of this Summary Report is to compare measured SNF isotopic concentrations to calculated isotopic concentrations for the following reactors:

Pressurized Water Reactors (PWRs):	Calvert Cliffs,
	Obrigheim,
	H. B. Robinson,
	Turkey Point,
	Trino Vercelles,
	Yankee Rowe, and
	Mihama.
Boiling Water Reactors (BWRs):	Cooper .

Assay measurements may be performed on Three Mile Island Unit 1, Quad Cities Unit 1, and Dresden. Also, search is underway for other samples for which measurements have already been performed (e.g. French data). Similar isotopic comparison analyses may be performed on these samples if data becomes available. Additional discussion concerning the isotopic concentration measurements are to be provided in future revision(s) of this report.

1.4 Quality Assurance

The Civilian Radioactive Waste Management System (CRWMS) Management and Operating Contractor (M&O) Quality Assurance (QA) program applies to the development of this report. The results provided in this report will be used to develop the methodology for evaluating the Mined Geologic Disposal System (MGDS) waste package and engineered barrier segment; the waste package and engineered barrier segment have been identified as MGDS Q-List items important to safety and waste isolation (Reference 1). The waste package is on the Q-List by direct inclusion by the DOE; a QAP-2-3 evaluation has yet to be conducted. There are no determination of importance evaluations developed in accordance with Nevada Line Procedure, NLP-2-0, since the report does not involve any field activity.

The Waste Package Development Department responsible manager has evaluated the technical document development activity in accordance with QAP-2-0 Conduct of Activities. The "Develop Technical Documents" (Reference 2) evaluation has determined the preparation and review of this technical documents is subject to *Quality Assurance Requirements and Description* (QARD, Reference 3) controls.

The results provided in this report are drawn from various evaluations developed under the CRWMS M&O QA program. The data used in the evaluations are drawn from various reports and have supported prior licensing submittals in which the NRC has accepted such data as established fact. The results therefore will be considered acceptable for quality affecting activities and for use in analyses affecting procurement, construction, or fabrication.

No computer software subject to the requirements of the QARD was used in the development of this report. The results reported in this document were drawn from various analyses which did use software subject to the requirements of the QARD. The details of the computer software approved for quality affecting work used to generate the results are provided in the various individual analyses referenced by this report.

2.0 ANALYSIS MODEL

This section provides a description of the isotopic model used in generating the supporting analysis results reported in this document. The isotopic model was used to calculate material isotopic concentrations of the irradiated commercial LWR fuel for comparison with the measure isotopic concentrations. The comparison of the calculated and measured concentrations will be used in developing and validating the isotopic model for use in determining commercial SNF fissionable and absorbing isotope concentrations for disposal criticality evaluations.

The code system used in the isotopic model is the SAS2H sequence of the SCALE 4.3 computer code system (Reference 4). SAS2H is the control module for the analytical sequence. The functional modules (or codes) within the sequence are BONAMI-S, NITAWL-S, XSDRNPM-S, COUPLE, and ORIGEN-S. SAS2H converts user input data into the forms required by the functional modules. BONAMI-S and NITAWL-S perform problem-dependent resonance processing of neutron cross sections. XSDRNPM-S is a one-dimensional discrete-ordinates code that produces a weighted cross section library and spectra data. This data is used by COUPLE to update an ORIGEN-S data library. ORIGEN-S is a point-depletion/decay code that computes the time-dependent isotopic concentrations using the matrix exponential expansion technique. For short-lived nuclides, a form of the Bateman equation is used to ensure better accuracy. ORIGEN-S computes the isotopic concentrations (actinides and fission products) for all required conditions. This includes both power operation and shutdown intervals while the fuel is in the reactor. ORIGEN-S is also used in calculating radioactive decay and daughter isotope buildup after the fuel is withdrawn from the reactor core. Since ORIGEN-S is a point model, spatial and spectral effects are not explicitly modeled. However, spatial and spectral effects are incorporated in the model through the one-dimensional spatial and the 44 energy group spectral weighting of cross section data by XSDRNPM-S.

A fuel assembly is modeled with SAS2H in one-dimensional (1-D) cylindrical geometry. This modeling is a two step process. First, the fuel is represented as an infinite lattice of fuel rods with XSDRNPM-S, where resonance data is obtained from BONAMI-S and NITAWL-S. Second, cell-spectrum-weighted cross sections from XSDRNPM-S are then applied to the fuel zone in a larger cell model representing part or all of a fuel assembly within an infinite lattice. Material and volume ratios for the zones must be appropriate for the physical system being represented. Weighted cross section and spectra data from this model are used by COUPLE to update the ORIGEN-S data library. ORIGEN-S performs point depletion calculations to provide updated isotopic concentrations that are fed back to the one-dimensional model. The first step is then repeated and new weighted cross section and spectra data are determined for the next depletion calculation. Updating of the ORIGEN-S library for depletion time steps is performed to appropriately represent changes (with depletion) in the neutron energy spectrum within the fuel assembly. A more detailed discussion of the SAS2H modeling for PWR and BWR fuel is presented below.

[Note: For BWR fuel, additional weighting of cross section data is necessary to accommodate the additional heterogeneities present within the fuel assemblies. A BWR SAS2H model is currently under development to accommodate these heterogeneities.]

2.1 SAS2H

The description of the SAS2H control module and the associated calculational modules presented in this paper is a summary of the discussion presented in the SCALE 4.3 users manual (Reference 5).

In the analysis procedure for calculation of isotopic concentrations, the SAS2H control module of the SCALE modular code system is used to perform a sequence of fuel depletion and decay calculations required to obtain spent fuel isotopic compositions. The objectives of SAS2H with respect to these analyses include the following:

1) predict spent fuel characteristics for spent fuel assemblies having a specified reactor history;
2) apply standard analytical models that represent the physics of the system being analyzed (within the 1-D transport limits of the problem);
3) apply acceptable and documented data bases that can be updated in the future;
4) automate the use of known methods of calculating some of the input parameters and the selection of appropriate control options for the various codes applied in the analysis.

SAS2H calculates the time-dependent fuel composition of a reactor fuel assembly by sequencing five independently tasked calculational modules of the SCALE code system. The sequence implemented by SAS2H results in an iterative burnup calculational procedure in which two separate lattice-cell calculations are performed for each iteration to determine the appropriate neutron spectrum and associated nuclide cross sections. At specified times during the burnup, the cross-sections are updated using resonance processing codes and 1-D transport analyses. These updated cross-sections are used in point depletion calculations that produce the time-dependent fuel compositions required for the next cross-section update. This procedure is repeated numerous times over the operating history of the reactor to obtain the desired burnup of the fuel composition.

The 1-D transport analyses required to obtain the relevant neutron flux distribution necessary for cross-section weighting is performed on two separate lattice-cells to approximate two-dimensional (2-D) effects that are introduced in fuel assemblies containing guide tubes, burnable poison rods (BPRs), control rods, and axial power shaping rods. A general description of the two-part neutron flux distribution calculation is provided in Section 2.4. The axial variation in the neutron flux is not considered in the SAS2H sequence.

The SAS2H control module reads a set of well defined user input. The user input is converted by the SAS2H control module into the data required by each calculational module to perform the necessary calculations relevant to fuel depletion and decay. The basic user input required by the SAS2H control sequence includes the following:

1) the material zone dimensions of the fuel-pin cell and the larger unit cell representation of the fuel assembly used to incorporate 2-D effects;
2) the material densities of the fresh fuel assembly;
3) the material temperatures;
4) the specific power, exposure time and shutdown time of the fuel assembly in each appropriate cycle of the reactor history;

5) the various control parameters used to select libraries, the optional parameters preferred over the defaults for each calculational module, the level of output printout, and the modifications to the transport computations (e.g., the fineness of mesh intervals or the problem convergence criteria).

The SCALE system driver invokes the execution of the various calculational modules in the SAS2H control sequence and returns control to the SAS2H sequence. The pertinent results obtained from a calculational module are processed by SAS2H and used to generate the input data for subsequent calculational modules. Passes through the functional modules are repeated until the case is completed.

2.2 Overview of Calculational Modules

The SAS2H control sequence accesses five calculational modules of the SCALE code system for performing fuel depletion and decay calculations. The five calculational modules include BONAMI-S, NITAWL-S, XSDRNPM-S, COUPLE, and ORIGEN-S. Each of the calculational modules have a specific purpose in the sequence to perform the fuel depletion and decay calculations.

The BONAMI-S calculational module applies the Bondarenko method of resonance self-shielding to nuclides for which Bondarenko data is available.

The NITAWL-II calculational module performs Nordheim resonance self-shielding corrections for nuclides that have resonance parameter data available.

The XSDRNPM-S calculational module performs a 1-D neutron transport calculation on a specified geometry to facilitate production of cell-weighted cross-sections for fuel depletion calculations.

The COUPLE calculational module updates all cross-section constants included on an ORIGEN-S nuclear data library with data from the cell-weighted cross-section library obtained from the XSDRNPM-S calculation. Additionally, the weighting spectrum produced by XSDRNPM-S is applied to update all nuclides in the ORIGEN-S library which were not included in the XSDRNPM-S calculation.

The ORIGEN-S calculational module performs a zero- dimensional nuclide generation and depletion calculation for a specified reactor fuel history. A decay calculation is also performed by ORIGEN-S for prescribed down times during the reactor history.

2.3 General Description of Method

The method applied by SAS2H starts with the data describing a fuel assembly or node of a fuel assembly as it is initially loaded into a particular reactor. The composition, temperatures, geometry, and time-dependent specific power of the fuel assembly are required inputs to SAS2H. For each time-dependent fuel composition, the SAS2H sequence performs a 1-D neutron transport analysis using XSDRNPM-S and a two-part procedure incorporating two separate lattice-cell models. The first model is a unit fuel-pin cell from which cell-weighted cross-sections are obtained. The second

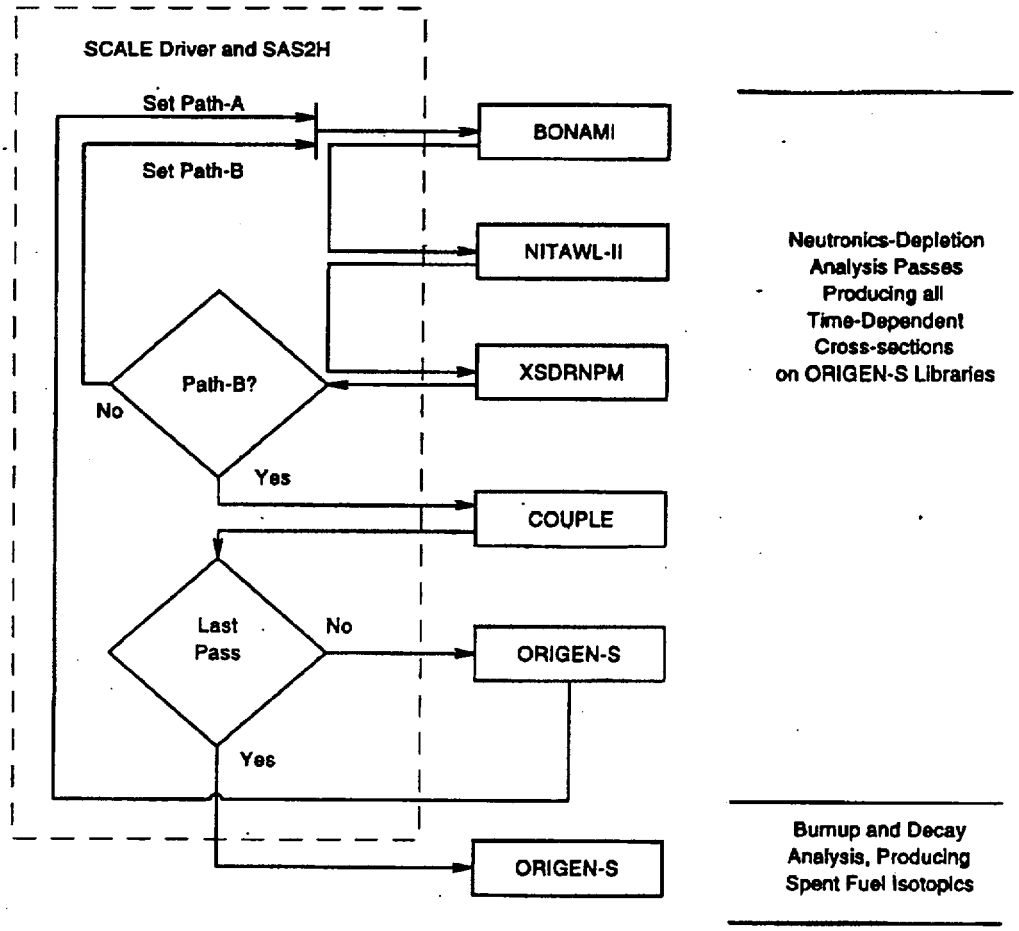
model represents a larger unit cell within an infinite lattice. The material zones of the larger unit cell can be structured for different types of light-water reactor fuel assemblies containing water holes, burnable absorber rods, gadolinium fuel rods, etc. Problem-dependent resonance self-shielding of the cross-sections is performed using the BONAMI-S and NITAWL-II calculational modules (Reference 5, p. S2.2.2).

The neutron flux spectrum obtained from the larger unit cell model is used to determine the appropriate nuclide cross-sections for the specified burnup-dependent fuel composition. The cross-sections derived from a transport analysis at each time step are used in an ORIGEN-S point-depletion calculation that produces the burnup-dependent fuel compositions to be used in the next spectrum calculation. This sequence is repeated over the prescribed operating history of the reactor. Ultimately, the nuclide inventory (actinides, fission products, and light elements) is computed at the burnup corresponding to the discharge of the assembly from the reactor. The buildup and decay of the nuclides in the fuel assembly are computed by ORIGEN-S for the down times relevant to reactor operation (Reference 5, p. S2.2.2).

2.4 Preparation of Fuel Cross-Sections

The preparation of fuel cross-sections employs a two-part calculational procedure that utilizes two separate 1-D neutron transport calculations performed on different models to account for 2-D variations in fuel assembly design. The calculational flow path invoked by SAS2H is illustrated in Figure 2-1 (Reference 5, p. S2.2.4).

Figure 2-1. Calculational Flow Path Invoked by SAS2H



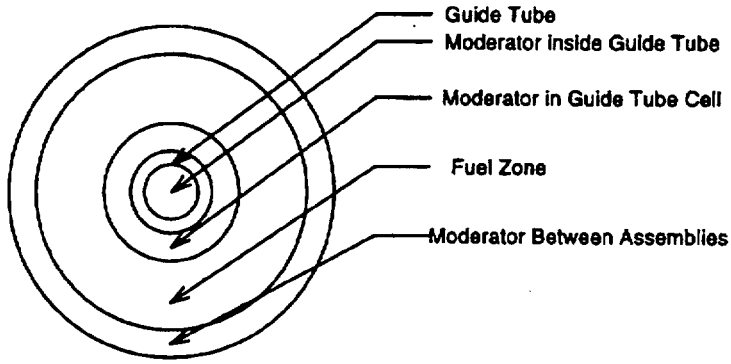
The upper part of Figure 2-1 shows the flow path for the neutronics-depletion analysis "passes" that create a cross-section library at specified burnup intervals. First, in path A, BONAMI-S, NITAWL-II, and XSDRNPM-S are invoked to produce the cell-weighted cross-sections of the fuel zone. The second return to the driver for path B of the reactor pass invokes all five calculational modules. The compositions for the first reactor pass are simply the nuclide mixtures of the new, or freshly loaded, fuel assembly. After completion of the path A and path B computations, execution continues with COUPLE updating an ORIGEN-S working library with data on the XSDRNPM-S weighted working library. The ORIGEN-S calculational module is invoked to compute the time-dependent densities of the nuclides in the fuel and burnable poison for the specified power and exposure times. SAS2H is then invoked for the next control function in the sequence.

The path A and path B models both utilize the same calculational modules (BONAMI-S, NITAWL-II, and XSDRNPM), but the models themselves are quite different. The path A model is simply a one-dimensional representation of an assembly unit cell containing a fuel rod. The fuel rod is modeled explicitly with the square unit cell perimeter converted to a circular perimeter maintaining the same total unit cell area. A white boundary condition is applied to the perimeter of the path A unit cell to simulate an infinite array of unit cells. The resonance self-shielding calculations and a 1-D neutron transport calculation are then performed on the path A model to obtain the neutron flux

and cell-weighted cross-sections for the fuel region. The cell-weighted cross-sections from the path A model are then applied to the fuel region in the path B model.

The path B model is a larger unit cell representation of all or part of the fuel assembly in an infinite lattice. The path B model is used to calculate an "assembly-averaged" fuel region flux that considers the effects due to the path A model, the assembly lattice locations containing different types of rods or water holes, and the moderator present in assembly-to-assembly spacings. The use of cell-weighted cross-sections from the path A model in the 1-D neutron transport calculation of the path B model is an approximate method for simulating 2-D effects present in fuel assemblies containing guide tubes and burnable poison rods. An example of a typical path B larger unit cell model for a PWR assembly containing guide tubes is presented in Figure 2-2.

Figure 2-2. Typical Path B Model for PWR Control Rod Assembly



Typical PWR Control Rod Assembly, After Withdrawal of Control Rods

The essential rule in deriving the zone radii is to maintain the fuel-to-moderator volume ratio in the actual assembly. The central region of the larger cell can be modeled as an assembly guide tube, a burnable poison rod containing no fuel, an orifice rod, an axial power shaping rod, a fuel rod containing a burnable poison, or almost any other pin-cell type rod. The moderator of the central region in the path B model is the moderator associated with the assembly lattice unit cell modeled in the central region. A fuel region surrounds the central unit cell moderator. The radius of the fuel region is determined such that the volume ratio of fuel to moderator in the assembly is maintained in the path B model. The region surrounding the fuel in the path B model may be composed of assembly housing material (for BWRs) or moderator between assemblies by conserving volumes. The assembly spacer grids and other hardware are typically either ignored or homogenized into the assembly moderator material due to their limited effect on the neutron flux and associated energy spectrum.

There are certain approximations made in developing the path B model. Two important approximations relevant to these analyses include:

1) the path B model assumes that the distribution of the non-fuel pin-cell locations are equidistantly spaced throughout the assembly;

2) the path B model allows placement of an assembly-to-assembly moderator region around the fuel region even though the path B model may only represent a portion of the entire fuel assembly.

The significance of these approximations appears to be less for the path B larger unit cell than if the additional zones representing the guide tubes or burnable poison rods were placed directly around the fuel rod unit cell (path A model).

The isotopic compositions for the various materials in the path A and path B models are prepared by the Material Information Processor of SCALE using both the user input and the SCALE Standard Composition Library. The user is required to input the compositions of the materials as defined in the fresh fuel assembly. Materials in the SAS2H input are defined by mixture numbers. The first three mixture numbers are reserved for the materials in the path A model. Mixture number one is reserved for the fresh fuel composition. Mixture number two is reserved for the cladding composition. Mixture number three is reserved for the moderator composition. Additional mixture numbers may then be defined to represent other materials (i.e., burnable absorber). The input mixtures define the "input mixing table" which is composed of the nuclide identification number, the mixture number, and the number density of the nuclide in the mixture. The input mixing table is combined with trace amounts (1E-20 atoms/b-cm) of nuclides present in the specified neutron cross-section library used in the SAS2H sequence to produce a "master mixing table". Additional trace amounts of selected nuclides, presented in Table 2-1, are also included to ensure that appropriate resonance processing data is utilized for important nuclides that build up in the fuel during depletion. The user may also define additional trace nuclides in mixture number one of the SAS2H input to ensure that appropriate resonance processing data is utilized.

Table 2-1. Selected Nuclides Automatically Added by SAS2H for Neutronics Processing

Xe-135	Cs-133	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	1/v-absorbers	

After the neutronics code interfaces are completed, SAS2H generates interface files for codes that couple burnup-dependent densities into the model for producing time-dependent cross-sections. First, an interface data set is produced for COUPLE, which updates cross-section constants on libraries input to ORIGEN-S. Finally, an input data set for ORIGEN-S is developed to execute a depletion case in which computed densities of the fuel are saved in a data set at prescribed time intervals.

2.5 Time-Dependent Depletion and Decay Calculation

During the irradiation of fuel in a reactor, nuclide densities vary as a function of the neutron flux and its associated energy spectrum. SAS2H performs the neutronics depletion calculations previously described in Section 2.4 at a number of user defined irradiation intervals to account for the variations in neutron flux and its associated energy spectrum that effect the fuel isotopic composition as a function of time. The irradiation intervals defined by the user are called "passes". The SAS2H sequence performs a number of passes prescribed by the user to adequately simulate the reactor history so that the resulting fuel isotopic composition for the assembly or node of the assembly may be determined. Referring to Figure 2-1, each pass through the procedure involves the following five steps:

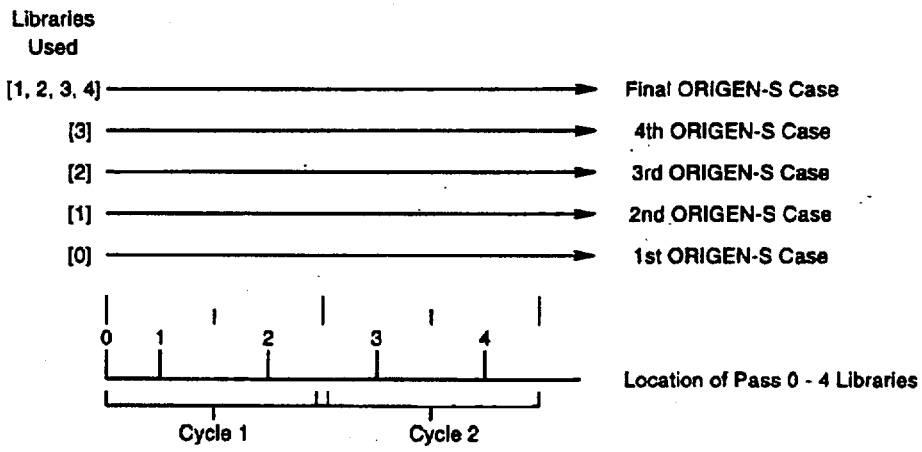
1) preparation of new data interfaces by SAS2H;
2) return of control to the SCALE driver for execution of the three codes required in the path A model;
3) preparation of the data interfaces for the path B model by SAS2H;
4) return of control to the SCALE driver for execution of the five codes required in the path B model;
5) return to SAS2H.

The user inputs the number of irradiation steps requested, the number of cross-section libraries to make per step, the specific power of the assembly or assembly node at each step, the total operation time of each step, and the downtime following each step. The irradiation steps are determined based on the reactor history and the detail required by the user. A single irradiation step or multiple irradiation steps may be specified to represent each reactor cycle. The irradiation-time associated with each cross-section library is derived from the input.

The moderator density does not change from the initial material specification (mixture 3) unless requested by the user. The soluble boron fraction in the moderator varies with reactor operation time. To account for this, the SAS2H sequence applies a default linear interpolation that specifies a boron concentration in the initial irradiation step which is 1.9 times the boron concentration specified on the mixture 3 material specification card. The boron concentration in the final irradiation step is 0.1 times the mixture 3 specified concentration. As an alternative to the default linear boron letdown scheme, the user may specify a fraction of the mixture 3 boron concentration for each irradiation step in the depletion calculation with one cross section library update per irradiation step. The boron concentration does not change as a function of time over each irradiation step. The specified boron concentration at each irradiation step should be the average boron concentration over the duration of the irradiation step.

With the exception of the fresh fuel library, each cross-section library is based on the number densities obtained for the midpoint of the irradiation-time interval. The midpoint number densities for an irradiation interval are computed from an ORIGEN-S case that uses the cross-section library from the previous irradiation interval. This procedure is graphically illustrated in Figure 2-3 for a two-step case where two libraries are requested per step (Ref. 5, p. S2.2.8).

Figure 2-3. Schematic of Successive ORIGEN-S Cases Used to Produce the Burnup-Dependent Number Densities



In reference to Figure 2-3, the first step is to produce the "PASS 0" library prepared using the fresh-fuel isotopic. This initial library is used in the first ORIGEN-S case to generate number densities at the midpoint of the first irradiation interval. Next, the SAS2H module:

1) computes density-dependent parameters for the resonance calculations;
2) increments the required data set unit numbers;
3) adds "PASS 1" to the ORIGEN-S library title;
4) updates the ORIGEN-S input for the second case to save number densities for the starting point and the midpoint of the second irradiation interval;
5) rewrites all code interfaces using the new data.

Then the "PASS 1" library is produced by invoking execution of the five codes in both path A and path B a second time with the new input interfaces. Each additional pass applies the same procedure as used for "PASS 1". The midpoint densities are applied to the neutronics analysis to produce a new library. The depletion computation applies this library and the densities calculated for the start of the pass. A decay computation with zero power is applied for reactor downtime, if specified for the end of a cycle, before deriving densities for the next pass. All ORIGEN-S libraries are saved, starting with the "PASS 1" library. The last pass is the only one in which there is a major difference in the procedure. After the completion of COUPLE in the final pass, the required libraries have been produced. The final ORIGEN-S case corresponding to the last pass uses all the libraries and runs through the entire reactor history input to the SAS2H module. All the cross-section libraries produced during all previous passes are combined into the final multi-burnup-dependent ORIGEN-S binary library made for the case.

The final ORIGEN-S case utilizes all previously determined cross-section libraries for each step to deplete the fuel from its fresh fuel state to its discharge state. All ORIGEN-S cases include over 1600 nuclides in the ORIGEN-S binary library. Cross-section constants are either updated directly from previous XSDRNPM-S output, or for those nuclides not included in the pin-cell analysis, from broad-group flux weight factors.

In the example shown in Figure 2-3, the final ORIGEN-S case begins with the nuclide generation and depletion calculation performed using the cross-section library, power, and time interval for "PASS 1". Four equal-size time steps are used during the irradiation time, followed by a single downtime interval. If no downtime was specified, a zero-time interval is applied. Next, a similar computation is performed using the compositions determined at the end of the "PASS 1" calculation and the cross-section data on the "PASS 2" library. The analysis proceeds with each succeeding library and corresponding assembly power and time interval. Ultimately, the discharge composition of the fuel assembly is determined. Finally, a decay-only subcase using six equal-size time steps is performed for the final requested downtime.

2.6 SAS2H Results Relative to the Measured Isotopic Concentrations

The number densities for the nuclides of the fuel, together with their activation products and fission products, are all computed by ORIGEN-S. In addition, ORIGEN-S calculates the depletion of most light elements, including the burnable poisons (e.g., boron), and most isotopes of the specified structural materials. However, the densities of alloys or elements in the clad, moderator, or structural materials, and oxygen in the fuel remain constant (Reference 5, p. S2.2.9).

The fuel isotopic compositions are extracted from the final ORIGEN-S output for comparison with corresponding measured compositions. Through such comparison, the adequacy of the model and accuracy of the code may be determined.

3.0 DESCRIPTION OF THE SAMPLES

This section provides a general description of the radiochemical assay samples analyzed in the supporting evaluations. The specific rod and fuel assembly location the sample was taken from as well as the reactor conditions for the sample used in the supporting analyses will be described.

3.1 PWRs

3.1.1 Calvert Cliffs

Calvert Cliffs Unit 1 (CC1) operated by Baltimore Gas and Electric Company is a 825 MWe Combustion Engineering (CE) PWR. CC1 is loaded with CE 14 × 14 assemblies. The samples were taken from assemblies D047, D101, and BT03. A full description of the design and model used in the SAS2H calculation are provided in Reference 6.

General spent fuel characteristics for each pellet sample from CC1 are presented in Table 3-1 and include the initial ^{235}U enrichment, final burnup and the cooling time. A cross section of the assemblies from CC1 are presented in Figures 3-1 through 3-3.

Table 3-1. Spent Fuel Characteristic Parameters for CC1 PWR

Assembly	Rod	Axial Location from Bottom of Assembly, cm	Enrichment, wt % ^{235}U	Burnup, GWd/MTU	Cooling Time, days
D047	MKP109	13.20	3.038	27.35	1870
		27.70	3.038	37.12	1870
		165.22	3.038	44.34	1870
D101	MLA098	8.90	2.72	18.68	2374
		24.30	2.72	26.62	2374
		161.70	2.72	33.17	2374
BT03	NBD107	11.28	2.453	31.40	2447
		19.92	2.453	37.27	2447
		161.21	2.453	46.46	2447

Figure 3-1. Location of Fuel Rod MKP109 in Assembly D047

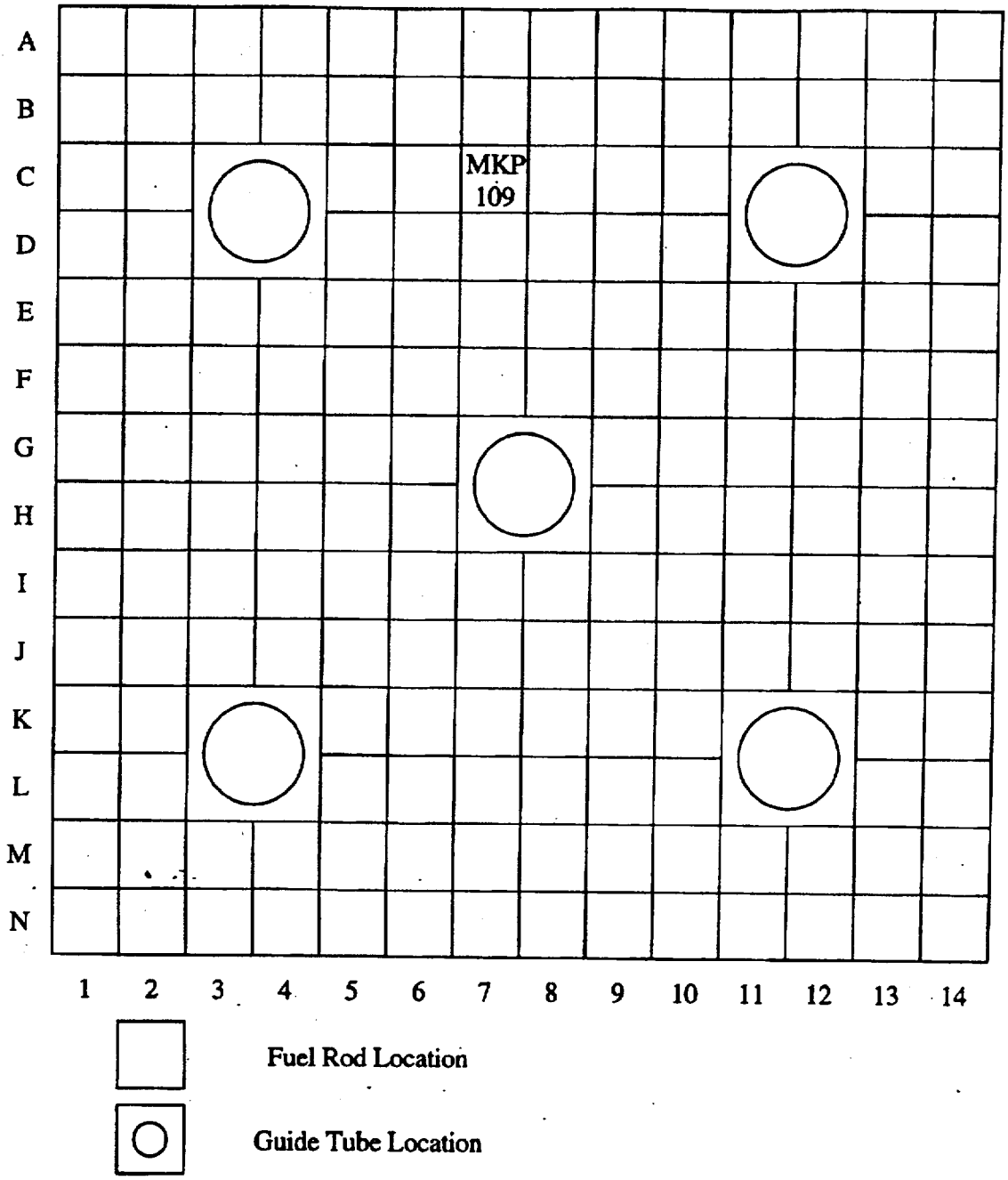


Figure 3-2. Location of Fuel Rod MLA098 in Assembly D101

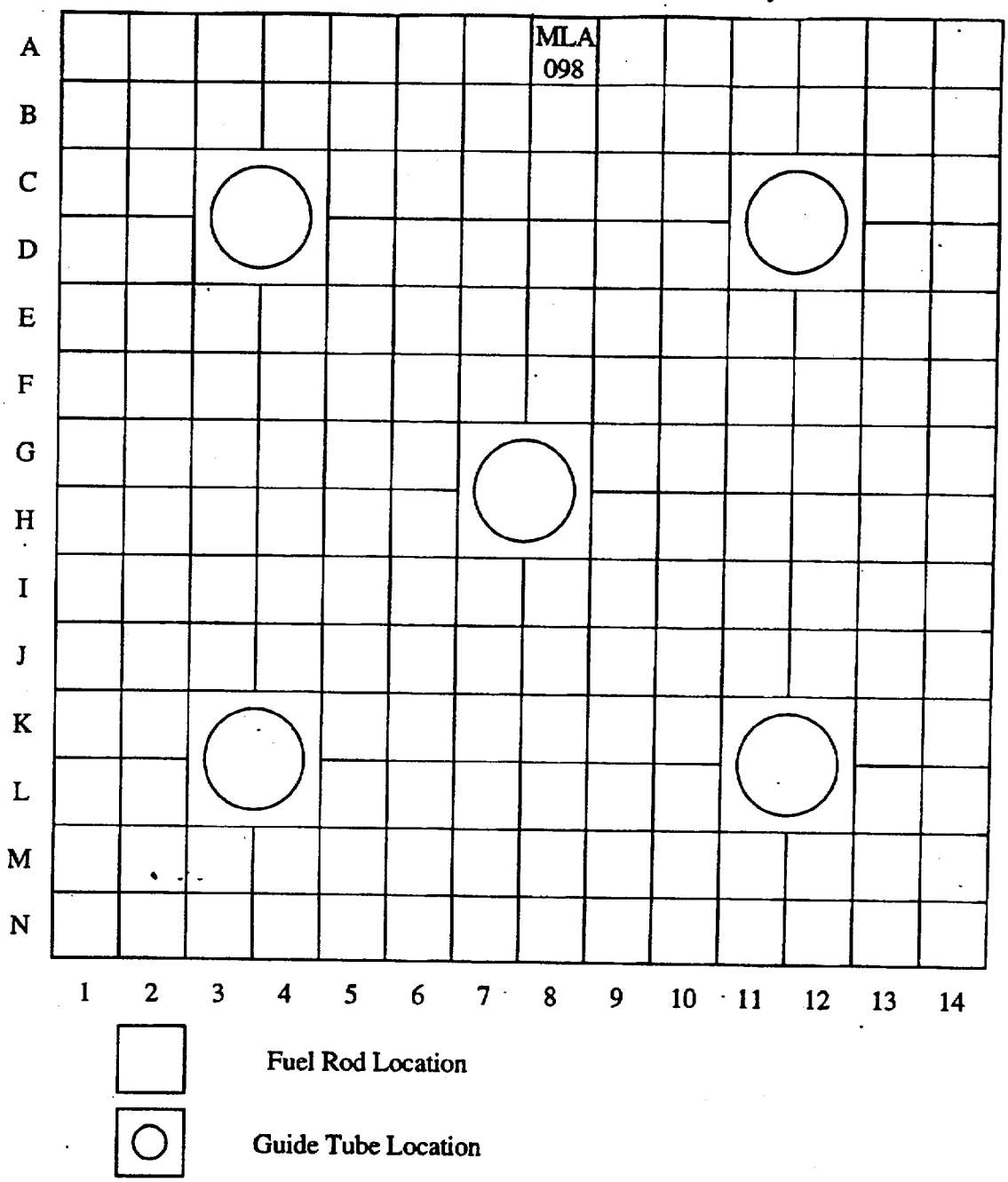
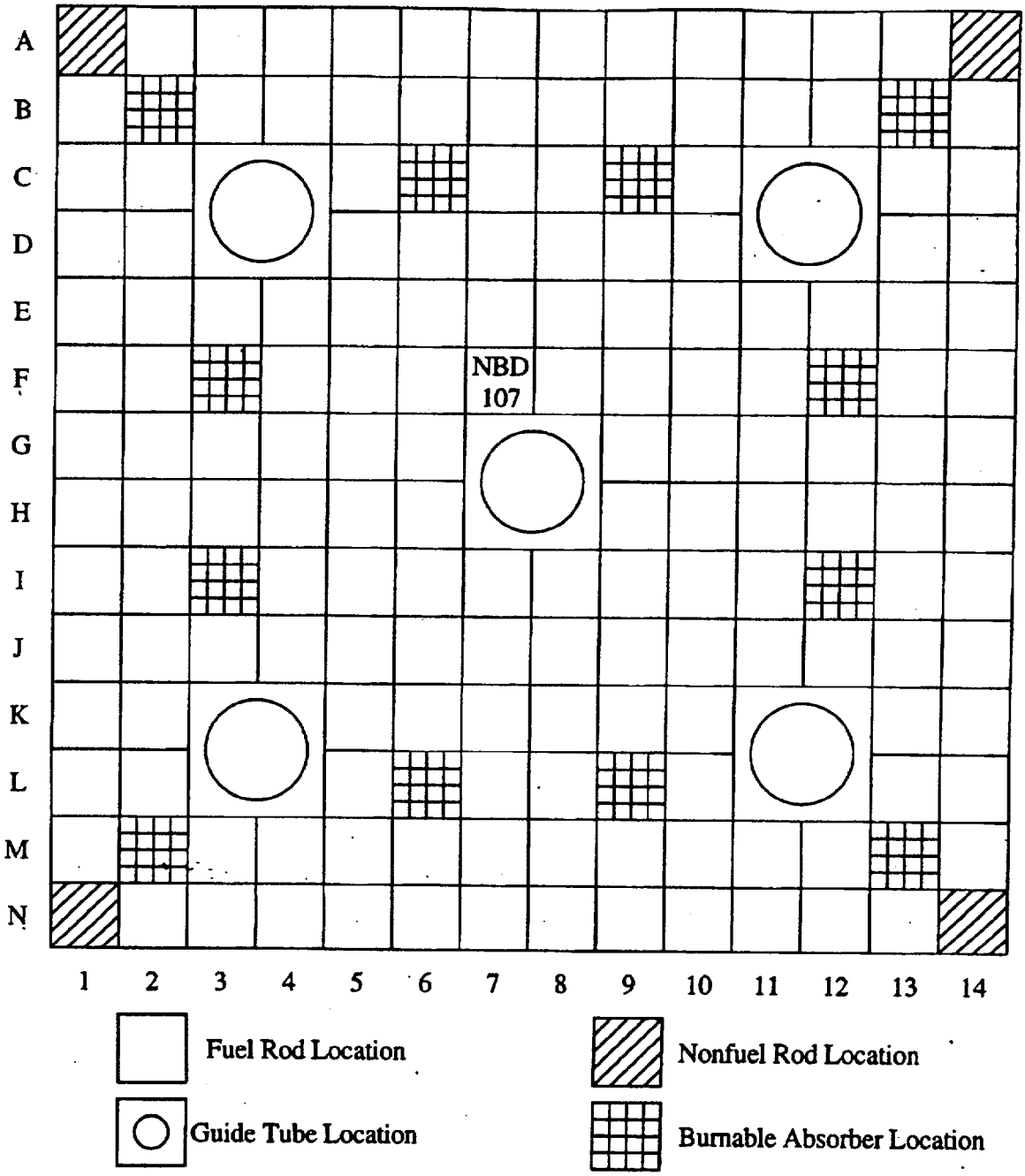


Figure 3-3. Location of Fuel Rod NBD107 in Assembly BT03



3.1.2 Obrigheim

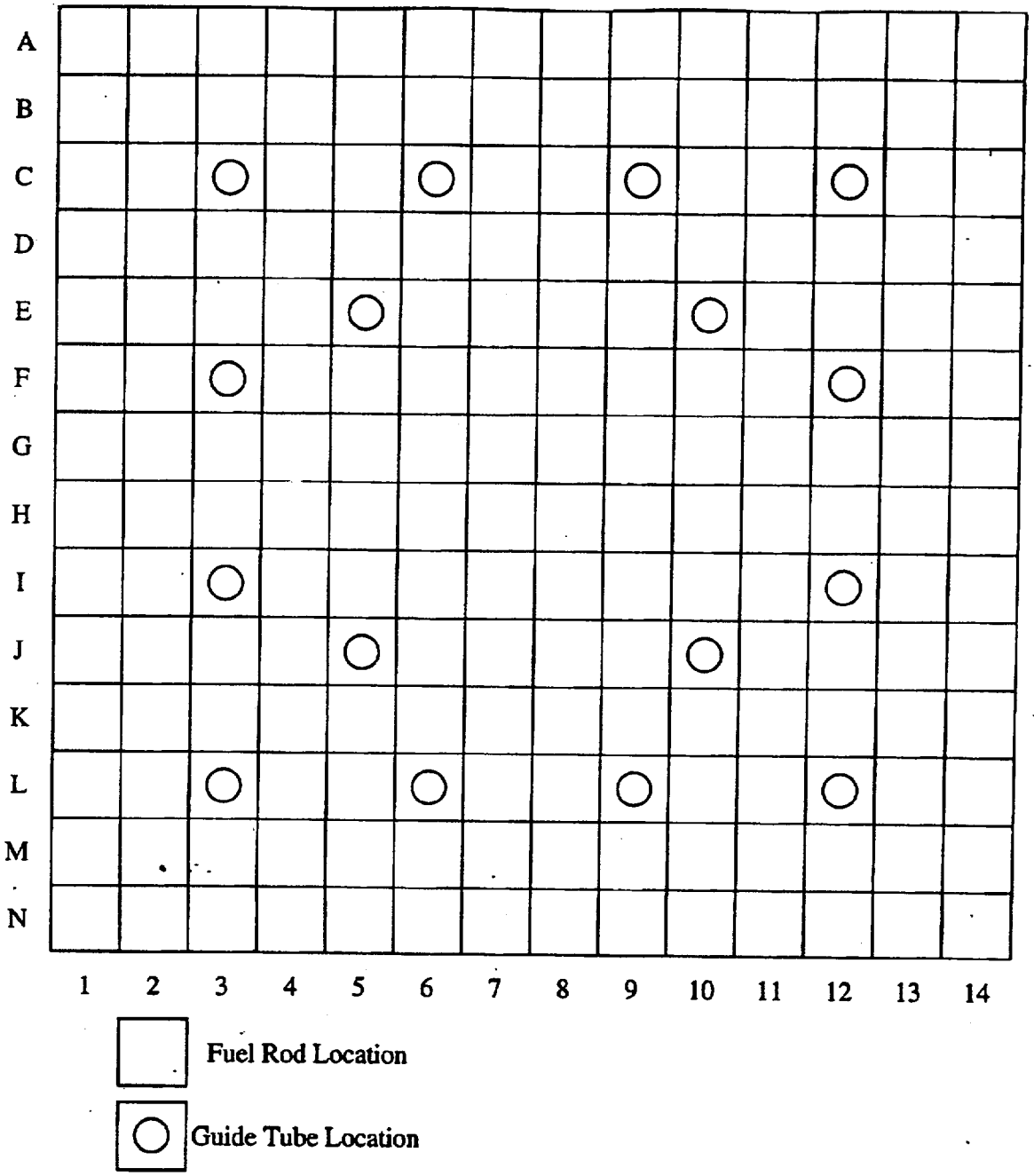
Obrigheim operates in Germany and is loaded with Siemens 14 × 14 assemblies. Assays were performed on assemblies 168, 170, 171, 172 and 176. A full description of the design and model used in the SAS2H calculation are provided in Reference 7.

General spent fuel characteristics for each assembly from Obrigheim are presented in Table 3-2 and include the initial ^{235}U enrichment, final burnup and the cooling time. A cross section of an assembly from Obrigheim is presented in Figure 3-4.

Table 3-2. Spent Fuel Characteristic Parameters for Obrigheim PWR

Test Assembly	Enrichment, wt % ^{235}U	Burnup, GWd/MTU	Cooling Time, days
168	3.13	28.40	10
170	3.13	25.93	10
171	3.13	29.04	10
172	3.13	26.54	10
176, batch 90	3.13	29.52	10
176, batch 91	3.13	27.99	10

Figure 3-4. Cross Section of Obrigheim Assembly



3.1.3 H. B. Robinson

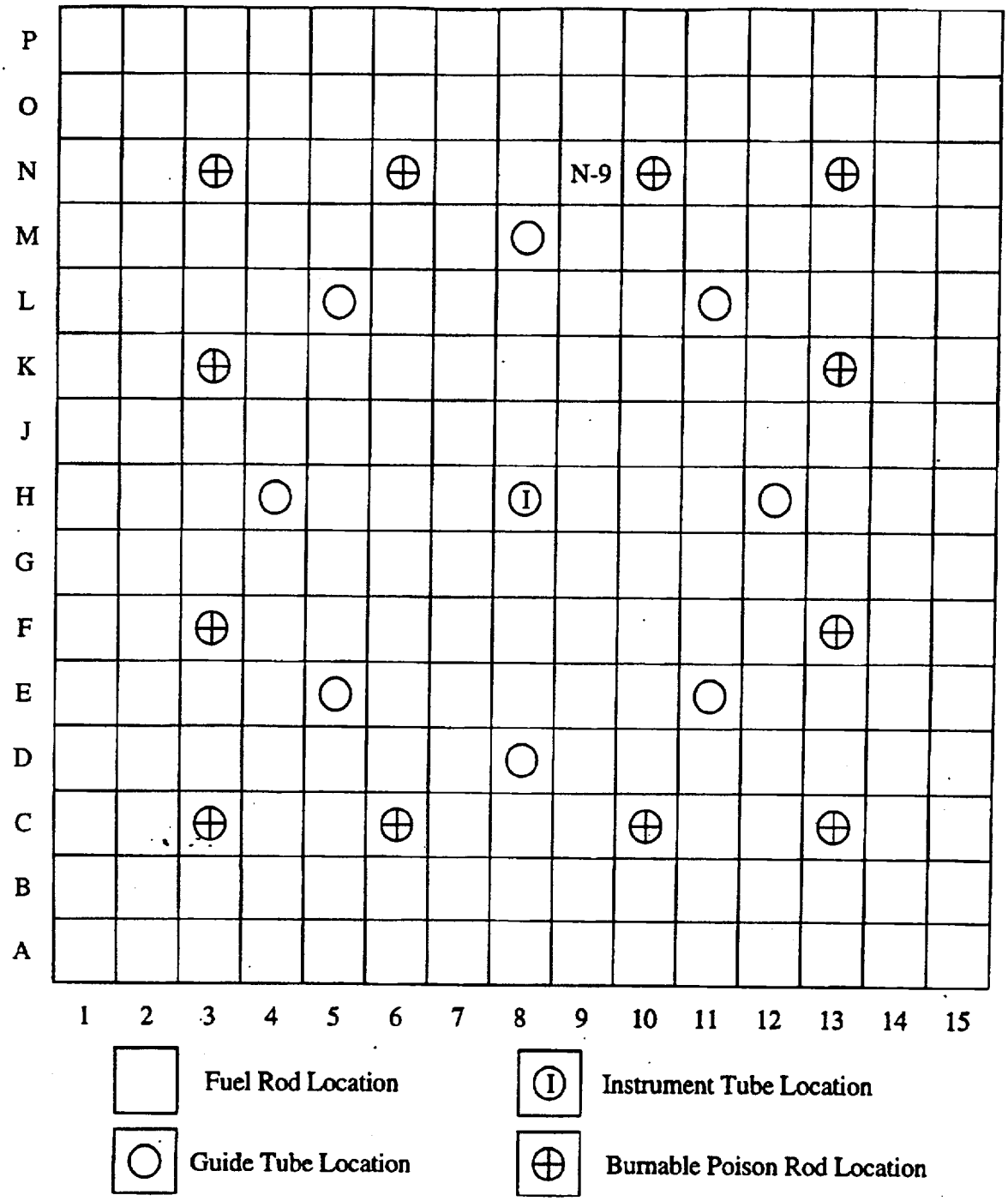
H. B. Robinson Unit 2 (HBR2) operated by Carolina Power & Light Company is a 683 MWe Westinghouse (W) PWR. HBR2 is loaded with W 15 × 15 assemblies. The samples were taken from assembly B05. A full description of the design and model used in the SAS2H calculation are provided in Reference 8.

General spent fuel characteristics for each pellet sample from HBR2 are presented in Table 3-3 and include the initial ^{235}U enrichment, final burnup and the cooling time. A cross section of the assembly from HBR2 is presented in Figure 3-5.

Table 3-3. Spent Fuel Characteristic Parameters for HBR2 PWR

Test Assembly B05, Rod N-9		
Enrichment: 2.561 wt % ^{235}U		
Axial Location from Bottom of Assembly, cm	**Burnup, GWd/MTU**	**Cooling Time, days**
11	16.02	3936
26	23.81	3936
199	28.47	3631
226	31.66	3631

Figure 3-5. Cross Section of HBR2 Assembly



3.1.4 Turkey Point

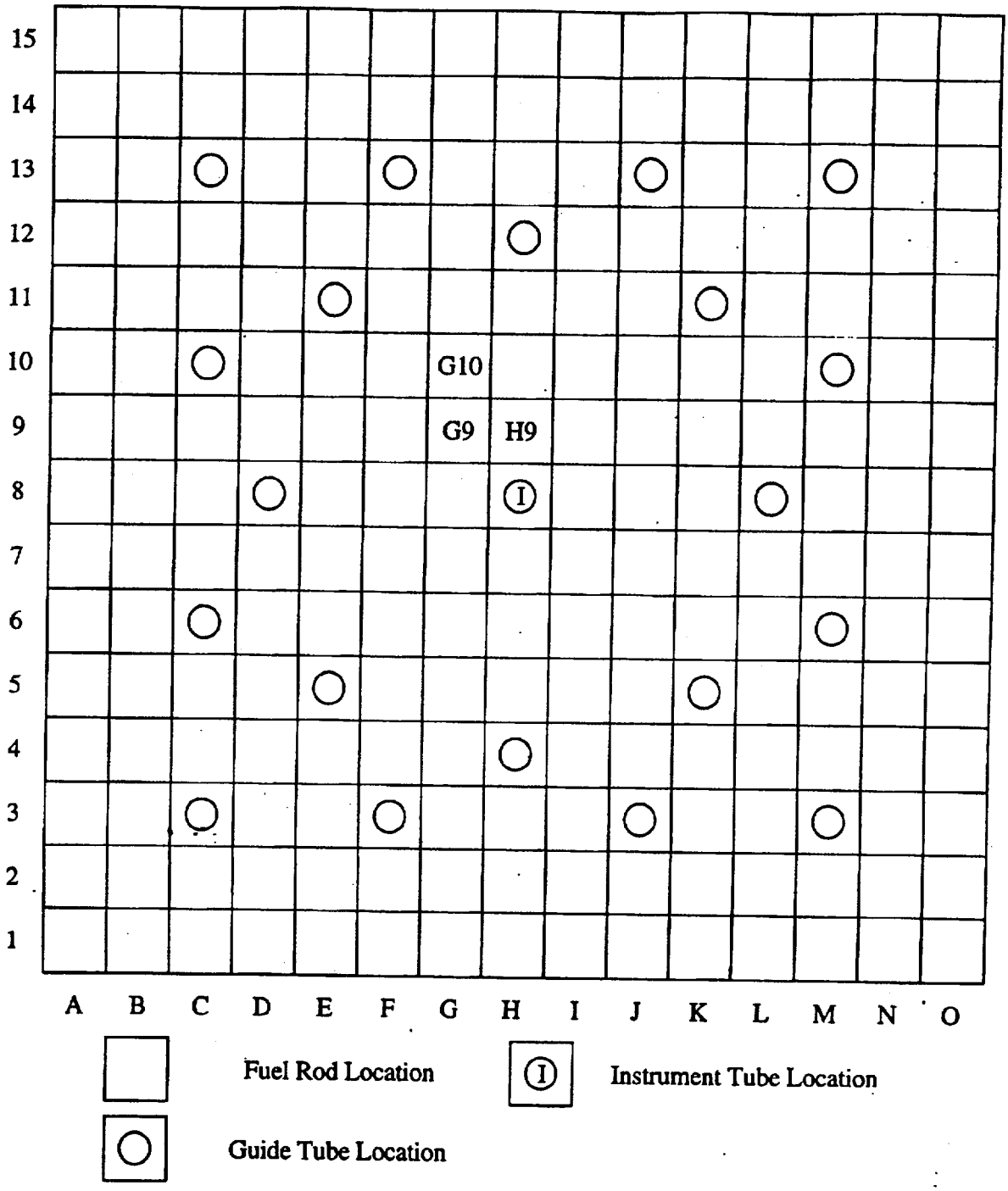
Turkey Point Unit 3 (TP3) operated by Florida Power & Light Company is a 1129 MWe W PWR with 193 fuel assemblies. TP3 is loaded with W 15 × 15 assemblies. The samples were taken from assemblies D01 and D04. A full description of the design and model used in the SAS2H calculation are provided in Reference 9.

General spent fuel characteristics for each pellet sample from Turkey Point are presented in Table 3-4 and include the initial ^{235}U enrichment, final burnup and the cooling time. A cross section of an assembly from Turkey Point is presented in Figure 3-6.

Table 3-4. Spent Fuel Characteristic Parameters for Samples from Turkey Point Unit 3 PWR

Assembly and Pin Number	Axial Location from Bottom of Assembly, cm	Enrichment, wt % ^{235}U	Burnup, GWd/MTU	Cooling Time, days
D01 (G09)	167.6	2.556	30.720	927
D01 (G10)	167.0	2.556	30.510	927
D01 (H09)	167.0	2.556	31.560	927
D04 (G09)	167.6	2.556	31.260	927
D04 (G10)	167.0	2.556	31.310	927

Figure 3-6. Cross Section of Turkey Point Assembly



3.1.5 Trino Vercelles

Trino Vercelles operates in Italy and is loaded with modified W 15 × 15 and cruciform assemblies. The samples were taken from assemblies 509-032, 509-069 and 509-104. A full description of the design and model used in the SAS2H calculation are provided in Reference 10.

General spent fuel characteristics for each pellet sample from Trino Vercelles are presented in Table 3-5 and include the initial ^{235}U enrichment, final burnup and the cooling time. A cross section of the square and cruciform assemblies as they fit together is presented in Figure 3-7, while the rod locations for the samples from each of the three square assemblies are included in Figures 3-8 through 3-10.

Table 3-5. Spent Fuel Characteristic Parameters for Trino Vercelles PWR

Test Assembly (Rod Number)	Axial Level Number	Axial Location from Bottom, cm	Enrichment, wt % ^{235}U	Burnup, GWd/MTU	Cooling Time, days
509-104 (M11)	7	79.2	3.87	12.042	0
509-032 (E11)	4	158.5	3.13	15.377	0
	7	79.2		15.898	0
	9	26.4		11.529	0
509-069 (E11)	1	237.7	3.13	12.859	0
	2	211.3		20.602	0
	4	158.5		23.718	0
	7	79.2		24.304	0
509-069 (E05)	4	158.5		23.867	0
	7	79.2		24.548	0
509-069 (L11)	4	158.5		23.928	0
	7	79.2		24.362	0
509-069 (L5)	4	158.5		24.330	0
	7	79.2		24.313	0

Figure 3-7. Cross Section of the Square and Cruciform Assemblies for Trino Vercelles

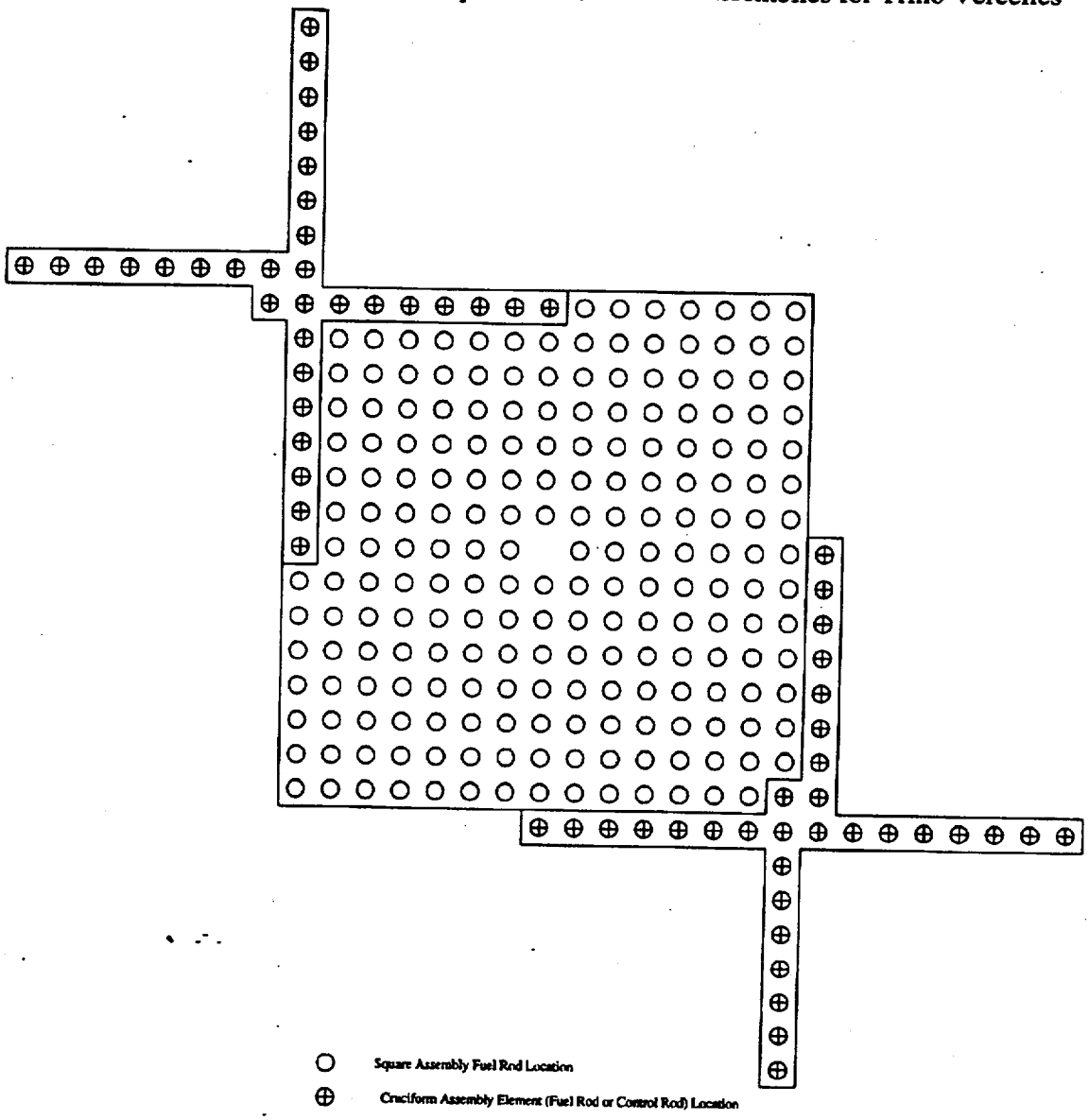
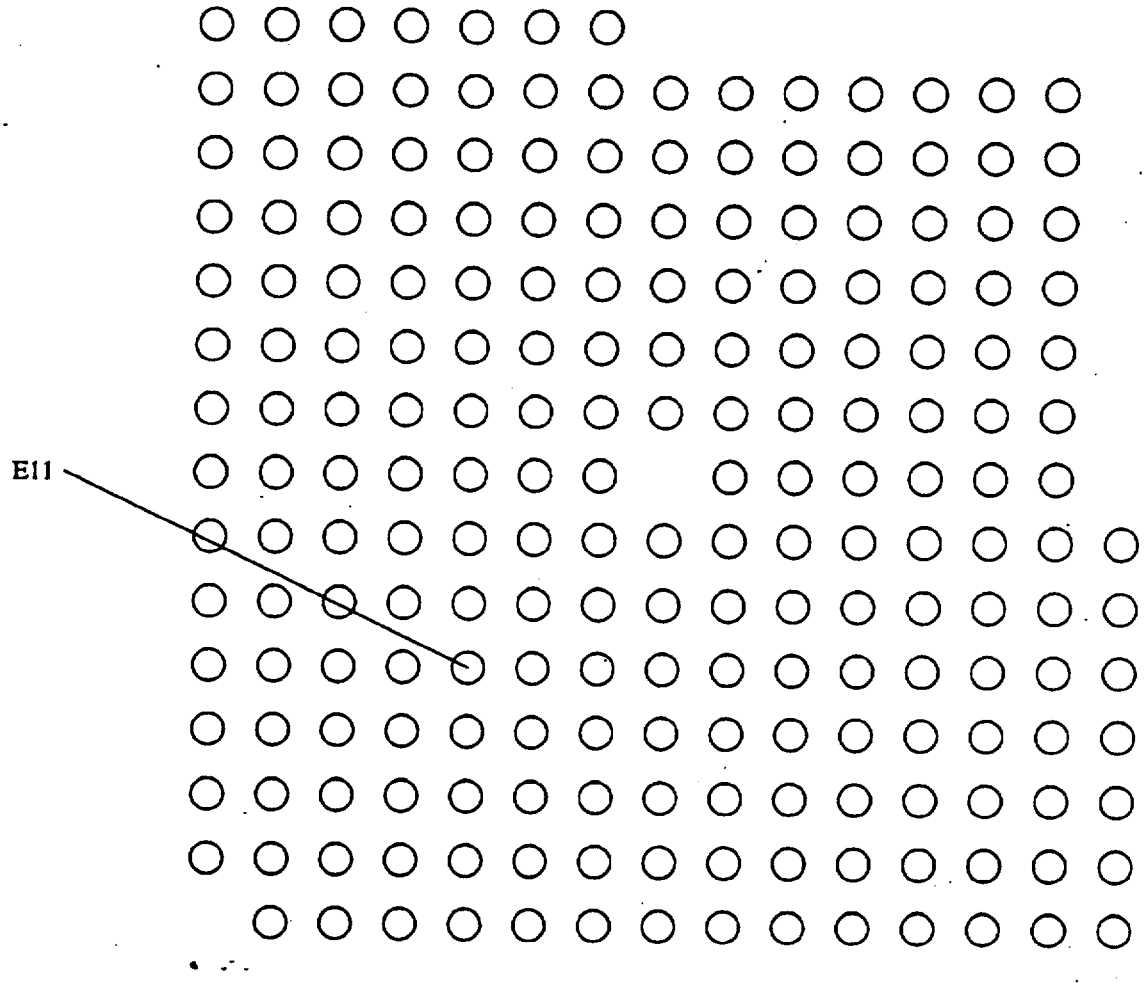
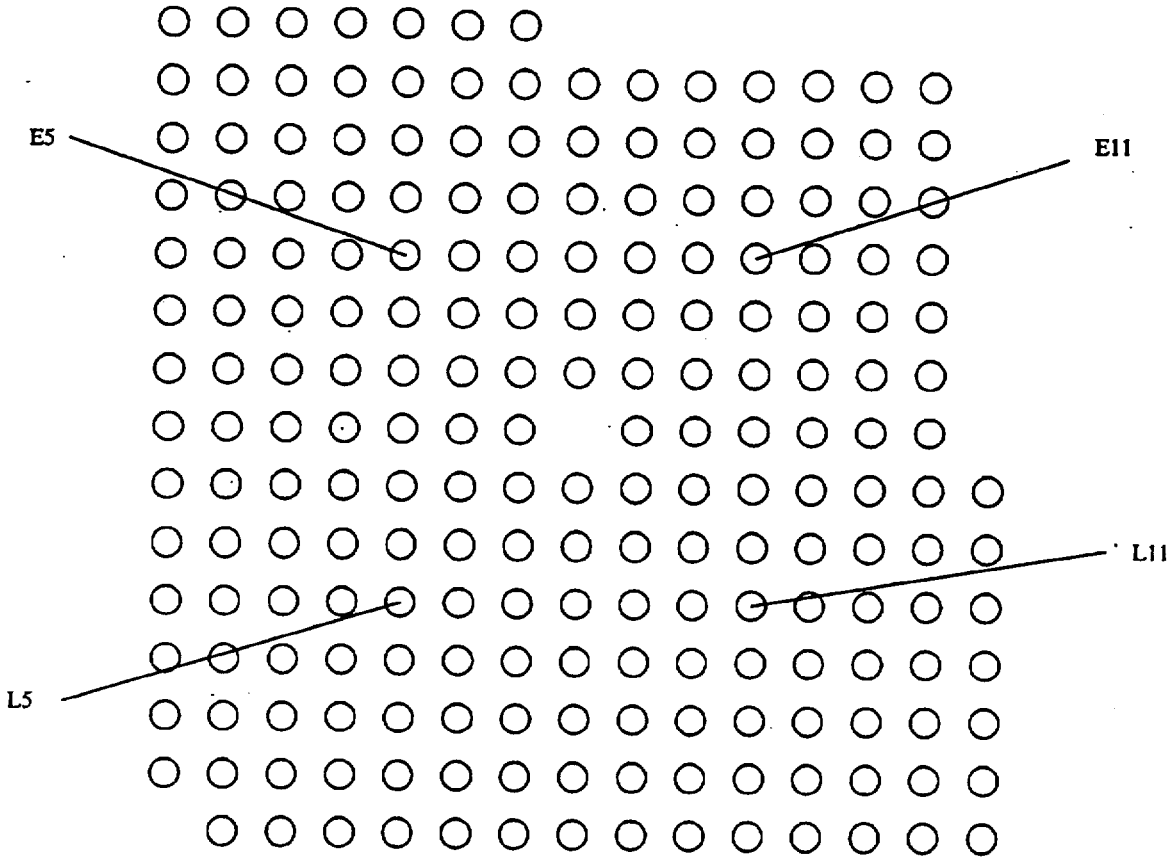


Figure 3-8. Fuel Rod Locations for Assembly 509-032



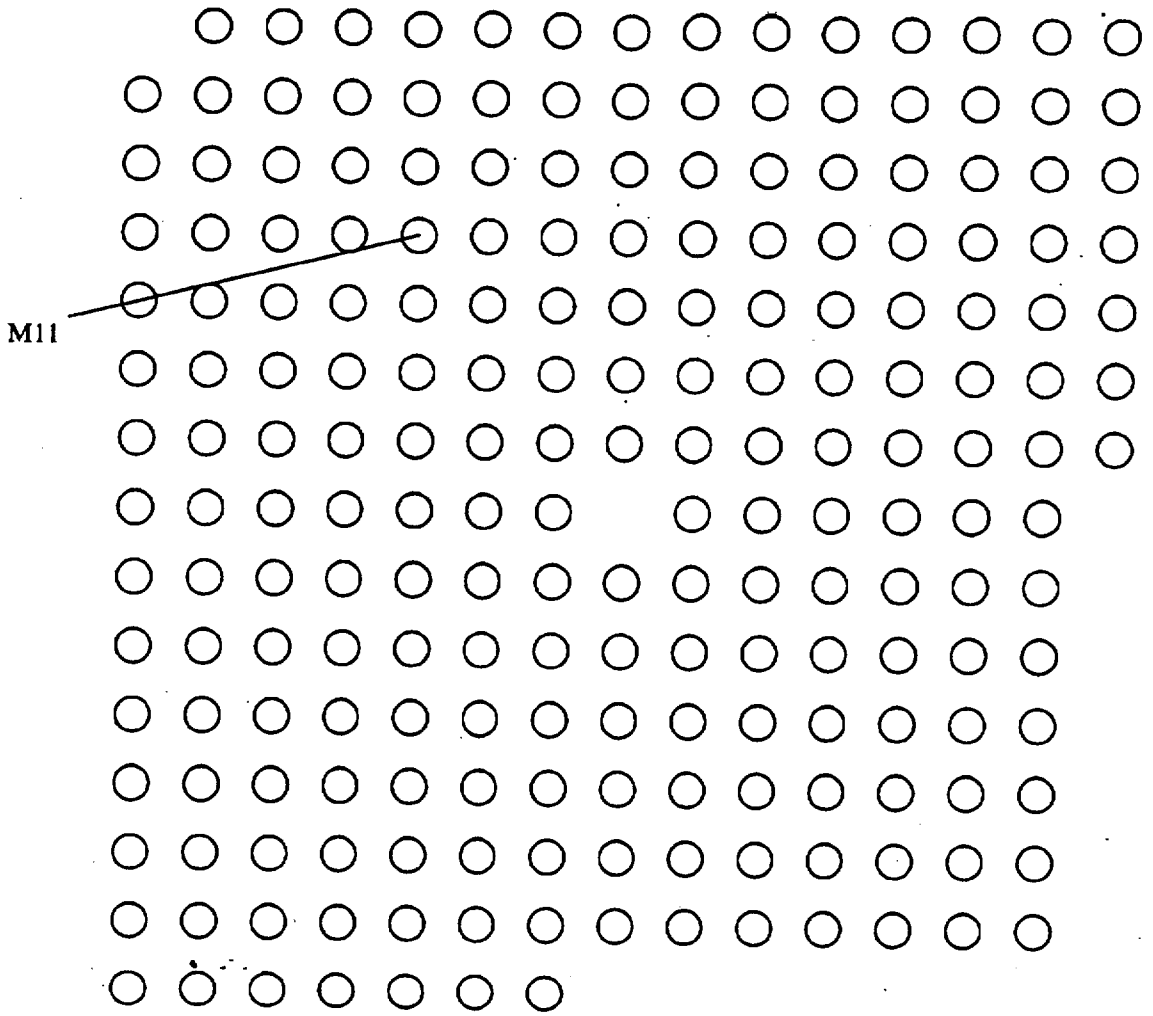
509-032

Figure 3-9. Fuel Rod Locations for Assembly 509-069



509-069

Figure 3-10. Fuel Rod Locations for Assembly 509-104



509-104

3.1.6 Yankee Rowe

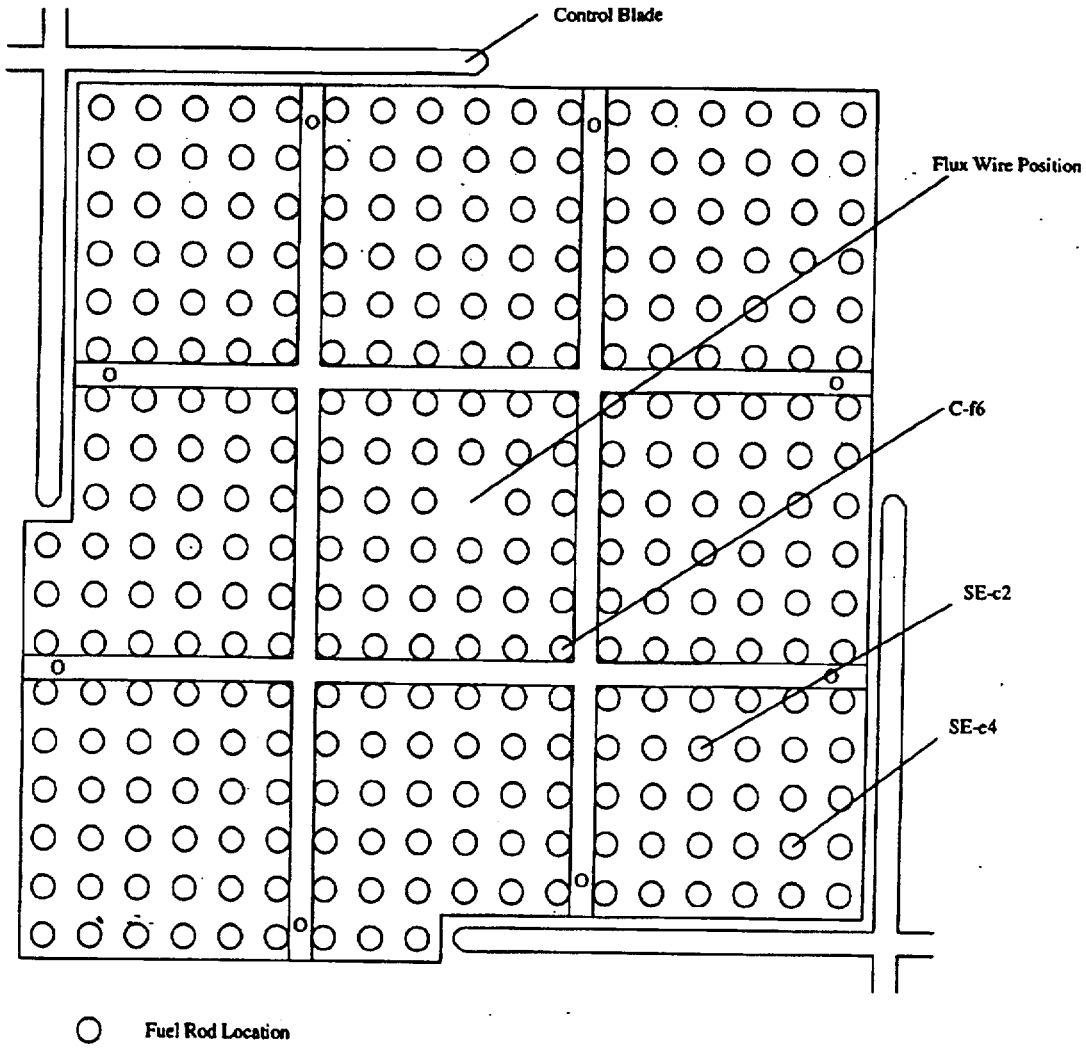
Yankee Rowe (YR) was operated by Yankee Nuclear Corporation and was a PWR with 76 fuel assemblies. YR was loaded with W 17 × 18 assemblies. The samples were taken from assembly E6. A full description of the design and model used in the SAS2H calculation are provided in Reference 11.

General spent fuel characteristics for each pellet sample from Yankee Rowe are presented in Table 3-6 and include the initial ^{235}U enrichment, final burnup and the cooling time. A cross section of an assembly from Yankee Rowe is presented in Figure 3-11.

Table 3-6. Spent Fuel Characteristic Parameters for Yankee Rowe PWR

Assembly and Rod Number	Axial Location from Bottom of Assembly, cm	Enrichment, wt % ^{235}U	Burnup, GWd/MTU	Cooling Time, days
E6-C-f6	220.22	3.400	15.95	281.5
E6-C-f6	138.94	3.400	30.39	717.0
E6-C-f6	57.66	3.400	31.33	281.5
E6-C-f6	17.02	3.400	20.19	281.5
E6-SE-c2	138.94	3.400	32.03	281.5
E6-SE-c2	57.66	3.400	31.41	281.5
E6-SE-e4	138.94	3.400	35.97	281.5
E6-SE-e4	57.66	3.400	35.26	281.5

Figure 3-11. Cross Section of Yankee Rowe Assembly



3.1.7 Mihama-3

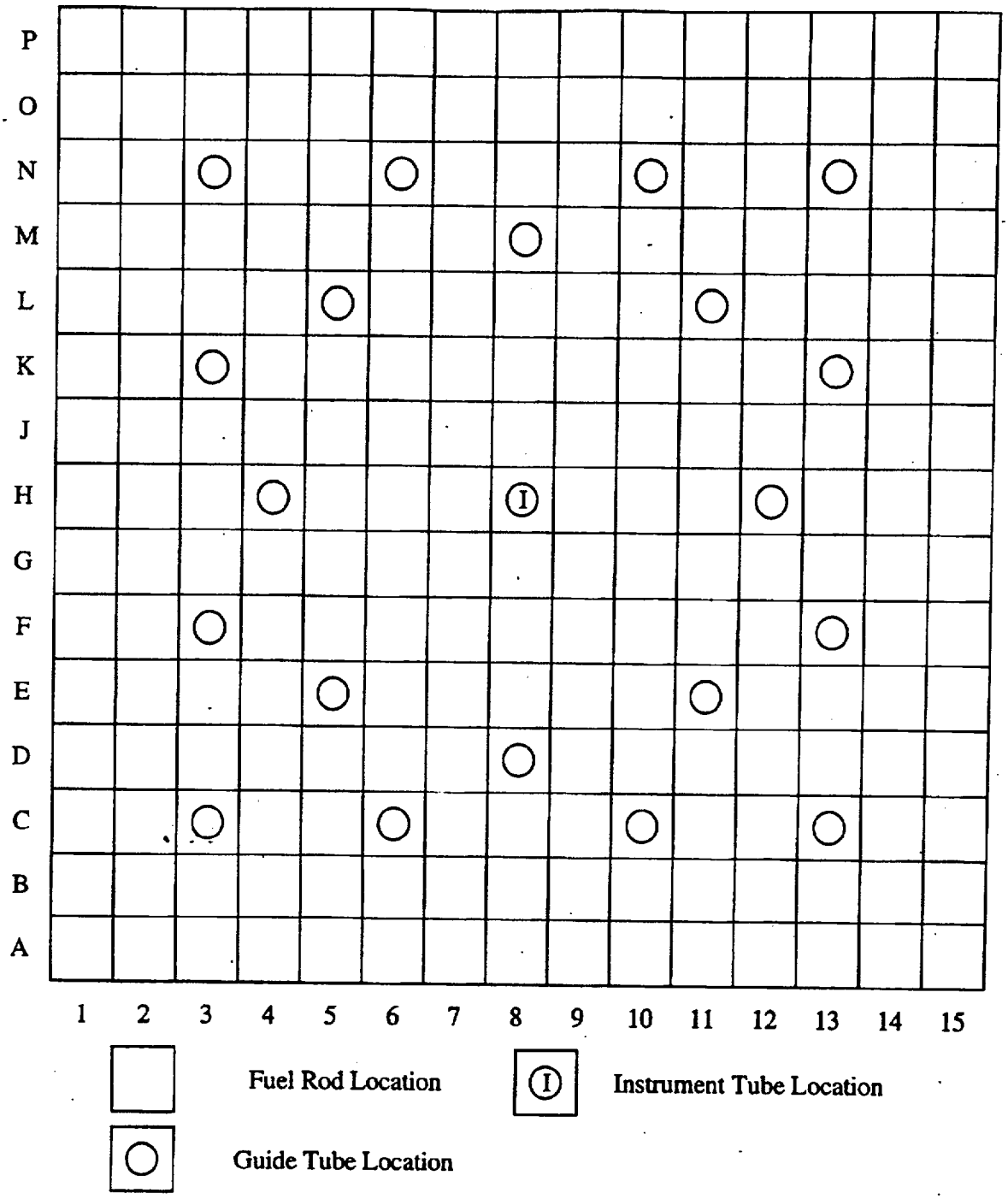
Mitsubishi Heavy Industries is the plant vendor for Mihama-3 which is a W PWR and is loaded with W 15 × 15 assemblies. The sample identifications are 86b02, 86b03, 86g03, 86g05, 87c03, 87c04, 87c07, and 87c08. A full description of the design and model used in the SAS2H calculation are provided in Reference 12.

General spent fuel characteristics for each pellet sample from Mihama are presented in Table 3-7 and include the initial ^{235}U enrichment, final burnup and the cooling time. A cross section of an assembly from Mihama is presented in Figure 3-12.

Table 3-7. Spent Fuel Characteristic Parameters for Samples from Mihama-3 PWR

Assembly	Enrichment, wt % ^{235}U	Burnup , GWd/MTU	Cooling Time, days
86b02	3.208	8.30	1825
86b03	3.208	6.92	1825
86g03	3.203	21.29	1825
86g05	3.203	15.36	1825
86g07	3.203	14.66	1825
87c03	3.210	29.50	1825
87c04	3.210	32.20	1825
87c07	3.210	33.71	1825
87c08	3.210	34.32	1825

Figure 3-12. Cross Section of Mihama Assembly



3.2 BWRs

3.2.1 Cooper

Cooper operated by Nebraska Public Power District is a 764 MWe General Electric (GE) class 4 BWR with 548 fuel bundles. Cooper is a source for GE 7 × 7 fuel assembly data. The samples were taken from Bundle CZ346, and a full description is provided in Reference 13.

General spent fuel characteristics for each pellet sample from Cooper are presented in Table 3-8 and include the initial ^{235}U enrichment, final burnup and the cooling time. A cross section of an assembly from Cooper is presented in Figure 3-13 with fuel rod enrichments and types listed in Table 3.9.

Table 3-8. Spent Fuel Characteristic Parameters for Cooper BWR

Sample	Axial Location from Top of Assembly, cm	Enrichment, wt % ^{235}U	Burnup, MWd/kgM	Cooling Time, years
ADD2966-B	55.107	2.93	18.96	5.35
ADD2966-K	218.869	2.93	33.07	5.35
ADD2966-T	274.777	2.93	33.94	5.35
ADD2974-B	55.723	2.93	17.84	5.28
ADD2974-J	115.042	2.93	29.23	5.28
ADD2974-U	291.087	2.93	31.04	5.28

Figure 3-13. Cross Section of Cooper BWR Assembly

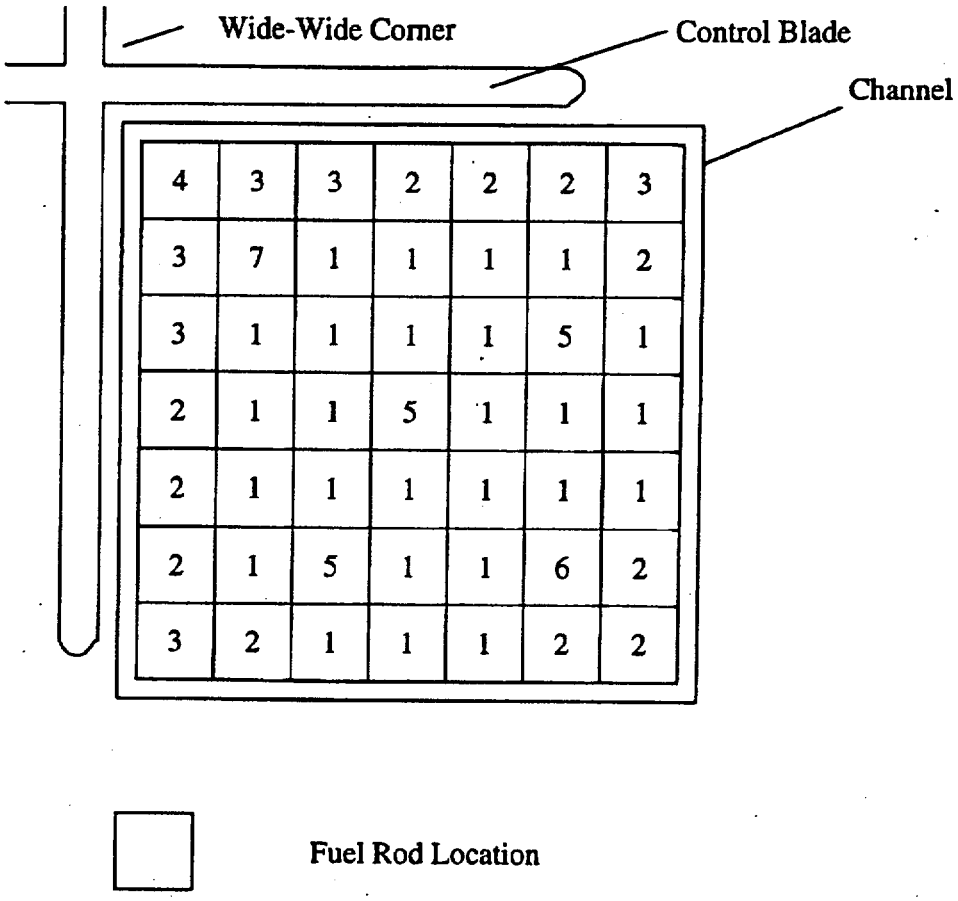


Table 3-9. Rod Enrichments for Cooper BWR

Rod Type	Enrichment, wt % ^{235}U	wt % Gd_2O_3	Number of Rods
1	2.93	0	26
2	1.94	0	11
3	1.69	0	6
4	1.33	0	1
5	2.93	3.0	3
6	2.93	4.0	1
7	1.94	4.0	1

4.0 COMPARISON RESULTS FOR MEASURED AND CALCULATED ISOTOPICS

This section contains a summary of the results from analyses comparing measured and calculated isotopic concentrations. Results are presented in percent differences of the calculated from the measured concentration.

4.1 PWRs

4.1.1 Calvert Cliffs

Table 4-1. Percent Difference Between Measured and Calculated [(C/M-1)*100] for CC1

Assembly	D047	D047	D047	D101	D101	D101	BT03	BT03	BT03
Axial Height	13.20 cm	27.70 cm	165.22 cm	8.90 cm	24.30 cm	161.70 cm	11.28 cm	19.92 cm	161.21 cm
^{99}Tc	5.27	6.59	12.04	0.62	4.48	4.63	44.30	43.48	40.63
^{234}U	-0.63	-1.43	1.67	12.86	15.70	6.67	-22.88	-14.17	30.31
^{235}U	-1.65	-2.13	-6.78	0.49	1.59	7.95	20.73	21.40	38.69
^{236}U	2.87	3.40	1.63	-2.40	-2.01	-2.45	1.75	0.66	2.96
^{238}U	-0.65	-0.32	-0.10	-1.06	-1.62	-0.85	-0.90	-1.28	-0.27
^{237}Np	3.73	12.36	7.05	-4.48	-11.98	1.00	18.53	14.24	18.49
^{238}Pu	-5.35	-3.17	-7.81	-21.44	-8.36	-0.20	3.79	2.72	2.04
^{239}Pu	-13.93	-14.85	3.74	-14.52	-19.57	-17.36	-7.71	-11.86	-11.84
^{240}Pu	4.71	1.83	-0.51	6.19	7.02	6.58	9.34	7.28	5.81
^{241}Pu	-2.20	-5.76	-2.45	-6.45	-5.01	-1.66	-0.41	-2.21	-0.47
^{242}Pu	16.61	15.80	0.48	7.60	13.30	12.53	4.89	4.86	3.51
^{241}Am	-5.26	-14.46	-10.67	-7.66	-6.43	-5.90	0.62	-13.05	-37.85
^{143}Nd	1.79	1.82	1.57	-	-	-	-	-	-
^{145}Nd	-0.20	-0.77	-0.81	-	-	-	-	-	-
^{149}Sm	-35.52	-32.33	-52.55	-	-	-	-	-	-
^{150}Sm	0.00	9.96	1.66	-	-	-	-	-	-
^{152}Sm	14.94	25.00	24.79	-	-	-	-	-	-
^{153}Eu	0.76	11.01	2.03	-	-	-	-	-	-

Table 4-1. Percent Difference Between Measured and Calculated [(C/M-1)*100] for CC1

Assembly	D047	D047	D047	D101	D101	D101	BT03	BT03	BT03
Axial Height	13.20 cm	27.70 cm	165.22 cm	8.90 cm	24.30 cm	161.70 cm	11.28 cm	19.92 cm	161.21 cm
Total U	-0.65	-0.32	-0.12	-1.05	-1.59	-0.81	-0.80	-1.20	-0.19
Total Pu	-6.88	-6.93	1.20	-9.01	-9.91	-6.83	-0.99	-3.29	-2.90

Note: Measured values (M) are taken from Reference 15

Reference 6

4.1.2 Obrigheim

Table 4-2. Percent Difference Between Measured and Calculated [(C/M-1)*100] for Obrigheim

Batch	86	94	89	92	90	91
Assembly	168	170	171	172	176	176
^{235}U	3.10	1.37	1.25	2.08	3.27	2.54
^{236}U	0.80	0.28	1.33	0.55	0.52	1.08
^{238}Pu	2.47	8.86	12.54	3.71	11.11	10.76
^{239}Pu	-16.02	-13.22	-15.07	-10.04	-14.83	-14.11
^{240}Pu	7.43	10.56	10.50	12.57	10.29	11.46
^{241}Pu	-0.27	3.27	2.08	5.32	1.95	2.08
^{242}Pu	4.18	10.90	10.62	5.79	5.25	8.87

Note: Measured values (M) are taken from Reference 15

Reference 7

Table 4-3. Sensitivity Analysis for Assembly 170 Batch 94

	Calculated Concentration, g/MTU		% Change in Calculated Concentrations
	Modeled Conditions	Boron Concentration Increase of 100 ppm	
^{235}U	1.11E4	1.12E4	0.90
^{236}U	3.60E3	3.60E3	0.00
^{238}Pu	8.72E1	8.80E1	0.92
^{239}Pu	4.17E3	4.21E3	0.96
^{240}Pu	1.99E3	2.00E3	0.50
^{241}Pu	1.01E3	1.01E3	0.00
^{242}Pu	3.46E2	3.47E2	0.29

Reference 7

Table 4-4. Sensitivity Analysis for Assembly 176 Batch 90

	Calculated Concentration, g/MTU		% Change in Calculated Concentrations
	Modeled Conditions	Boron Concentration Increase of 100 ppm	
^{235}U	9.48E3	9.54E3	0.63
^{236}U	3.83E3	3.83E3	0.00
^{238}Pu	1.19E2	1.20E2	0.84
^{239}Pu	4.21E3	4.26E3	1.19
^{240}Pu	2.25E3	2.25E3	0.00
^{241}Pu	1.15E3	1.16E3	0.87
^{242}Pu	4.61E2	4.61E2	0.00

Reference 7

4.1.3 H. B. Robinson

Table 4-5. Percent Difference Between Measured and Calculated [(C/M-1)*100] for HBR2

Sample Identification	N-9B-S	N-9B-N	N-9C-J	N-9C-D
^{99}Tc	12.40	8.66	14.88	11.52
^{235}U	3.74	5.96	0.49	9.47
^{236}U	-2.74	-2.92	2.13	-0.33
^{238}U	0.00	-0.59	0.48	-0.83
^{237}Np	-3.87	-5.00	2.63	6.31
^{238}Pu	-2.47	-4.75	-12.28	-3.85
^{239}Pu	10.44	9.45	5.01	11.43
^{240}Pu	6.42	3.59	3.05	4.25
^{241}Pu	3.29	1.59	-3.96	3.76

Note: Measured values (M) are taken from Reference 15

Reference 8

Table 4-6. Sensitivity Analysis for Sample N-9B-S

	Calculated Concentration, g/MTUO$_2$		% Change in Calculated Concentrations
	Modeled Conditions	Fuel Temperature Decrease of 100 K	
^{99}Tc	3.61E2	3.61E2	0.00
^{235}U	1.11E4	1.11E4	0.00
^{236}U	2.13E3	2.14E3	0.47
^{238}U	8.47E5	8.47E5	0.00
^{237}Np	1.49E2	1.49E2	0.00
^{238}Pu	2.76E1	2.76E1	0.00
^{239}Pu	4.02E3	3.98E3	-1.00
^{240}Pu	1.16E3	1.16E3	0.00
^{241}Pu	3.14E2	3.11E2	-0.96

Reference 8

Table 4-7. Sensitivity Analysis for Sample N-9C-D

	Calculated Concentration, g/MTUO$_2$		% Change in Calculated Concentrations
	Modeled Conditions	Fuel Temperature Decrease of 100 K	
^{99}Tc	6.65E2	6.65E2	0.00
^{235}U	5.32E3	5.27E3	-0.94
^{236}U	2.99E3	3.00E3	0.33
^{238}U	8.35E5	8.35E5	0.00
^{237}Np	3.54E2	3.52E2	-0.56
^{238}Pu	1.25E2	1.25E2	0.00
^{239}Pu	4.68E3	4.62E3	-1.28
^{240}Pu	2.21E3	2.21E3	0.00
^{241}Pu	7.18E2	7.10E2	-1.11

Reference 8

4.1.4 Turkey Point

Table 4-8. Percent Difference Between Measured and Calculated [(C/M-1)*100] for Turkey Point

Axial Location (cm)	167.6	167.0	167.0	167.6	167.0
Sample Identification	D01 (G09)	D01 (G10)	D01 (H09)	D04 (G09)	D04 (G10)
Burnup (GWd/MTU)	30.720	30.510	31.560	31.260	31.310
^{234}U	1.44	2.20	7.76	17.60	0.76
^{235}U	-5.37	-1.16	-5.27	-2.34	-5.16
^{236}U	2.95	2.61	6.18	6.46	3.63
^{238}U	-0.13	-0.17	-0.16	-0.09	-0.08
^{238}Pu	-1.10	-2.21	-0.42	1.30	2.04
^{239}Pu	4.38	4.34	2.64	2.41	5.68
^{240}Pu	3.27	1.57	4.14	2.16	4.48
^{241}Pu	0.85	-0.75	-1.27	-3.91	0.75
^{242}Pu	8.57	2.32	5.35	4.09	8.31

Note: Measured values (M) are taken from Reference 16

Reference 9

4.1.5 Trino Vercelles

Table 4-9. Percent Difference Between Measured and Calculated [(C/M-1)*100] for Trino Vercelles

Assembly	509-104 M11	509-032 E11	509-032 E11	509-032 E11	509-069 E11	509-069 E11	509-069 E11
Location	7	4	7	9	1	2	4
Burnup (GWd/MTU)	12.042	15.377	15.898	11.529	12.859	20.602	23.718
^{235}U	1.05	2.43	4.15	0.64	2.26	5.15	3.37
^{236}U	-10.09	-7.55	-2.15	-14.07	-7.46	-6.84	-5.54
^{238}U	0.07	0.02	0.02	-0.05	-0.07	0.02	-0.03
^{239}Pu	-2.97	-0.30	0.11	-1.09	2.84	3.04	5.51
^{240}Pu	-5.51	-0.72	0.26	-2.84	3.33	-0.66	1.42
^{241}Pu	-11.94	-5.21	-3.24	-8.40	-1.50	-5.20	0.00
^{242}Pu	-13.24	-4.38	-6.61	-7.44	-1.09	-5.81	-1.44
^{243}Am	-	-	-	-	-	-3.09	-10.88
Assembly	509-069 E11	509-069 E5	509-069 E5	509-069 L11	509-069 L11	509-069 L5	509-069 L5
Location	7	4	7	4	7	4	7
Burnup (GWd/MTU)	24.304	23.867	24.548	23.928	24.362	24.330	24.313
^{235}U	1.21	-0.85	1.56	-0.16	2.04	-2.85	1.54
^{236}U	-4.89	-2.84	-1.98	-8.87	-0.14	-0.61	-3.05
^{238}U	-0.02	-0.02	-0.03	0.05	0.08	-0.06	0.19
^{239}Pu	1.48	4.71	3.34	2.97	2.75	3.47	3.18
^{240}Pu	-1.37	1.70	1.96	0.00	0.00	2.82	0.56
^{241}Pu	-1.89	-0.95	-0.47	-0.95	-1.42	0.00	-1.89
^{242}Pu	-2.14	1.25	1.57	-0.81	-2.32	4.51	0.80
^{243}Am	-7.07	-	-4.44	-6.56	1.25	-	-

Note: Measured values (M) are taken from Reference 16

Reference 10

4.1.6 Yankee Rowe

Table 4-10. Percent Difference Between Measured and Calculated [(C/M-1)*100] for Yankee Rowe

Sample	E6-C-f6	E6-C-f6	E6-C-f6	E6-C-f6	E6-SE-c2	E6-SE-c2	E6-SE-e4	E6-SE-e4
Location (cm)	220.22	138.94	57.66	17.02	138.94	57.66	138.94	57.66
Burnup (GWd/MTU)	15.95	30.39	31.33	20.19	32.03	31.41	35.97	35.26
^{234}U	-0.65	-11.97	2.52	0.69	5.26	6.09	-4.24	-5.00
^{235}U	0.00	-2.38	-0.84	-0.58	-1.69	-0.84	4.29	4.67
^{236}U	-1.04	-0.25	-0.48	-0.30	-0.24	0.98	-2.02	-2.48
^{238}U	0.42	0.32	0.53	1.50	0.43	0.43	0.21	0.21
^{238}Pu	-18.82	1.70	-13.55	-15.80	-11.26	-11.85	1.62	-0.83
^{239}Pu	-9.92	-16.52	-18.60	-14.09	-16.54	-15.10	-1.15	-1.61
^{240}Pu	5.36	11.32	6.64	7.64	3.80	6.61	5.06	6.85
^{241}Pu	-5.88	-0.65	-4.88	-3.72	-2.99	-1.27	8.33	8.64
^{242}Pu	4.23	23.41	13.82	10.34	13.03	13.75	9.42	9.26

Note: Measured values (M) are taken from Reference 17

Reference 11

4.1.7 Mihama-3

It has been determined that the reported burnup of sample 86g07 is lower than what would be expected by examining the relative measured isotopic concentrations. The results from sample 86g07 are not used as an indication of the accuracy of the SAS2H modules ability to predict isotopic concentrations; however, they are provided for informational purposes.

Table 4-11. Percent Difference Between Measured and Calculated [(C/M-1)*100] for Mihama

Sample	86b02	86b03	86g03	86g05	86g07	87c03	87c04	87c07	87c08
Burnup (GWd/ MTU)	8.30	6.92	21.29	15.36	14.66	29.50	32.20	33.71	34.32
^{234}U	-5.24	-	-	-	-	-	4.60	2.30	-
^{235}U	-2.09	-1.59	-4.14	-4.32	-0.54	-3.98	-8.38	-3.30	-3.36
^{236}U	6.06	4.79	-0.61	-0.75	-4.51	6.53	5.75	3.11	2.86
^{238}U	0.00	0.10	0.00	0.10	0.00	-0.11	0.00	-0.11	0.00
^{238}Pu	0.67	-3.23	-12.41	-15.83	-24.25	-12.21	-11.32	-8.33	-9.14
^{239}Pu	0.99	-0.71	-1.97	-7.53	-9.49	-3.58	-4.75	4.43	2.44
^{240}Pu	1.90	0.87	1.34	-1.94	-8.58	-2.38	-1.76	-0.86	-1.65
^{241}Pu	0.00	-1.45	-5.68	-11.27	-18.35	-11.73	-12.17	-2.54	-4.63
^{242}Pu	7.48	3.64	0.00	-4.74	-15.71	-6.62	-4.29	-2.81	-4.39

Note: Measured values (M) are taken from Reference 17

Reference 12

Table 4-12. Sensitivity Analyses for Sample 86b02

Case	Modeled Conditions	Fuel Temperature Decrease of 100 K		Boron Concentration Increase of 100 ppm	
	Calculated Concentration, g/MTU	Calculated Concentration, g/MTU	% Change in Calculated	Calculated Concentration, g/MTU	% Change in Calculated
^{234}U	2.53E2	2.53E2	0.00	2.53E2	0.00
^{235}U	2.34E4	2.34E4	0.00	2.34E4	0:00
^{236}U	1.75E3	1.75E3	0.00	1.75E3	0.00
^{238}U	9.62E5	9.62E5	0.00	9.62E5	0.00
^{238}Pu	4.54E0	4.53E0	-0.22	4.60E0	1.32
^{239}Pu	3.05E3	3.02E3	-0.98	3.07E3	0.66
^{240}Pu	4.30E2	4.28E2	-0.47	4.33E2	0.70
^{241}Pu	1.09E2	1.08E2	-0.92	1.10E2	0.92
^{242}Pu	1.02E1	1.01E1	-0.98	1.03E1	0.98

Reference 12

Table 4-13. Sensitivity Analyses for Sample 87c07

Case	Modeled Conditions	Fuel Temperature Decrease of 100 K		Boron Concentration Increase of 100 ppm	
Isotope	Calculated Concentration, g/MTU	Calculated Concentration, g/MTU	% Change in Calculated Concentrations	Calculated Concentration, g/MTU	% Change in Calculated Concentrations
^{234}U	1.78E2	1.78E2	0.00	1.78E2	0.00
^{235}U	7.63E3	7.57E3	-0.79	7.70E3	0.92
^{236}U	4.31E3	4.32E3	0.23	4.30E3	-0.23
^{238}U	9.43E5	9.43E5	0.00	9.43E5	0.00
^{238}Pu	1.54E2	1.53E2	-0.65	1.55E2	0.65
^{239}Pu	5.19E3	5.12E3	-1.35	5.24E3	0.96
^{240}Pu	2.30E3	2.30E3	0.00	2.31E3	0.43
^{241}Pu	9.58E2	9.47E2	-1.15	9.67E2	0.94
^{242}Pu	5.19E2	5.17E2	-0.39	5.19E2	0.00

Reference 12

4.2 BWRs

4.2.1 Cooper

Table 4-14. Percent Difference Between Measured and Calculated [(C/M-1)*100] for Cooper

Sample	ADD2966-B	ADD2966-K	ADD2966-T	ADD2974-B	ADD2974-J	ADD2974-U
Burnup, MWd/kg	18.96	33.07	33.94	17.84	29.23	31.04
^{99}Tc	14.18	15.44	15.37	9.53	7.19	13.65
^{234}U	-1.76	2.96	-4.17	-2.30	-1.37	-5.84
^{235}U	0.76	-2.25	-6.83	-3.85	-6.96	-15.29
^{236}U	-0.76	-1.98	-3.04	1.61	-2.08	-2.30
^{238}U	-0.20	-0.07	-0.61	-1.35	-1.65	-1.01
^{237}Np	26.76	-4.72	-5.05	19.41	-1.51	-12.66
^{238}Pu	10.84	-8.20	-9.73	-1.15	-12.20	-10.01
^{239}Pu	17.98	10.37	7.01	6.51	1.86	-5.40
^{240}Pu	6.56	-5.23	-5.02	2.20	-8.50	-7.78
^{241}Pu	25.77	7.51	3.85	15.08	4.23	-5.20
^{242}Pu	23.33	4.38	3.65	20.11	5.33	4.11
^{241}Am	37.39	19.25	15.55	25.61	15.38	2.37

Note: Measured values (M) are taken from Reference 18

Reference 13

Table 4-15. Sensitivity Analyses for Sample ADD2966-T

Case	Modeled Conditions	Fuel Temperature Increase of 100 K		Moderator Density Increase of 10%	
Isotope	Calculated Concentration, g/MTU	Calculated Concentration, g/MTU	% Change in Calculated	Calculated Concentration, g/MTU	% Change in Calculated
^{99}Tc	7.22E2	7.22E2	0.00	7.24E2	0.28
^{234}U	1.38E2	1.38E2	0.00	1.38E2	0.00
^{235}U	4.50E3	4.54E3	0.89	4.31E3	-4.22
^{236}U	3.51E3	3.50E3	-0.28	3.52E3	0.28
^{238}U	8.34E5	8.34E5	0.00	8.35E5	0.12
^{237}Np	3.32E2	3.34E2	0.60	3.23E2	-2.71
^{238}Pu	1.54E2	1.55E2	0.65	1.48E2	-3.90
^{239}Pu	3.57E3	3.61E3	1.12	3.42E3	-4.20
^{240}Pu	2.08E3	2.08E3	0.00	2.06E3	-0.96
^{241}Pu	6.44E2	6.50E2	0.93	6.21E2	-3.57
^{242}Pu	4.91E2	4.92E2	0.20	4.92E2	0.20
^{241}Am	2.83E2	2.86E2	1.06	2.71E2	-4.24

Reference 13

Table 4-16. Sensitivity Analyses for Sample ADD2974-B

Case	Modeled Conditions	Fuel Temperature Increase of 100 K		Moderator Density Increase of 50%	
Isotope	Calculated Concentration, g/MTU	Calculated Concentration, g/MTU	% Change in Calculated	Calculated Concentration, g/MTU	% Change in Calculated
^{99}Tc	3.99E2	3.99E2	0.00	4.02E2	0.75
^{234}U	1.70E2	1.70E2	0.00	1.72E2	1.18
^{235}U	1.25E4	1.26E4	0.80	1.22E4	-2.40
^{236}U	2.52E3	2.51E3	-0.40	2.51E3	-0.40
^{238}U	8.43E5	8.43E5	0.00	8.44E5	0.12
^{237}Np	1.85E2	1.86E2	0.54	1.69E2	-8.65
^{238}Pu	5.15E1	5.17E1	0.39	4.53E1	-12.04
^{239}Pu	4.32E3	4.36E3	0.93	3.93E3	-9.03
^{240}Pu	1.21E3	1.21E3	0.00	1.16E3	-4.13
^{241}Pu	3.93E2	3.97E2	1.02	3.64E2	-7.38
^{242}Pu	1.05E2	1.05E2	0.00	1.03E2	-1.90
^{241}Am	1.92E2	1.94E2	1.04	1.77E2	-7.81

Reference 13

4.3 Summary of Results

In general, the SAS2H module of SCALE is adequate in predicting isotopic concentrations for samples from each of the reactors. While over-prediction or under-prediction is significant for a few isotopes, the majority of calculated concentrations are very close to the measured concentrations. The measurement uncertainties for CC1 and Obrigheim may be expected to account for some deviation between measured and calculated concentrations. More detailed operating data would be expected to improve the accuracy of the calculated concentrations in relation to the corresponding measurements. It is recommended that future analyses use more detailed data if possible.

The accuracy with which the SAS2H module is able to predict isotopic concentrations is indicated by the percent differences presented in Tables 4-1 through 4-16. Inspection of such results reveals that the code does not consistently over-predict or under-predict concentrations for all samples. However, some isotopes are consistently over-predicted or under-predicted for samples within the same reactor. Percent differences from these analyses are compared with results from similar analyses in which calculations were performed with a previous version of SCALE and the 27burnuplib cross section library. The concentrations calculated in the similar analysis agree, for the most part, with the concentrations calculated in this analysis; however, significant differences are seen for the plutonium isotopes. Table 4-17 includes a summary of the percent differences from each of the samples. Included are the averages of the percent differences and the standard deviations of the percent differences for each of the isotopes. The average percent differences and standard deviations of percent difference indicate that the code is not entirely accurate or consistent for all samples. This is evident in the fact that the standard deviation of percent difference is larger than the average percent difference for each of the isotopes.

Table 4-17. Summary of Percent Differences

Isotope	Number of Samples	Average Percent Difference	Standard Deviation of Percent Difference
^{99}Tc	19	14.99	13.08
^{234}U	36	1.10	8.98
^{235}U	60	0.79	7.52
^{236}U	60	-0.49	3.97
^{238}U	54	-0.17	0.56
^{237}Np	19	4.28	11.33
^{238}Pu	46	-3.98	8.25
^{239}Pu	60	-2.85	9.23
^{240}Pu	60	3.02	4.76
^{241}Pu	60	-0.81	6.07
^{242}Pu	56	4.94	7.59
^{241}Am	15	0.99	18.87
^{243}Am	6	-3.67	6.07
^{143}Nd	9	0.58	0.87
^{145}Nd	9	-0.20	0.34
^{149}Sm	9	-13.38	20.79
^{150}Sm	9	1.29	3.30
^{152}Sm	9	7.19	11.17
^{153}Eu	9	1.53	3.62

Possible explanations for the differences between the results from the previous analyses and the results presented within are: 1) change from 27burnuplib to 44GROUPNDF5 cross section library, 2) use of SCALE 4.3 instead of SCALE 4.2, and 3) differences in the modeling of individual reactors. "This broad group library {44GROUPNDF5} has a similar structure as that provided in the SCALE 27 group ENDF/B-IV library, except that additional groups were added to ensure more accurate treatment of the 0.3 eV resonance of ^{239}Pu" (p. IX, Reference 14). "The cross section processing portion of the SCALE system has been upgraded to add major improvements to the NITAWL-II code. NITAWL-II has been modified to perform the resonance calculation in double precision. The mesh generation for a resonance has been modified to better span higher energy resonances and to reduce excessive numbers of mesh points. In addition, this new version of NITAWL-II is able to interpolate the available thermal-scattering matrices to obtain data for the

temperature requested by user input (via direct input to NITAWL-II or via the SCALE Standard Composition data)" (p. XI, Reference 14). Differences in the individual modeling of reactors in the previous analyses and the analyses summarized within are mainly due to improved data and modifications to maintain "in house" consistency.

Furthermore, the SAS2H code normally predicts isotopic concentrations as a radial assembly average; however, measurements are performed on individual pellet samples for all reactors except Obrigheim. Therefore, local pellet conditions are modeled as closely as possible in this analysis, so that a more realistic pellet composition can be determined. However, approximations made to obtain local pellet conditions will influence the calculated isotopic concentrations, as is shown in the sensitivity analyses discussed later.

Uncertainty in the measured concentration of isotopes helps to explain the deviation of the calculated concentrations from the measured concentrations. For example, in CC1, the calculated concentration of total U is always within the ±1.6% measurement uncertainty. However, such is not always the case for the total Pu, ^{99}Tc or ^{237}Np, which generally deviate only slightly more than the measurement uncertainty. For these, the deviation (not accounted for by the measurement uncertainty) may be explained by the lack of detailed operating data. For instance, calculated concentrations for samples from assembly BT03 deviate much more than the calculated concentrations for samples from the other assemblies for the isotopes of ^{99}Tc, ^{234}U, and ^{241}Am. This may be a result of the Path B model containing an effective infinite array of BT03 assemblies, while in reality there were few BT03 assemblies in the core. Therefore, the neutron spectrum calculated by SAS2H would be slightly different than the actual spectrum effecting the calculated concentrations. For Obrigheim the calculated concentration of ^{235}U, ^{236}U, ^{238}Pu, and ^{241}Pu are either within or very close to the measurement uncertainties of ±2%, ±1%, ±15% and ±3%, respectively. However, such is not the case for the isotopes of ^{238}Pu, ^{240}Pu and ^{242}Pu, which deviate by more than the respective measurement uncertainties.

An analysis of the sensitivity of isotopic concentrations in relation to the fuel temperature reveals that for a 100 K decrease in the fuel temperature, most of the plutonium isotopic concentrations decrease by around 1.35% or less. For the 86b02 Mihama sample at relatively low burnup, the isotopes of ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, and ^{242}Pu decrease by 1% or less; and the remaining isotopes are unchanged. For the 87c07 Mihama sample at relatively high burnup, the isotopes of ^{235}U, ^{238}Pu, and ^{242}Pu all decrease by less than 1% or less, isotopes ^{239}Pu and ^{241}Pu decrease by little more than 1%, ^{236}U increases by less that 1% and the remaining isotopes remain unchanged. For the N-9B-S HBR2 sample at relatively low burnup, the isotopes of ^{239}Pu and ^{241}Pu decreased by 1.00% and 0.96%, respectively; ^{236}U increased by 0.47% and the remaining isotopes are unchanged. For the N-9C-D HBR2 sample at relatively high burnup, the isotopes of ^{235}U, ^{237}Np, ^{239}Pu and ^{241}Pu all decreased by 1.28% or less, while ^{236}U increased by 0.33%. For a 100 K increase in the fuel temperature, the ADD2974-B Cooper sample, at relatively low burnup, shows that the isotopes of ^{235}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{241}Pu and ^{241}Am increase by 1.04% or less; ^{236}U decreases by 0.4% and the remaining isotopes are unchanged. For the ADD2966-T Cooper sample at relatively high burnup, the isotopes of ^{235}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{241}Pu, ^{242}Pu and ^{241}Am all increase by 1.12% or less; ^{236}U decreases by 0.28% and the remaining isotopes remain unchanged. The actual fuel temperature is not expected to deviate more than 200 K from the temperature assumed.

An analysis of the sensitivity of isotopic concentrations in relation to the boron concentration reveals that for a 100 ppm increase in the boron concentration, the isotopic concentrations mostly increase. For the 86b02 Mihama sample at relatively low burnup, the isotopes of ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu and ^{242}Pu increase by around 1.32% or less, and the remaining isotopes are unchanged. For the 87c07 Mihama sample at relatively high burnup, the isotopes of ^{235}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, and ^{241}Pu increase by less than 1%, the ^{236}U isotope decreases by less than 1%, and the remaining isotopes are unchanged. The sensitivity analysis also indicates that calculated isotopic concentrations increase by around 1% or less with a 100 ppm increase in boron concentration for samples from Obrigheim. Although, for Obrigheim, a slightly lower average boron concentration would improve calculated concentrations for most isotopes, it would also create a larger deviation for ^{239}Pu which already has some of the largest deviation. The average boron concentration is not expected to deviate more than 250 ppm from the assumed value. Therefore, it is expected that the assumption of an average boron concentration of 450 ppm for Obrigheim does not significantly effect the calculated isotopic concentrations.

An analysis of the sensitivity of isotopic concentrations in relation to the moderator density reveals that for a 10 percent increase in the moderator density of Cooper sample ADD2966-T and a 50 percent increase in Cooper sample ADD2974-B, the isotopic concentrations change significantly. For the ADD2974-B Cooper sample at relatively low burnup, the isotopes of ^{235}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu and ^{241}Am decrease between 2.4 to 12.04%, and the remaining isotopes change by less than 2%. For the ADD2966-T Cooper sample at relatively high burnup, the isotopes of ^{235}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{241}Pu and ^{241}Am decrease between 2.72 to 4.24% or less, and the remaining isotopes change by less than 2%. The moderator density is not expected to deviate more than 10 percent from the assumed value near the bottom of the assembly or 50 percent from the assumed value near the top of the assembly. Therefore, an incorrect assumption of the moderator density would significantly effect the calculated isotopic concentrations.

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