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1. PURPOSE

The objective of the *Limerick Unit 1 Radiochemical Assay Comparisons to SAS2H Calculations* is to determine the accuracy of the SAS2H control module of the baselined modular code system SCALE, Version 4.4A (STN: 10129-4.4A-00), in predicting the isotopic concentrations of spent fuel, and to quantify the overall effect that the differences between the calculated and measured isotopic concentrations have on the system reactivity. The scope of this calculation covers eight different spent fuel samples from a fuel assembly that was irradiated in the Limerick Unit 1 boiling water reactor (BWR). The spent fuel samples evaluated are from a three-cycle burn period, representing burnups from 37.02 GWd/MTU through 65.54 GWd/MTU (Reager 2003).

This report is an engineering calculation supporting the development of validation reports to be used for License Application of the proposed Monitored Geologic Repository (MGR), and was performed under Administrative Procedure-3.12Q, *Design Calculations and Analyses.* This calculation is subject to the *Quality Assurance Requirements and Description* (DOE 2003) per the activity evaluation under work package number ACRM01 in the technical work plan TWP-EBS-MD-000014 REV 00 (BSC 2002).

The control of the electronic management of data was accomplished in accordance with methods specified in BSC (2002).

2. METHOD

The calculational method used to determine the spent nuclear fuel isotopics consisted of using the SAS2H control sequence of the baselined modular code system SCALE to deplete the fuel for two initial fuel enrichments and eight burnups. The isotopic predictions are then compared against measured concentrations from the fuel assembly that was represented in the depletion calculations to determine the accuracy of the predicted values.

The analytical methods employed for this evaluation were the SAS2H control module of the baselined modular code system SCALE and baselined code system MCNP, Version 4B2LV (CSCI: 30033-V4B2LV). Based upon fuel assembly design, power history, and operating data for the specific assembly in the Limerick Unit 1 core, a computational representation was developed for use with SAS2H. The SAS2H module is used to perform a fuel depletion analysis to predict the isotopic concentrations in localized areas of assembly pins. The isotopic concentrations predicted by the SAS2H module are then compared with measured concentrations of the same localized areas (axial locations) of the assembly pins to determine the accuracy of the developed calculational representation. The measured and calculated isotopic compositions from SCALE were then used as input to the baselined MCNP code to calculate the neutron multiplication factor in order to quantify the overall effect that the variations between measured and calculated isotopic concentrations have on system neutron multiplication. The measured isotopic concentrations used for comparisons in this evaluation are taken from Reager (2003).

3. ASSUMPTIONS

3.1 It is assumed that the YJ1433 fuel assembly channel was made of Zircaloy-4. Although specific information about the YJ1433 assembly channel material could not be found, various sources indicate that the material used for the assembly channel in other similar General Electric fuel designs was Zircaloy-4 (CRWMS M&O 2000a, Table S2.6.4 and BSC 2001, p. 25). This assumption is used in Section 5.

3.2 It was assumed that the ^{234}U wt% in the fresh fuel composition was approximately 0.9 % of ^{235}U wt%. The rationale for this assumption is that no information about the ^{234}U content in the fresh fuel rods in YJ1433 assembly at the Limerick Unit 1 BWR is available, therefore the information about ^{234}U and ^{235}U contents in similar fuel types is used to approximate the correlation between the wt% contents for the two isotopes (CRWMS M&O 2000a, p. S2.6.11 and BSC 2001, p. 15). This assumption is used in Section 5.

3.3 It is assumed that there is no ^{236}U in the fresh fuel composition. The rationale for this assumption is that no information about the ^{236}U content in the fresh fuel rods in YJ1433 assembly at the Limerick Unit 1 BWR was available, and ^{236}U is only present in ^{235}U that has been obtained from reprocessed uranium. This assumption is used in Section 5.

3.4 The heat transfer between the outer surface of the fuel rod and the coolant is assumed to be completely efficient (i.e., there is no temperature jump across the boundary layer). The rationale for this assumption is that is reasonable for boiling heat transfer and should have an acceptably small effect on fuel temperature. This assumption is used in Section 5.

3.5 The fuel thermal conductivity is assumed to be invariant with radial temperature distribution and fuel exposure. The rationale for this assumption is that since the fuel temperature is lumped in the SAS2H depletion model, this is acceptable. This assumption is used in Section 5.

3.6 It is assumed that the omission of the isotopes ^{146}Nd, ^{148}Nd, ^{150}Nd, ^{242}Cm, ^{243}Cm, and ^{245}Cm from the MCNP cases has a negligible effect on system reactivity. The rationale for these isotopes being omitted is that the MCNP cross section libraries for these isotopes are not available, and their concentrations are very small (< 0.15 wt%). This assumption is used in Section 6.

3.7 It is assumed that using the Al material cross-section for Zn in the MCNP cases has a negligible impact on the results of criticality calculations. The basis for this assumption is that the neutronic characteristics for Zn and Al are sufficiently similar. The Zn neutron cross-section libraries are not available for MCNP. Also, the Zn material that is substituted only appears in Al6061 and is in trace amounts. This assumption is used in Section 5.

3.8 It is assumed that the length of each axial node in the core follow information for Limerick Unit 1 (Scaglione 2003) is 15.24 cm (6 in.). The basis for this assumption is the core follow information for LaSalle BWR (CRWMS M&O 1999, Table 3-4), which has a similar design with Limerick Unit 1 and the core follow information is reported for both reactors in the same (25 node) format. This assumption is used in Section 5.

4. USE OF COMPUTER SOFTWARE AND MODELS

4.1 SOFTWARE APPROVED FOR QA WORK

4.1.1 SAS2H

The SAS2H control module of the baselined modular code system SCALE, Version 4.4A (STN: 10129-4.4A-00), was used to perform the fuel assembly depletion calculations required for this evaluation. The software specifications are as follows:

- Program Name: SAS2H of the SCALE Modular Code System
- Version/Revision Number: Version 4.4A
- Status/Operating System: Qualified/HP-UX B.10.20
- Software Tracking Number: 10129-4.4A-00
- Computer Type: Hewlett Packard (HP) 9000 Series Workstations
- Computer Processing Unit number: 700887.

The input and output files for the various SAS2H calculations were documented in Attachments II and III to this calculation so that an independent repetition of the software use could be performed. The SAS2H code sequence of SCALE that was used was (1) appropriate for the application of commercial fuel assembly depletion, (2) used only within the range of validation documented in *Users Manual for SCALE-4.4A* (CRWMS M&O 2000a) and *Validation Test Report (VTR) for SCALE-4.4A* (CRWMS M&O 2000b), and (3) obtained from Software Configuration Management in accordance with appropriate procedures.

4.1.2 MCNP

The baselined code MCNP, Version 4B2LV (CSCI: 30033-V4B2LV), was used to calculate the neutron multiplication factor for the various spent nuclear fuel compositions. The software specifications are as follows:

- Program Name: MCNP
- Version/Revision Number: Version 4B2LV
- Status/Operating System: Qualified/HP-UX B.10.20
- Computer Software Configuration Item Number: 30033-V4B2LV
- Computer Type: HP 9000 Series Workstations
- CPU number: 700887.

The input and output files for the various MCNP calculations are documented in Attachments II and III to this calculation so that an independent repetition of the software use may be performed. The MCNP software used was (1) appropriate for the application of multiplication factor calculations, (2) used only within the range of validation as documented throughout *Software Qualification Report for MCNP Version 4B2, A General Monte Carlo N-Particle Transport Code* (CRWMS M&O 1998) and *MCNP-A General Monte Carlo N-Particle Transport Code* (Briesmeister 1997), and (3) obtained from Software Configuration Management in accordance with appropriate procedures.

5. CALCULATION

This report evaluates the accuracy to which the SAS2H control module can predict the composition of spent nuclear fuel for eight different radiochemical assay (RCA) samples from assembly YJ1433 that operated at the Limerick Generation Station Unit 1 BWR.

5.1 CALCULATION METHOD

The method of calculation is based upon the calculation of isotopic concentrations of irradiated fuel using the SAS2H sequence of the SCALE modular code system. All SAS2H inputs were set up to represent the assembly axial node where the measured fuel sample was located.

5.1.1 SAS2H Fuel Depletion Description

The SAS2H control sequence accesses five calculation modules of the SCALE code system for performing fuel depletion and decay calculations. The five modules include BONAMI, NITAWL-II, XSDRNPM, COUPLE, and ORIGEN-S. Each of the modules has a specific purpose in the sequence to perform the fuel depletion and decay calculations. The following provides a brief description of what each module does with a more detailed description being provided in CRWMS M&O (2000a).

- BONAMI – applies the Bondarenko method of resonance self-shielding to nuclides for which Bondarenko data are available.
- NITAWL-II – performs Nordheim resonance self-shielding corrections for nuclides that have resonance parameter data available.
- XSDRNPM – performs a one-dimensional (1-D) neutron transport calculation on a specified geometry to facilitate production of cell-weighted cross sections for fuel depletion calculations.
- COUPLE – updates all cross section constants included on an ORIGEN-S working nuclear data library with data from the cell-weighted cross section library obtained from the XSDRNPM calculation. Additionally, the weighting spectrum produced by XSDRNPM is applied to update all nuclides in the ORIGEN-S working library, which were not included in the XSDRNPM calculation.
- ORIGEN-S – performs point depletion, buildup, and decay calculations for the specified assembly irradiation history. Additionally, can be run as a stand-alone case to provide isotopic concentrations at various decay times.

The SAS2H control module uses ORIGEN-S to perform a point depletion calculation for the fuel assembly section described in the SAS2H input file. The ORIGEN-S module uses cell-weighted cross sections based on 1-D transport calculations performed by XSDRNPM. One-dimensional transport calculations are performed on two models, Path A and Path B, to calculate energy dependent spatial neutron flux distributions necessary to perform cross section cell-weighting calculations.

The Path A model is simply a unit cell of the fuel assembly lattice containing a fuel rod. In the Path A model, the fuel, cladding, and moderator are modeled explicitly. The only modification

required to develop the Path A model is the conversion of the fuel assembly's square lattice unit cell perimeter to a radial perimeter conserving moderator volume within the unit cell (exterior to the fuel rod cladding). This modification is performed automatically by the SAS2H control module. A 1-D transport calculation is performed on the Path A model for each energy group, and the spatial flux distributions for each energy group are used to calculate cell-weighted cross sections for the fuel.

The Path B model is a larger representation of the assembly than the Path A model. The Path B model approximates spectral effects due to heterogeneity within the fuel assembly such as water gaps, burnable poison rods, control rods, or axial power shaping rods. The structure of the Path B model is based on a uniform distribution of non-fuel lattice cells. In reality, most fuel assemblies do not have uniformly distributed non-fuel lattice cells, but the approximation of uniformly distributed non-fuel lattice cells is considered acceptable within the fidelity of these calculations as documented in Section S2.2.3.1 of Volume 1, Rev. 6 in CRWMS M&O (2000a).

The basic structure of the Path B model for the fuel assembly depletion calculations performed in this analysis included an inner region composed of a representation of the non-fuel assembly lattice cell. A region containing the homogenization of the Path A model surrounds the inner region in the Path B model. A final region representing the moderator in the assembly-to-assembly spacing surrounds the homogenized region in the Path B model. The size of each radial region that surrounds the inner region in the Path B model is determined by conserving both the fuel-to-moderator mass ratio and the fuel-to-absorber (burnable poison) mass ratio in the corresponding section of the fuel assembly. The cell-weighted cross sections from the Path A model are applied to the homogenized region during the Path B model transport calculations. New cell-weighted cross sections for each energy group are then developed using the unit cell spatial flux distribution results from the Path B model transport calculations. These cell-weighted cross sections are ultimately used in the point depletion calculations performed by ORIGEN-S to calculate the depleted fuel isotopic compositions in the corresponding fuel assembly. A detailed description of the calculations used to produce burnup-dependent cross sections by SAS2H is documented in Section S2.2.4 of Volume 1, Rev. 6 in CRWMS M&O (2000a).

The Path B model for the fuel assembly configuration is provided to the SAS2H control module. The essential rule in deriving the zone radii is to maintain the relative volumes for all zones in the actual assembly (p. S2.2.5, CRWMS M&O 2000a).

5.2 SAMPLE DESCRIPTION

Eight representative cross-sectional samples (approximately ½-inch thick) were obtained from three extended exposure fuel rods operated at the Limerick Unit 1 BWR to measure the concentrations of 37 selected isotopes (Reager 2003, pp. 1-1 and 2-1). The sampled fuel rods consisted of one full-length standard UO_2 rod from fuel bundle lattice location D9; a gadolinia-bearing UO_2 rod from location D8; and a part-length rod from location H5, all of which were retrieved from a GE11 9x9 fuel bundle assembly, identified as YJ1433. The 9x9 fuel rod array contains two water rods that span seven fuel rod positions, and eight part-length fuel rods (DOE 1996, p. 120). The samples were cut from various axial locations of the three fuel rods and were

dissolved and processed for the measurement of concentrations of the selected isotopes. Sample locations and basic characteristics are provided in Table 5-1.

Table 5-1. Fuel Sample Characteristic Parameters

Rod Location in Assembly Lattice	Sample Identifier	Axial Position[a] (in. / cm)	Initial Enrichment (Wt% ^{235}U)	Measured Burnup[b] (MWd/MTU)
D8	D8-3D2B D8 – 3D2C[c]	82.30 / 209.04 82.05 / 208.41	3.60	54,840
D8	D8-4G3 D8 – 4G4[c]	130.45 / 331.34 130.95 / 332.61	3.60	37,020
D9	D9-1D2 D9 – 1D3[c]	30.75 / 78.11 30.50 / 77.47	3.95	62,110
D9	D9-2D2 D9 – 2D3[c]	62.25 / 158.12 62.00 / 157.48	3.95	65,540
D9	D9-4D4 D9 – 4D3[c]	102.20 / 259.59 101.70 / 258.32	3.95	64,950
D9	D9-4G1E1 D9 – 4G1D1[c]	123.06 / 312.57 122.51 / 311.18	3.95	56,520
H5	H5-3A1C H5 – 3A1B[c]	85.25 / 216.54 85.00 / 215.90	3.95	57,915
H5	H5-3A1G H5 – 3A1E[c]	88.90 / 225.81 88.40 / 224.54	3.95	57,810

Source: Reager (2003, pp. 1-4 and 1-5).

NOTES: [a] Axial position of each sample is measured in inches from the tip of bottom end plug of the fuel rod; cm value provided was converted from inches.
[b] Measured burnup via ^{148}Nd method.
[c] Since the dissolution technique for samples assayed through the inductive coupled plasma mass spectroscopy (used for measurement of ^{95}Mo, ^{99}Tc, ^{101}Ru, ^{103}Rh, and ^{109}Ag concentrations) was significantly different than the conditions used for the rest of the analyses, duplicate "matched" full cross-sectional fuel samples (approximately ¼-inch thick) were excised from the fuel rods. The "matched" fuel samples were immediately adjacent or as close as possible to one another. No distinction will be made hereafter between the matched samples, i.e. the ^{95}Mo, ^{99}Tc, ^{101}Ru, ^{103}Rh, and ^{109}Ag concentrations will be associated to the first sample in each pair in column "Sample Identifier".

For convenience, the rods will be identified hereafter by their lattice position within the fuel bundle.

The dates of the measurements were used to calculate the amount of decay time associated with each sample. Reager (2003, pp. 4-3 through 4-7) indicated measurement dates of May 30, June 12 and July 15, 2002 for various samples. The date of July 15, 2002 was used as the reference date for all samples, and the measurements performed at other dates were corrected for decay to the reference date. This date corresponds to a downtime of 1510 days for all the samples investigated.

The radiochemical assay measured isotopic concentrations for all eight samples from assembly YJ1433 are presented in Table 5-2.

Table 5-2. Measured Concentrations for Assembly YJ1433 Samples

Sample	D8-3D2B	D8-4G3	D9-1D2	D9-2D2	D9-4D4	D9-4G1E1	H5-3A1C	H5-3A1G
Average Burnup (MWd/MTU)	54840	37020	62110	65540	64950	56520	57915	57810
Isotope	Concentration (mg/mg ^{238}U)							
^{234}U	1.61E-04	1.94E-04	1.66E-04	1.63E-04	1.65E-04	1.85E-04	1.80E-04	1.87E-04
^{235}U	4.26E-03	8.72E-03	1.70E-03	2.19E-03	2.69E-03	4.31E-03	4.80E-03	4.88E-03
^{236}U	5.71E-03	5.18E-03	6.00E-03	6.01E-03	6.05E-03	6.01E-03	6.21E-03	6.21E-03
^{238}Pu	4.39E-04	2.55E-04	4.00E-04	5.08E-04	5.43E-04	4.45E-04	5.07E-04	5.08E-04
^{239}Pu	5.46E-03	5.52E-03	3.94E-03	4.77E-03	5.30E-03	5.44E-03	6.14E-03	6.18E-03
^{240}Pu	3.70E-03	2.90E-03	3.12E-03	3.50E-03	3.61E-03	3.35E-03	3.76E-03	3.77E-03
^{241}Pu	1.38E-03	1.14E-03	1.06E-03	1.31E-03	1.43E-03	1.39E-03	1.50E-03	1.50E-03
^{242}Pu	1.19E-03	6.33E-03	1.54E-03	1.62E-03	1.56E-04	1.23E-04	1.16E-03	1.14E-03
^{143}Nd	1.02E-03	9.19E-04	8.52E-04	9.85E-04	1.04E-03	1.04E-03	1.11E-03	1.11E-03
^{145}Nd	1.01E-03	7.99E-04	1.13E-03	1.17E-03	1.16E-03	1.06E-03	1.07E-03	1.07E-03
^{146}Nd	1.23E-03	8.52E-04	1.43E-03	1.52E-03	1.50E-03	1.28E-03	1.32E-03	1.31E-03
^{148}Nd	6.15E-04	4.44E-04	6.96E-04	7.36E-04	7.29E-04	6.37E-04	6.51E-04	6.49E-04
^{150}Nd	3.09E-04	2.16E-04	3.42E-04	3.68E-04	3.65E-04	3.15E-04	3.25E-04	3.23E-04
^{134}Cs	5.74E-05	3.35E-05	5.90E-05	7.17E-05	7.22E-05	5.66E-05	6.24E-05	6.21E-05
^{137}Cs	1.87E-03	1.35E-03	1.99E-03	2.17E-03	2.09E-03	1.78E-03	1.95E-03	1.94E-03
^{151}Eu	4.77E-07	4.32E-07	3.42E-07	4.04E-07	4.38E-07	4.52E-07	5.19E-07	5.26E-07
^{153}Eu	1.94E-04	1.41E-04	2.09E-04	2.21E-04	2.15E-04	2.01E-04	1.97E-04	1.97E-04
^{155}Eu	7.96E-06	5.36E-06	8.01E-06	9.01E-06	8.74E-06	8.00E-06	8.11E-06	8.10E-06
^{147}Sm	2.88E-04	2.58E-04	2.95E-04	2.96E-04	2.90E-04	2.99E-04	2.94E-04	2.95E-04
^{149}Sm	2.69E-06	2.91E-06	1.67E-06	2.35E-06	2.81E-06	3.08E-06	2.94E-06	2.95E-06
^{150}Sm	4.81E-04	3.34E-04	4.98E-04	5.51E-04	5.43E-04	4.90E-04	5.07E-04	5.04E-04
^{151}Sm	1.35E-05	1.23E-05	1.01E-05	1.24E-05	1.35E-05	1.35E-05	1.54E-05	1.53E-05
^{152}Sm	1.52E-04	1.20E-04	1.79E-04	1.76E-04	1.66E-04	1.58E-04	1.49E-04	1.48E-04
^{155}Gd[a]	1.19E-05	9.68E-06	7.80E-06	8.78E-06	9.18E-06	7.79E-06	8.60E-06	8.09E-06
^{241}Am	3.89E-04	3.17E-04	2.83E-04	3.26E-04	3.81E-04	3.69E-04	4.08E-04	4.14E-04
^{241m}Am	1.18E-06	1.16E-06	6.68E-07	8.18E-07	9.90E-07	1.06E-06	1.42E-06	1.46E-06
^{243}Am	3.03E-04	1.30E-04	3.62E-04	3.92E-04	4.19E-04	3.01E-04	2.96E-04	2.97E-04
^{237}Np	7.92E-04	5.40E-04	7.67E-04	9.00E-04	8.86E-04	8.22E-04	8.60E-04	8.65E-04
^{95}Mo	1.27E-03	9.94E-04	1.43E-03	1.42E-03	1.37E-03	1.27E-03	1.28E-03	1.28E-03
^{99}Tc[b]	1.27E-03	9.99E-04	1.39E-03	1.36E-03	1.40E-03	1.16E-03	1.22E-03	1.18E-03
^{101}Ru	1.28E-03	9.56E-04	1.50E-03	1.51E-03	1.47E-03	1.33E-03	1.32E-03	1.36E-03
^{103}Rh	7.45E-04	6.07E-04	7.22E-04	7.59E-04	8.00E-04	7.41E-04	7.54E-04	7.84E-04
^{109}Ag	1.61E-04	1.10E-04	1.46E-04	1.53E-04	1.55E-04	1.21E-04	1.34E-04	1.51E-04
^{242}Cm	4.91E-08	3.73E-08	3.75E-08	3.76E-08	5.28E-08	5.56E-08	4.81E-08	4.27E-08
^{243}Cm	1.15E-06	6.48E-07	8.49E-07	1.13E-06	1.37E-06	1.21E-06	1.24E-06	1.30E-06
^{244}Cm	1.56E-04	4.61E-05	1.81E-04	2.21E-04	2.43E-04	1.51E-04	1.62E-04	1.63E-04
^{245}Cm	1.28E-05	3.28E-06	9.50E-06	1.53E-05	1.90E-05	1.13E-05	1.53E-05	1.53E-05
^{246}Cm	2.94E-06	4.17E-07	3.46E-06	5.10E-05	5.54E-06	2.47E-06	3.10E-06	3.10E-06

Source: Reager (2003, pp. 4-2 through 4-9).

NOTE: [a] Not including ^{155}Gd from the decay of ^{155}Eu.
[b] Includes any ^{99}Ru present in the sample solution.

5.3 FUEL ASSEMBLY DESIGN AND OPERATING PARAMETERS

The general fuel assembly design parameters are presented in Table 5-3.

Table 5-3. YJ1433 Fuel Assembly Geometric and Material Information

Fuel Assembly Data	
Lattice	9x9
Number of lattice positions occupied by water rods (DOE 1996, p. 120)	7
Number of fuel rods	74
Number of rods containing Gd_2O_3	9
Number of part-length fuel rods (DOE 1996, p. 120)	8
Rod pitch (cm)	1.440
Assembly pitch (cm)	15.240
Assembly channel material (see Assumption 3.1)	Zircaloy-4
Fuel Rod Data	
Cladding outer diameter (cm)	1.1176
Cladding thickness (cm)	0.0711
Cladding inner diameter (cm) (= Outer diameter - 2*Thickness)	0.9754
Fill gas (DOE 1992, p. 2.2-3)	Helium
Cladding material	Zircaloy-2
Fuel Pellet Data	
Diameter (cm)	0.9550
Pellet material	UO_2

Source: Nuclear Engineering International (1998, p. 63), unless otherwise noted.

The nominal characteristics of the fuel rods from which the samples were cut are presented in Table 5-4.

Table 5-4. Nominal Characteristics of Sampled Fuel Rods

Fuel Rod Number	As-Built ^{235}U (Wt.%)	As-Built Gd_2O_3 (Wt.%)	Active Fuel Column (in./cm)	As-Built Rod Length (in./cm)	Average Exposure (GWd/MTU)
D8[a]	3.60	5.00	138.0 / 350.5	160.97 / 408.9	43.5
D9[b]	3.95	0.00	146.0 / 370.8	160.97 / 408.9	54.2
H5	3.95	0.00	90.0 / 228.6	102.99 / 261.6	51.0

Source: Reager (2003, Table 1-2).

NOTES: [a] D8: bottom 6 inches: UO_2 (natural U), 112 g; top 132 inches: 95 wt% UO_2 (3.60 wt% ^{235}U) and 5 wt% Gd_2O_3, 2349g.
[b] D9: bottom 6 inches: UO_2 (natural U), 114 g; middle 132-inches: UO_2 (3.95 wt% ^{235}U), 2510g; top 8 inches UO_2 (natural U), 152 g.

There are eight part-length fuel rods like H5 in assembly YJ1433. Therefore, two main axial zones can be distinguished for assembly YJ1433:

- The lower zone, consisting of the lower 248.13 cm (97.69 in.) of the assembly fuel rods, as measured from the lower end plug tips of the rods. The length of this zone is the sum between the length of the active fuel column for the partial-length fuel rods (90 in. - see Table 5-4) and the remaining length of the fuel rod, from bottom end of active fuel

column to the end plug tip (7.69 in. - from Martinez 2001). This zone has 74 fuels rods (81 total lattice positions minus 7 positions occupied by water rods), of which 9 contain Gd_2O_3. Samples D8-3D2B, D8-3D2C, D9-1D2, D9-1D3, D9-2D2, D9-2D3, H5-3A1C, H5-3A1B, H5-3A1G, and H5-3A1E are axially located in this zone.

- The upper zone, which is between the top of the lower zone and the top end of the active fuel column of the standard rods. This zone has 66 fuels rods (81 total lattice positions minus 7 positions occupied by water rods, and minus 8 positions occupied by water above the top of part-length rods), of which 9 contain Gd_2O_3. Samples D8-4G3, D8-4G4, D9-4D4, D9-4D3, D9-4G1E1, and D9-4G1D1 are axially located in this zone.

5.3.1 SAS2H Material Specifications

The material specification section defines the UO_2 fresh fuel composition to which the SAS2H calculation pertains, along with the other materials necessary to describe the fuel assembly. The UO_2 fresh fuel composition is characterized by the fuel density, fuel temperature, and weight percentages of ^{234}U, ^{235}U, and ^{238}U. In SAS2H inputs, a number of additional isotopes are specified in trace amounts in the fresh fuel composition to assure that their buildup and decay is tracked during the depletion calculation. Table 5-5 contains a list of trace isotopes, which are specified as each having a concentration of 10^{-21} atoms/barn-cm in the fresh fuel composition.

Table 5-5. Trace Isotopes Specified in Fresh Fuel Compositions

^{83}Kr	^{85}Kr	^{90}Sr	^{89}Y	^{95}Mo	^{93}Zr	^{94}Zr
^{95}Zr	^{94}Nb	^{95}Nb	^{99}Tc	^{103}Rh	^{105}Rh	^{101}Ru
^{106}Ru	^{105}Pd	^{108}Pd	^{109}Ag	^{124}Sb	^{126}Sn	^{131}Xe
^{132}Xe	^{135}Xe	^{136}Xe	^{134}Cs	^{135}Cs	^{137}Cs	^{136}Ba
^{139}La	^{144}Ce	^{141}Pr	^{143}Pr	^{143}Nd	^{144}Nd	^{145}Nd
^{146}Nd	^{147}Nd	^{148}Nd	^{150}Nd	^{147}Pm	^{148}Pm	^{149}Pm
^{147}Sm	^{148}Sm	^{149}Sm	^{150}Sm	^{151}Sm	^{152}Sm	^{154}Gd
^{155}Gd	^{157}Gd	^{158}Gd	^{160}Gd	^{151}Eu	^{153}Eu	^{154}Eu
^{155}Eu	^{232}U	^{233}U				

The wt% ranges for Zircaloy-2 and Zircaloy-4 compositions as given in MO9906RIB00048.000 and the values selected from these ranges for the SAS2H inputs are presented in Table 5-6.

Table 5-6. Zircaloy-2 and Zircaloy-4 Compositions

Element	Wt% in Zircaloy-2[a]	SAS2H Wt% in Zircaloy-2	Wt% in Zircaloy-4[a]	SAS2H Wt% in Zircaloy-4
Cr	0.05-0.15	0.10	0.07-0.13	0.10
Fe	0.07-0.20	0.135	0.18-0.24	0.21
O	0.09-0.16	0.125	0.09-0.16	0.125
Sn	1.20-1.70	1.45	1.20-1.70	1.45
Ni	0.03-0.08	0.055	-	-
Fe+Cr	0.18-0.38	-	0.28-0.37	-
Zr	Remainder	98.135	Remainder	98.115
Density[a]	6.55 g/cm^3		6.56 g/cm^3	

Source: [a] MO9906RIB00048.000.

In the SAS2H Path A model, the moderator density and temperature must be provided, and both remain unchanged unless new values are added to the input irradiation history. The Limerick Unit 1 core follow report (Scaglione 2003) contains axial profile information for core averaged moderator void fraction, power, and exposure, and for YJ1433 assembly channel averaged power and exposure. The axial profile information for each of these physical quantities is provided as a sequence of 25 values, one for each axial node, which is a slice 15.24-cm- (6-in.-) thick of the active core (see Assumption 3.8). The lower end of the first node coincides with the lower end of the active fuel column of the standard fuel pin, which is 3.97 cm (1.563 in.) from the bottom end plug tip (Martinez 2001). The axial profile information in Scaglione (2003) is provided for 20 accounting cases for core operating cycle 5, 35 for cycle 6, and 32 for cycle 7. This information can be used to estimate the axial profile of the moderator density inside assembly YJ1433 channel, for each exposure accounting case. Therefore, it is possible to develop a more realistic Path A model than the simplified model that uses a constant moderator density for the entire residence time of the assembly in the core.

Since the moderator flows upward through the channel, the moderator density at any location is dependent not only on the power at that location but also on the power at lower locations. A correlation between the core averaged node moderator density was developed as a function of the node integrated relative core power. The node integrated relative core power is defined as the sum of the powers for that node and all the nodes below:

$$P_i = \sum_{1}^{i} p_k \qquad \text{(Eq. 1)}$$

where

p_k = relative core power for node k (normalized to 1);
P_i = integrated core relative power for node i.

The variation of core averaged node moderator density with node integrated relative core power is well fit as a fifth degree polynomial (BSC 2001, Section 5.2.7):

$$\rho_i = \sum_{j=0}^{5} C_j \cdot P_i^j \qquad \text{(Eq. 2)}$$

The coefficients C_j are calculated using the least squares method (Walpole et al. 1998, p. 411). As explained below, these coefficients are used to calculate the node averaged moderator density inside the channel containing assembly YJ1433.

The node integrated relative core power is defined as the sum of the powers for that node and all the nodes below:

$$P_{1433i} = \sum_{1}^{i} p_{1433k} \qquad \text{(Eq. 3)}$$

where

p_{1433k} = relative channel (containing assembly YJ1433) power for node k (normalized to 1);

P_{1433i} = integrated channel (containing assembly YJ1433) relative power for node i.

The node averaged moderator density in the channel containing assembly YJ1433 is calculated using the coefficients calculated via the least squares method in the following equation:

$$\rho_{1433i} = \sum_{j=0}^{5} C_j \cdot P_{1433i}^{j} \qquad \text{(Eq. 4)}$$

The isotopic composition of ^{234}U in fresh fuel was calculated using the following equation based on Assumption 3.2:

$$^{234}U \text{ wt\%} = 0.009 * {}^{235}U \text{ wt\%} \qquad \text{(Eq. 5)}$$

The ^{238}U wt% is then the remainder from the total of 100 wt%:

$$^{238}U \text{ wt\%} = 100 \text{ wt\%} - {}^{234}U \text{ wt\%} - {}^{235}U \text{ wt\%} \qquad \text{(Eq. 6)}$$

The fresh fuel densities and compositions used in this calculation are specified in Table 5-7.

Table 5-7. SAS2H Compositions Specific to Assembly YJ1433

Description	SAS2H Mixture #	Density[b] (g/cm^3)		SAS2H Identifier	Concentration[c] (wt%)	
		Rod D8 samples	Rod D9 and H5 samples		Rod D8 samples	Rod D9 and H5 samples
Fuel	1	9.37605	10.45128	92234	0.03240	0.03555
				92235	3.60000[a]	3.95000[a]
				92238	96.36760	96.01445
UO_2-Gd_2O_3 Rod	4	9.37605	10.45128	64000	5.0[a]	0[a]
				16000		

Source: [a] Reager (2003, Table 1-2).

NOTES: [b] The fuel density was calculated using the fuel column masses in pins D8 and D9 given in Reager (2003, Table 1-2), and by expanding the rod UO_2 loading to fill the cladding-pellet gap.
[c] The ^{234}U and ^{238}U wt.% were calculated using Equations 5 and 6, and the ^{235}U wt.% given in Reager (2003, Table 1-2).

5.3.2 SAS2H Operating History Specifications

The core follow report (Scaglione 2003) provides cumulative burnup information for assembly YJ1433. The average burnups for each axial node of the assembly are provided for 20 accounting cases for core operating cycle 5, 35 for cycle 6, and 32 for cycle 7. For each sample is known only the final burnup (see Table 5-1), which was measured through radiochemical assay. Sample cumulative burnup histories were estimated considering each sample was burned at the same relative rate as the full assembly. Thus, sample burnups per accounting case were obtained by normalizing the assembly burnup history and multiplying by the final sample burnup.

The axial power and burnup profile information in Scaglione (2003) was used to calculate the average values for assembly node power, moderator density, and temperatures of fuel, cladding and moderator in 37 irradiation steps, with lengths between 35 and 81 days. Irradiation steps that are less than 90 days are considered sufficiently short to have a negligible impact on SAS2H depletion results.

The fuel temperature corresponding to the nodal power was calculated from the nodal power in agreement with assumptions 3.4 and 3.5, by using equations 7 through 12, and the physical constants listed in Table 5-8.

Table 5-8. Constants for Fuel Temperature Calculations

Constant	Value used	Reference
Cladding-pellet gap mean diameter, D_G (cm)	0.965	(Cladding Inner Diameter + Pellet Outer Diameter)/2 (diameters taken from Table 5.3)
Effective gap thickness (cm)	0.0112	Calculated using Equation 10
Stefan-Boltzmann constant ($kW \cdot cm^{-2} \cdot K^{-4}$)	5.67E-15	Parrington et al. 1996, p. 59
Fuel conductivity ($kW \cdot cm^{-1} \cdot K^{-1}$)	3.17E-05	Hagrman et al. 1981, p. 29
Cladding conductivity ($kW \cdot cm^{-1} \cdot K^{-1}$)	1.64E-04	Hagrman et al. 1981, p. 219
Fuel emissivity	0.7993	Hagrman et al. 1981, p. 48
Cladding emissivity	0.325	Hagrman et al. 1981, p. 230

The linear heat generation rate ($\dot{q}$) for a single fuel rod is calculated using Equation 7.

$$\dot{q} = \frac{P_{node} \cdot K_{235}}{N_{rods} \cdot L_{node}} \qquad \text{(Eq. 7)}$$

where

P_{node} = average assembly power in node (kW);
K_{235} = ratio between pin and assembly ^{235}U wt.% (used to correct the power in pin);
N_{rods} = the number of fuel rods in lattice;
L_{node} = the active length of the node (cm).

The heat flux at the surface of the fuel pellet ($\ddot{q}$) is calculated using Equation 8.

$$\ddot{q} = \frac{\dot{q}}{\pi \cdot D_P} \qquad \text{(Eq. 8)}$$

where D_P is the diameter of the fuel pellet (cm).

The temperature change across the cladding (ΔT_C) is calculated using Equation 9 (Todreas and Kazimi 1990, p. 336).

$$\Delta T_C = \frac{\ddot{q} \cdot \delta_C}{k_C} \qquad \text{(Eq. 9)}$$

where

δ_C = the thickness of the cladding (cm);
k_C = the cladding conductivity ($kW \cdot cm^{-1} \cdot K^{-1}$).

The effective gap thickness (δ_{eff}) is estimated using Equation 10 (Todreas and Kazimi 1990, p. 334).

$$\delta_{eff} = \delta_G + \delta_{jump1} + \delta_{jump2} \quad \text{(Eq. 10)}$$

where δ_G is the geometrical gap thickness (cm), and δ_{jump1} and δ_{jump2} are corrections for temperature discontinuities near the surfaces (at atmospheric pressure, the sum of the last two terms is known to be 10^{-3} cm for helium; Todreas and Kazimi 1990, p. 334).

The gap thermal conductance (h_G) is calculated as follows (Todreas and Kazimi 1990, p. 334):

$$h_G = \frac{k_G}{\delta_{eff}} + \frac{\sigma \cdot T_S^3}{\frac{1}{\varepsilon_F} + \frac{1}{\varepsilon_C} - 1} \quad \text{(Eq. 11)}$$

where

T_S = the fuel pellet surface temperature (K);
k_G = the thermal conductivity of the gas in the gap ($kW \cdot cm^{-1} \cdot K^{-1}$);
σ = the Stefan-Boltzmann constant ($5.67 \cdot 10^{-15}$ $kW \cdot cm^{-2} \cdot K^{-4}$);
ε_F and ε_C = the emissivities of the fuel and cladding, respectively.

The thermal conductivity of the gas in the gap (helium), k_G is dependent on temperature as follows (Todreas and Kazimi 1990, p. 334):

$$k_G = 15.8 \cdot 10^{-6} \cdot T^{0.79} \quad \text{(Eq. 12)}$$

where T (K) is the gas temperature that was approximated with the average temperature across the gap (T_{avgg}, which is calculated using Equation 15).

For the fuel/cladding gap without gap closure, the temperature jump is given as follows (Todreas and Kazimi 1990, p. 336):

$$\Delta T_G = \frac{\dot{q}}{\pi \cdot D_G \cdot h_G} \quad \text{(Eq. 13)}$$

where

D_G = the gap mean diameter (cm);
h_G = the gap conductance ($kW \cdot cm^{-2} \cdot K^{-1}$; calculated using Equation 11).

The bulk temperature in the coolant/moderator (T_{bulk}) was considered approximately equal to the core outlet temperature, which was calculated by adding 10 K to the core inlet temperature. The

value of 10 K (or 10 °C) is used because it is equal to the difference between the core outlet (288 °C) and inlet (278 °C) temperatures for the Grand Gulf Unit 1 BWR, which has a very similar design to that of Limerick Unit 1 BWR (Nuclear Engineering International 1998, pp. 54 and 63).

Assuming excellent heat transfer due to boiling (see Assumption 3.4) and given the bulk temperature (T_{bulk}) in the coolant, the surface temperature of the fuel pellet may be calculated as follows:

$$T_S = T_{bulk} + \Delta T_C + \Delta T_G \quad \text{(Eq. 14)}$$

The average temperature across the gap is calculated as follows:

$$T_{avgg} = T_{bulk} + \Delta T_C + \frac{\Delta T_G}{2} \quad \text{(Eq. 15)}$$

The surface temperature of the fuel pellet and the linear heat generation rate were used to determine the centerline temperature of the fuel as shown in Equation 16 (Todreas and Kazimi 1990, p. 336):

$$T_{CL} = \frac{\dot{q}}{4 \cdot \pi \cdot k_f} + T_S \quad \text{(Eq. 16)}$$

where

T_{CL} = fuel centerline temperature (maximum fuel temperature; K);
k_f = fuel thermal conductivity (3.17E-05 $kW \cdot cm^{-1} \cdot K^{-1}$, which is based on 93.4 % of theoretical density and an average temperature of 1071 K; from Hagrman et al. 1981, p. 29).

The average temperature across the cladding is calculated as follows:

$$T_{avgc} = T_{Bulk} + \frac{\Delta T_C}{2} \quad \text{(Eq. 17)}$$

The fuel, cladding, and moderator average temperatures for each sample and each irradiation step are presented in Table 5-9. The fuel conductivity was considered to be constant, thus the average fuel temperature (T_{avgf}) is the simple average of the pellet surface and centerline temperatures.

The source of information in Table 5-9 is spreadsheet 'LGS1RCA.xls' in Attachment III (in the worksheets that have identical names with the samples). The specific columns in the worksheets from where the information is retrieved are presented in the next eight paragraphs. The power, density and temperature values used in the 37 power steps for SAS2H input are highlighted in yellow in the worksheets. In Table 5-9 the column headings are the same as the keywords used in the power history data block of the SAS2H input:

power – nodal power for a given irradiation step (MW/node; in column with the header 'Linear Heat Gen. Rate'). It was calculated by dividing the YJ1433 assembly exposure for the node where the sample is located as given in Scaglione (2003) in MWD/ST for each time step to the length of the time step (days) and multiplied with a correction factor with the purpose of obtaining the same burnup as the sample (see also first paragraph in this section).

burn – duration of the irradiation step (days; in the second column with the header 'Days').

down – time at zero power (days; in cells D100, D191, and D281).

h2of – node averaged fraction of first power step moderator density (in column with the header 'H_2O fraction'). The method of calculating the moderator density is explained in Section 5.3.1.

tmpf – node averaged fuel temperature for the irradiation step (K; in column with the header 'Fuel T_{avgf}').

tmpc – node averaged fuel cladding temperature for the irradiation step (K; was taken from column with the header 'Cladding T_{avgc}').

tmpm – node averaged moderator temperature for the irradiation step (K, was taken from column with the header 'Moderator T_{bulk}').

Equations 7 through 17 were used to calculate the average temperatures for fuel, cladding and moderator. Because the pellet surface temperature and the average temperature in the fuel-cladding gap were unknowns in a system of two transcendental equations, these temperatures were determined by changing the given input values (in columns with the headers 'Input Value for T_S,' and 'Input Value for T_{avgg}') until they matched the calculated values.

Table 5-9. Operating History Information for Assembly YJ1433

		Node 14 (D8-3D2B)					Node 22 (D8-4G3)					Node 5 (D9-1D2)				
burn	down	power	h2of	tmpf	tmpc	tmpm	power	h2of	tmpf	tmpc	tmpm	power	h2of	tmpf	tmpc	tmpm
73.0	0	0.19348	1.000	1059	574	561	0.08331	1.000	854	568	561	0.19255	1.000	1026	573	561
45.5	0	0.19718	0.877	1068	575	561	0.08553	0.902	862	569	561	0.28620	0.939	1233	579	561
45.5	0	0.19718	0.877	1068	575	561	0.08553	0.902	862	569	561	0.28620	0.939	1233	579	561
45.5	0	0.20425	0.880	1085	575	561	0.10600	0.896	929	570	561	0.28423	0.900	1228	579	561
45.5	0	0.20425	0.880	1085	575	561	0.10600	0.896	929	570	561	0.28423	0.900	1228	579	561
45.5	0	0.20348	0.978	1083	575	561	0.12238	0.905	982	572	561	0.25907	0.974	1174	577	561
45.5	0	0.20348	0.978	1083	575	561	0.12238	0.905	982	572	561	0.25907	0.974	1174	577	561
55.0	0	0.23563	0.878	1160	578	562	0.12725	1.065	998	573	562	0.31797	0.927	1301	582	562
53.0	0	0.21628	0.934	1114	577	562	0.12981	1.027	1007	574	562	0.23395	0.965	1120	577	562
50.0	0	0.24685	1.073	1183	575	558	0.16590	0.916	1118	573	558	0.23235	1.035	1113	573	558
67.0	38.0	0.20453	1.272	1086	575	561	0.16060	0.827	1103	575	561	0.13960	1.073	905	570	561
57.0	0	0.26255	0.696	1220	577	559	0.12149	1.774	978	570	559	0.33150	0.848	1328	580	559
65.0	0	0.24847	0.678	1189	577	560	0.12530	1.511	991	572	560	0.36368	0.805	1396	584	560
42.5	0	0.23814	0.725	1164	576	559	0.11584	1.246	960	570	559	0.36585	0.835	1400	583	559
42.5	0	0.23814	0.725	1164	576	559	0.11584	1.246	960	570	559	0.36585	0.835	1400	583	559
37.0	0	0.23024	0.779	1147	577	562	0.13369	1.140	1019	574	562	0.29116	0.845	1244	580	562
67.0	0	0.23010	0.793	1146	576	560	0.13108	1.041	1010	572	560	0.30643	0.844	1276	580	560
37.0	0	0.20482	0.819	1086	574	560	0.15234	0.910	1077	573	560	0.26226	0.875	1180	576	560
67.0	0	0.22097	0.889	1124	575	560	0.16937	0.835	1130	575	560	0.23495	0.971	1120	575	560
35.0	0	0.19817	0.847	1070	574	560	0.11503	0.850	958	571	560	0.22000	0.932	1088	574	560
42.0	0	0.21758	0.947	1116	575	560	0.13324	0.900	1016	572	560	0.21928	0.984	1086	574	560
43.0	0	0.14627	0.955	945	572	562	0.10259	0.887	918	571	562	0.13279	1.001	890	570	562
43.0	0	0.14627	0.955	945	572	562	0.10259	0.887	918	571	562	0.13279	1.001	890	570	562
60.0	0	0.21285	1.078	1105	574	560	0.16603	0.966	1120	575	560	0.17655	1.040	989	571	560
45.0	27.0	0.19883	1.293	1072	574	560	0.16373	1.161	1113	575	560	0.13438	1.077	893	569	560
57.0	0	0.16851	0.926	1001	575	563	0.06781	0.951	804	569	563	0.15984	1.007	954	573	563
78.0	0	0.19549	0.873	1065	575	562	0.07698	0.906	834	569	562	0.20550	0.977	1057	575	562
60.5	0	0.20135	0.894	1079	576	562	0.09416	0.876	891	571	562	0.20948	0.948	1066	576	562
60.5	0	0.20135	0.894	1079	576	562	0.09416	0.876	891	571	562	0.20948	0.948	1066	576	562
71.0	0	0.19366	0.952	1061	576	562	0.11309	0.921	953	573	562	0.19830	1.001	1041	575	562
74.0	0	0.20782	0.961	1095	576	562	0.10944	0.935	941	572	562	0.18613	1.000	1013	574	562
71.0	0	0.18913	1.111	1051	576	563	0.14128	0.992	1044	576	563	0.16350	1.026	962	574	563
81.0	0	0.15965	1.157	979	574	563	0.13612	1.066	1028	575	563	0.17005	1.021	977	574	563
41.0	0	0.15220	1.101	960	572	562	0.13692	1.046	1029	574	562	0.18649	0.994	1014	574	562
48.0	0	0.16887	1.000	1002	575	563	0.12618	1.008	996	575	563	0.23810	0.920	1130	579	563
48.0	0	0.16091	1.073	983	574	563	0.12809	1.060	1003	575	563	0.18756	0.965	1017	575	563
63.0	1510	0.12927	1.307	902	569	560	0.10709	1.247	932	569	560	0.13378	1.052	891	568	560

Table 5-9. Operating History Information for Assembly YJ1433 (continued)

		Node 11 (D9-2D2)					Node 17 (D9-4D4)					Node 21 (D9-4G1E1)				
burn	down	power	h2of	tmpf	tmpc	tmpm	power	h2of	tmpf	tmpc	tmpm	power	h2of	tmpf	tmpc	tmpm
73.0	0	0.23202	1.000	1107	575	561	0.18271	1.000	1062	574	561	0.13137	1.000	930	570	561
45.5	0	0.26529	0.853	1180	578	561	0.18458	0.882	1067	575	561	0.13469	0.891	939	571	561
45.5	0	0.26529	0.853	1180	578	561	0.18458	0.882	1067	575	561	0.13469	0.891	939	571	561
45.5	0	0.25452	0.848	1156	577	561	0.21496	0.874	1143	576	561	0.16663	0.876	1022	573	561
45.5	0	0.25452	0.848	1156	577	561	0.21496	0.874	1143	576	561	0.16663	0.876	1022	573	561
45.5	0	0.23305	0.977	1110	576	561	0.24941	0.946	1228	579	561	0.19459	0.898	1093	575	561
45.5	0	0.23305	0.977	1110	576	561	0.24941	0.946	1228	579	561	0.19459	0.898	1093	575	561
55.0	0	0.29177	0.872	1237	580	562	0.26319	0.844	1263	581	562	0.20343	0.959	1116	577	562
53.0	0	0.25663	0.933	1162	578	562	0.24836	0.893	1226	580	562	0.20660	0.937	1124	577	562
50.0	0	0.28952	1.082	1229	576	558	0.28455	1.023	1312	579	558	0.25913	0.917	1252	577	558
67.0	38.0	0.23129	1.268	1106	575	561	0.23933	1.228	1204	578	561	0.24137	0.978	1210	579	561
57.0	0	0.33564	0.716	1327	580	559	0.25400	0.729	1238	578	559	0.19225	1.436	1086	573	559
65.0	0	0.32068	0.684	1296	581	560	0.24489	0.700	1217	578	560	0.19441	1.235	1092	574	560
42.5	0	0.30160	0.726	1256	578	559	0.23708	0.699	1197	576	559	0.18062	1.009	1056	572	559
42.5	0	0.30160	0.726	1256	578	559	0.23708	0.699	1197	576	559	0.18062	1.009	1056	572	559
37.0	0	0.27503	0.766	1201	579	562	0.25360	0.759	1239	580	562	0.20588	0.990	1122	577	562
67.0	0	0.27154	0.773	1193	578	560	0.26351	0.768	1263	580	560	0.20480	0.922	1119	575	560
37.0	0	0.23440	0.803	1112	574	560	0.23457	0.796	1191	577	560	0.23120	0.823	1184	577	560
67.0	0	0.24842	0.905	1142	575	560	0.25440	0.858	1240	578	560	0.25640	0.798	1246	578	560
35.0	0	0.23686	0.844	1118	575	560	0.20907	0.824	1128	576	560	0.17684	0.815	1048	573	560
42.0	0	0.25812	0.951	1164	576	560	0.22919	0.930	1178	577	560	0.20237	0.891	1112	575	560
43.0	0	0.16652	0.969	963	572	562	0.15925	0.953	1002	573	562	0.15184	0.907	984	573	562
43.0	0	0.16652	0.969	963	572	562	0.15925	0.953	1002	573	562	0.15184	0.907	984	573	562
60.0	0	0.24491	1.098	1135	575	560	0.23439	1.049	1191	577	560	0.23936	0.986	1204	577	560
45.0	27.0	0.22816	1.304	1099	575	560	0.21826	1.241	1151	576	560	0.23172	1.188	1186	577	560
57.0	0	0.21049	0.942	1062	576	563	0.15473	0.931	992	574	563	0.10735	0.948	868	571	563
78.0	0	0.25345	0.873	1155	578	562	0.17428	0.887	1041	575	562	0.12128	0.904	904	571	562
60.5	0	0.23769	0.888	1121	577	562	0.19138	0.896	1085	576	562	0.14585	0.882	969	573	562
60.5	0	0.23769	0.888	1121	577	562	0.19138	0.896	1085	576	562	0.14585	0.882	969	573	562
71.0	0	0.23943	0.972	1125	578	562	0.19113	0.943	1084	576	562	0.16984	0.928	1031	575	562
74.0	0	0.25311	0.983	1154	578	562	0.19808	0.955	1102	577	562	0.16665	0.942	1023	574	562
71.0	0	0.18066	1.119	996	575	563	0.21880	1.066	1154	579	563	0.21403	1.009	1144	579	563
81.0	0	0.17242	1.143	977	574	563	0.17623	1.138	1047	576	563	0.20274	1.086	1115	578	563
41.0	0	0.18265	1.069	999	573	562	0.17503	1.104	1043	574	562	0.20369	1.062	1117	577	562
48.0	0	0.19833	0.957	1035	576	563	0.17902	1.025	1054	576	563	0.18537	1.018	1072	577	563
48.0	0	0.18429	1.038	1004	575	563	0.17331	1.087	1040	576	563	0.18472	1.074	1070	577	563
63.0	1510	0.15039	1.256	925	569	560	0.13888	1.304	948	570	560	0.15201	1.264	983	571	560

Table 5-9. Operating History Information for Assembly YJ1433 (continued)

		Node 14 (H5-3A1C)					Node 15 (H5-3A1G)				
burn	down	power	h2of	tmpf	tmpc	tmpm	power	h2of	tmpf	tmpc	Tmpm
73.0	0	0.20433	1.000	1104	575	561	0.19860	1.000	1087	575	561
45.5	0	0.20823	0.877	1114	576	561	0.19891	0.881	1089	575	561
45.5	0	0.20823	0.877	1114	576	561	0.19891	0.881	1089	575	561
45.5	0	0.21570	0.880	1132	576	561	0.21298	0.882	1123	576	561
45.5	0	0.21570	0.880	1132	576	561	0.21298	0.882	1123	576	561
45.5	0	0.21489	0.978	1130	576	561	0.21974	0.972	1139	576	561
45.5	0	0.21489	0.978	1130	576	561	0.21974	0.972	1139	576	561
55.0	0	0.24884	0.878	1213	580	562	0.24720	0.871	1206	579	562
53.0	0	0.22841	0.934	1164	578	562	0.22941	0.927	1163	578	562
50.0	0	0.26069	1.073	1239	576	558	0.26297	1.062	1241	577	558
67.0	38.0	0.21600	1.272	1133	576	561	0.21927	1.261	1138	576	561
57.0	0	0.27727	0.696	1279	579	559	0.26841	0.689	1255	578	559
65.0	0	0.26241	0.678	1245	579	560	0.25473	0.673	1223	578	560
42.5	0	0.25149	0.725	1218	577	559	0.24569	0.715	1201	577	559
42.5	0	0.25149	0.725	1218	577	559	0.24569	0.715	1201	577	559
37.0	0	0.24315	0.779	1199	579	562	0.25029	0.772	1213	579	562
67.0	0	0.24300	0.793	1198	578	560	0.25549	0.788	1225	579	560
37.0	0	0.21630	0.819	1133	575	560	0.21936	0.817	1137	575	560
67.0	0	0.23336	0.889	1174	576	560	0.23707	0.883	1180	577	560
35.0	0	0.20928	0.847	1116	575	560	0.20801	0.844	1110	575	560
42.0	0	0.22978	0.947	1166	577	560	0.22823	0.944	1159	576	560
43.0	0	0.15448	0.955	980	573	562	0.15535	0.955	980	573	562
43.0	0	0.15448	0.955	980	573	562	0.15535	0.955	980	573	562
60.0	0	0.22478	1.078	1153	576	560	0.22645	1.069	1155	576	560
45.0	27.0	0.20997	1.293	1118	575	560	0.21121	1.275	1118	575	560
57.0	0	0.17795	0.926	1041	576	563	0.17272	0.926	1025	575	563
78.0	0	0.20645	0.873	1110	577	562	0.19865	0.877	1089	576	562
60.5	0	0.21264	0.894	1126	577	562	0.20975	0.895	1116	577	562
60.5	0	0.21264	0.894	1126	577	562	0.20975	0.895	1116	577	562
71.0	0	0.20451	0.952	1106	577	562	0.20211	0.947	1097	577	562
74.0	0	0.21947	0.961	1142	578	562	0.21509	0.958	1129	577	562
71.0	0	0.19974	1.111	1095	577	563	0.21091	1.095	1120	578	563
81.0	0	0.16860	1.157	1017	575	563	0.17305	1.152	1026	575	563
41.0	0	0.16073	1.101	996	573	562	0.16411	1.105	1003	573	562
48.0	0	0.17834	1.000	1042	576	563	0.18076	1.010	1045	576	563
48.0	0	0.16993	1.073	1021	576	563	0.17298	1.079	1026	576	563
63.0	1510	0.13652	1.307	933	570	560	0.13837	1.310	936	570	560

5.4 SAS2H PATH B REPRESENTATIONS

The Path B model for the fuel assembly configuration is provided to the SAS2H control module. The primary concern in the development of the Path B model for BWR assemblies is the conservation of the fuel-to-moderator and the fuel-to-absorber mass ratios. The Path B model used in this evaluation is for a GE11 9x9 fuel assembly with 9 rods that contain gadolinium as a burnable neutron absorber. Figure 5-1 illustrates the general diagram of the Path B model, where R_i (i = 1,…,6) refer to the radial dimensions.

Figure 5-1. SAS2H General Path B Model used for Assembly YJ1433

At any time during assembly YJ1433 residence inside Limerick Unit 1 BWR core, there is no control blade inserted fully or partially inside the blade position adjacent to the assembly (Scaglione 2003). Therefore no control blade region is represented in the Path B model.

SAS2H code sets the fuel composition to be uniform throughout the fuel and burnable absorber region (CRWMS M&O 2000a, p. S2.5.15). In the SAS2H representation of the fuel assembly node, the input value for the U fuel composition that most accurately represents the node assembly is the node-averaged U composition. However, for the purpose of this calculation the most accurate sample representation is needed. Therefore, the input value used for the U fuel composition in each case was the sample composition.

Equations 18 through 23 are used to calculate the Path B zone radii. For the first zone, which represents the burnable absorber rod (UO_2-Gd_2O_3 mixture), the pellet diameter was increased to the inner cladding diameter and the material density was adjusted (smeared) accordingly. Therefore, the radius of the first zone is:

R_1 = (Fuel Rod Cladding Inner Diameter)/2 = 0.4877 cm. (Eq. 18)

The second zone represents the fuel rod cladding. Its radius is:

R_2 = (Fuel Rod Cladding Outer Diameter)/2 = 0.5588 cm. (Eq. 19)

The third zone represents the moderator in the fuel rod lattice cell. Its radius is:

$$R_3 = \frac{\text{rodpitch}}{\sqrt{\pi}} = 0.81243 \text{ cm} \quad \text{(Eq. 20)}$$

where ‘rodpitch’ is the rod pitch in the 9x9 lattice.

The radii values for the first three zones are applicable to all eight samples.

The fourth zone represents the homogenized fuel zone. Its radius is:

$$R_4 = \sqrt{R_3^2 + \left(\frac{\#\text{fuelrods}}{\#\text{gdrods}} - 1\right) \cdot \frac{\text{rodpitch}^2}{\pi}} \quad \text{(Eq. 21)}$$

where

R_3 = the radius of the third Path B zone

#fuelrods = the total number of fuel rods in assembly (including those that contain Gd_2O_3)

#gdrods = the number of rods in assembly that contain Gd_2O_3.

As explained in Section 5.3, the fuel assembly has two axial zones with different numbers of fuel rods: 74 in the lower zone, and 66 in the upper zone. Therefore, Equation 21 gives two different results for R_4, 2.32960 cm for the lower zone, and 2.20008 cm for the upper zone.

The fifth zone represents the assembly channel zone. Its radius is:

$$R_5 = \sqrt{R_4^2 + \frac{\text{outwidth}^2 - \text{inwidth}^2}{\#\text{gdrods} \cdot \pi}} \quad \text{(Eq. 22)}$$

where

R_4 = the radius of the fourth Path B zone

outwidth = the outer width of the assembly channel

inwidth = the inner width of the assembly channel.

R_5 is 2.45181 cm for the lower zone, and 2.32909 cm for the upper zone.

The sixth zone represents the moderator outside the assembly channel zone, but inside the assembly lattice cell. Its radius is:

$$R_6 = \frac{\text{assemblypitch}}{\sqrt{\pi \cdot \#\text{gdrods}}} \quad \text{(Eq. 23)}$$

where 'assemblypitch' is the assembly pitch in the core zone lattice.

Equation 23 is independent of the axial zone of the assembly, therefore R_6 is 2.86608 cm for both zones.

5.5 MCNP SPECIFICATIONS

In order to quantify the overall effect that the differences between the calculated and measured isotopic concentrations have on system reactivity, MCNP calculations were performed to calculate the multiplication factor (k_{eff}) that results from using the different sets of isotopic concentrations and provide a comparison in terms of Δk_{eff}.

The axial nodes from which the samples came from were used to represent fuel assemblies in a flooded waste package configuration. The waste package design parameters used in the MCNP

representations are illustrated in Attachment I. Axially reflective boundary conditions were used for each representation. The general assembly design parameters were presented in Table 5-3.

The spent fuel isotopes used in the MCNP cases correspond to those from the SAS2H calculations and the measured sample isotopes. Isotopes were extracted from the SAS2H outputs and measured results, and then combined with the initial oxygen mass and renormalized to the total mass in terms of weight percents. Isotopes ^{146}Nd, ^{148}Nd, ^{150}Nd, ^{242}Cm, ^{243}Cm, ^{245}Cm, and ^{246}Cm were omitted from the MCNP cases as they have a negligible effect on system reactivity (see Assumption 3.6). The values from the SAS2H calculations are given in units of mols, which were converted to units of grams using Equation 24. In order to keep changes in reactivity limited to variations from isotopic concentrations, for the MCNP density input was used the value calculated for the fresh fuel. Each depleted fuel composition is listed in the MCNP input files contained in Attachment III in terms of ZAID's and weight percents, and can be verified by visual inspection from the SAS2H outputs along with the equation provided. The SAS2H output files for each calculation are contained on a compact disc attachment (Attachment III).

$$\text{Mass}_i = (\text{Mols Isotope}_i) * A_i \qquad \text{(Eq. 24)}$$

where 'i' is the particular isotope and A_i is the atomic mass value (from Audi and Wapstra 1995).

The outer barrier of the waste package was represented as SB-575 N06022 as described in Table 5-10. The inner barrier was represented as SA-240 S31600, which is nuclear grade 316 stainless steel (SS) with tightened control on carbon and nitrogen content (ASM International 1987, p. 931, and ASME 1998, Section II, SA-240, Table 1) as described in Table 5-11. The fuel basket plates were represented as Neutronit A978 with 1.62 wt% boron as described in Table 5-12, and the thermal shunts were represented as aluminum 6061 as described in Table 5-13. The basket side and corner guides were represented as Grade 70 A 516 carbon steel as described in Table 5-14. The basket stiffeners were represented as water since they are not solid over the length of the basket.

The chromium, nickel, and iron elemental weight percents obtained from the references were expanded into their constituent natural isotopic weight percents for use in MCNP. This expansion was performed by: (1) calculating a natural weight fraction of each isotope in the elemental state, and (2) multiplying the elemental weight percent in the material of interest by the natural weight fraction of the isotope in the elemental state to obtain the weight percent of the isotope in the material of interest. This process is described mathematically in Equations 25 and 26. The atomic mass values and atom percent of natural element values for these calculations are from Parrington et al (1996).

$$\begin{pmatrix} \text{Weight Fraction} \\ \text{of Isotope "i" in the} \\ \text{Natural Element} \end{pmatrix} = \frac{(\text{Atomic Mass of Isotope "i"})(\text{At\% of Isotope "i" in Natural Element})}{\sum_{i=1}^{I} (\text{Atomic Mass of Isotope "i"})(\text{At\% of Isotope "i" in Natural Element})} \qquad \text{(Eq. 25)}$$

where 'I' the total number of isotopes in the natural element

$$\begin{pmatrix}\text{Wt\% of Isotope "i" in}\\ \text{Material Composition}\end{pmatrix} = \begin{pmatrix}\text{Weight Fraction}\\ \text{of Isotope "i" in the}\\ \text{Natural Element}\end{pmatrix}\begin{pmatrix}\text{Reference Wt\% of}\\ \text{Element in Material Composition}\end{pmatrix} \quad \text{(Eq. 26)}$$

Table 5-10. Material Specifications for SB-575 N06022

Element/Isotope	ZAID	Wt%	Element/Isotope	ZAID	Wt%
C-nat	6000.50c	0.0150	^{59}Co	27059.50c	2.5000
^{55}Mn	25055.50c	0.5000	^{182}W	74182.55c	0.7877
Si-nat	14000.50c	0.0800	^{183}W	74183.55c	0.4278
^{50}Cr	24050.60c	0.8879	^{184}W	74184.55c	0.9209
^{52}Cr	24052.60c	17.7863	^{186}W	74186.55c	0.8636
^{53}Cr	24053.60c	2.0554	V	23000.50c	0.3500
^{54}Cr	24054.60c	0.5202	^{54}Fe	26054.60c	0.2260
^{58}Ni	28058.60c	36.8024	^{56}Fe	26056.60c	3.6759
^{60}Ni	28060.60c	14.6621	^{57}Fe	26057.60c	0.0865
^{61}Ni	28061.60c	0.6481	^{58}Fe	26058.60c	0.0116
^{62}Ni	28062.60c	2.0975	^{32}S	16032.50c	0.0200
^{64}Ni	28064.60c	0.5547	^{31}P	15031.50c	0.0200
Mo-nat	42000.50c	13.5000	Density = 8.69 g/cm^3		

Source: MO0003RIB00071.000.

Table 5-11. Material Specifications for SS316NG

Element/Isotope	ZAID	Wt%	Element/Isotope	ZAID	Wt%
C-nat	6000.50c	0.0200	^{54}Fe	26054.60c	3.6911
^{14}N	7014.50c	0.0800	^{56}Fe	26056.60c	60.0322
Si-nat	14000.50c	1.0000	^{57}Fe	26057.60c	1.4119
^{31}P	15031.50c	0.0450	^{58}Fe	26058.60c	0.1897
^{32}S	16032.50c	0.0300	^{58}Ni	28058.60c	8.0641
^{50}Cr	24050.60c	0.7103	^{60}Ni	28060.60c	3.2127
^{52}Cr	24052.60c	14.2291	^{61}Ni	28061.60c	0.1420
^{53}Cr	24053.60c	1.6443	^{62}Ni	28062.60c	0.4596
^{54}Cr	24054.60c	0.4162	^{64}Ni	28064.60c	0.1216
^{55}Mn	25055.50c	2.0000	Mo-nat	42000.50c	2.5000
Density = 7.98 g/cm^3					

Source: ASM International (1987), p. 931, and ASME 1998, Section II, SA-240, Table 1.

Table 5-12. Material Specifications for Neutronit A978 with 1.62 wt% Boron

Element/Isotope	ZAID	Wt%	Element/Isotope	ZAID	Wt%
^{10}B	5010.50c	0.2986	^{57}Fe	26057.60c	1.3928
^{11}B	5011.56c	1.3214	^{58}Fe	26058.60c	0.1872
C-nat	6000.50c	0.0400	^{59}Co	27059.50c	0.2000
^{50}Cr	24050.60c	0.7730	^{58}Ni	28058.60c	8.7361
^{52}Cr	24052.60c	15.4846	^{60}Ni	28060.60c	3.4805
^{53}Cr	24053.60c	1.7894	^{61}Ni	28061.60c	0.1539
^{54}Cr	24054.60c	0.4529	^{62}Ni	28062.60c	0.4979
^{54}Fe	26054.60c	3.6411	^{64}Ni	28064.60c	0.1317
^{56}Fe	26056.60c	59.2189	Mo-nat	42000.50c	2.2000
Density = 7.76 g/cm^3					

Source: MO0109RIB00049.001.

Table 5-13. Material Specifications for Al 6061

Element/Isotope	ZAID	Wt%	Element/Isotope	ZAID	Wt%
Si-nat	14000.50c	0.6000	Mg-nat	12000.50c	1.0000
^{54}Fe	26054.60c	0.0396	^{50}Cr	24050.60c	0.0081
^{56}Fe	26056.60c	0.6433	^{52}Cr	24052.60c	0.1632
^{57}Fe	26057.60c	0.0151	^{53}Cr	24053.60c	0.0189
^{58}Fe	26058.60c	0.0020	^{54}Cr	24054.60c	0.0048
^{63}Cu	29063.60c	0.1884	Ti-nat	22000.50c	0.1500
^{65}Cu	29065.60c	0.0866	^{27}Al	13027.50c	96.9300
^{55}Mn	25055.50c	0.1500	Density = 2.7065 g/cm^3		

Source: MO9906RIB00048.000.

NOTE: Zn cross-section data unavailable, therefore it was substituted as ^{27}Al (See assumption 3.7).

Table 5-14. Material Specifications for Grade 70 A516 Carbon Steel

Element/Isotope	ZAID	Wt%[a]	Element/Isotope	ZAID	Wt%[a]
C-nat	6000.50c	0.2700	^{54}Fe	26054.60c	5.5558
^{55}Mn	25055.50c	1.0450	^{56}Fe	26056.60c	90.3584
^{31}P	15031.50c	0.0350	^{57}Fe	26057.60c	2.1252
^{32}S	16032.50c	0.0350	^{58}Fe	26058.60c	0.2856
Si-nat	14000.50c	0.2900	Density[b] = 7.850 g/cm^3		

Sources: [a] ASTM A 516/A 516M-01 (2001), Table 1.
[b] ASTM A 20/A20M-99a (1999), p. 9.

Table 5-15. Material Specifications for Zircaloy-2

Element/Isotope	ZAID	Wt%[a]	Element/Isotope	ZAID	Wt%[a]
^{16}O	6000.50c	0.1250	^{58}Fe	26058.60c	0.0004
^{50}Cr	24050.60c	0.0042	^{58}Ni	28058.60c	0.0370
^{52}Cr	24052.60c	0.0837	^{60}Ni	28060.60c	0.0147
^{53}Cr	24053.60c	0.0097	^{61}Ni	28061.60c	0.0007
^{54}Cr	24054.60c	0.0024	^{62}Ni	28062.60c	0.0021
^{54}Fe	26054.60c	0.0076	^{64}Ni	28064.60c	0.0006
^{56}Fe	26056.60c	0.1241	Sn-nat	50000.35c	1.4500
^{57}Fe	26057.60c	0.0029	Zr-nat	40000.60c	98.1350
Density = 6.55 g/cm^3					

Source: MO9906RIB00048.000.

Table 5-16. Material Specifications for Zircaloy-4

Element/Isotope	ZAID	Wt%	Element/Isotope	ZAID	Wt%
^{50}Cr	24050.60c	0.0042	^{57}Fe	26057.60c	0.0045
^{52}Cr	24052.60c	0.0837	^{58}Fe	26058.60c	0.0006
^{53}Cr	24053.60c	0.0097	^{16}O	8016.50c	0.1250
^{54}Cr	24054.60c	0.0024	Zr-nat	40000.60c	98.1150
^{54}Fe	26054.60c	0.0119	Sn-nat	50000.35c	1.4500
^{56}Fe	26056.60c	0.1930	Density = 6.56 g/cm^3		

Source: MO9906RIB00048.000.

6. RESULTS

The Limerick Generating Station Unit 1 radiochemical assay comparison results are presented in this section. The criticality calculations were performed using two different sets of compositions for the fuel material while keeping unchanged all the other material compositions and geometry parameters for the waste package disposal configuration. One set consists of the concentrations for 32 of the isotopes measured in eight samples, and the other set consists of the concentrations for the same isotopes calculated using the SAS2H sequence of SCALE 4.4a. The results presented provide a comparison of the calculated isotopic concentrations with the measured isotopic concentrations on a percent difference basis. The difference between the measured and the calculated value was divided by the measured value to determine the accuracy of the SAS2H calculation. A positive percent difference represents an over prediction by the code, while a negative percent difference represents an under prediction by the code. Two additional calculations were performed, for the two fresh fuel compositions (and using the same geometry).

In order to quantify the overall effect that the differences between the calculated and measured isotopic concentrations have on system reactivity, MCNP calculations were performed to calculate the multiplication factor (k) that results from using the different sets of isotopic concentrations and provide a comparison in terms of Δk. The results represent the average combined collision, absorption, and track-length estimator from the MCNP calculations. The standard deviation (σ) represents the standard deviation of k about the average combined collision, absorption, and track-length estimate due to the Monte Carlo calculation statistics.

The SAS2H and MCNP input and output files used in this evaluation are contained on an attachment compact disc to this calculation file as listed in Attachment II. The outputs are considered reasonable compared to inputs.

The results are suitable for their intended use.

6.1 SAMPLE RESULTS FROM ASSEMBLY YJ1433

Table 6-1 presents the SAS2H calculated isotopic concentrations.

Table 6-1. SAS2H Calculated Isotopic Concentrations for Assembly YJ1433 Samples

Sample	D8-3D2B	D8-4G3	D9-1D2	D9 2D2	D9 4D4	D9-4G1E1	H5-3A1C	H5-3A1G
Node	15	23	6	11	18	22	15	16
Isotope	($g/g^{238}U$)							
^{234}U	1.49E-04	1.97E-04	1.62E-04	1.56E-04	1.50E-04	1.71E-04	1.73E-04	1.72E-04
^{235}U	2.63E-03	6.62E-03	2.13E-03	2.38E-03	1.68E-03	3.09E-03	4.09E-03	4.20E-03
^{236}U	5.57E-03	5.15E-03	6.11E-03	6.17E-03	6.18E-03	6.17E-03	6.15E-03	6.16E-03
^{238}Pu	4.45E-04	1.87E-04	4.27E-04	5.32E-04	4.61E-04	3.78E-04	4.62E-04	4.68E-04
^{239}Pu	4.85E-03	4.15E-03	4.32E-03	4.95E-03	4.17E-03	4.29E-03	5.31E-03	5.40E-03
^{240}Pu	3.54E-03	2.63E-03	3.33E-03	3.69E-03	3.52E-03	3.33E-03	3.58E-03	3.60E-03
^{241}Pu	1.26E-03	8.58E-04	1.13E-03	1.32E-03	1.11E-03	1.08E-03	1.35E-03	1.36E-03
^{242}Pu	1.50E-03	6.38E-04	1.61E-03	1.71E-03	1.70E-03	1.28E-03	1.33E-03	1.32E-03
^{143}Nd	1.04E-03	9.03E-04	1.00E-03	1.11E-03	9.79E-04	1.01E-03	1.14E-03	1.15E-03
^{145}Nd	1.12E-03	8.42E-04	1.20E-03	1.24E-03	1.22E-03	1.11E-03	1.14E-03	1.13E-03
^{146}Nd	1.40E-03	8.80E-04	1.50E-03	1.60E-03	1.60E-03	1.35E-03	1.38E-03	1.38E-03
^{148}Nd	6.83E-04	4.55E-04	7.27E-04	7.70E-04	7.59E-04	6.58E-04	6.78E-04	6.76E-04
^{150}Nd	3.48E-04	2.18E-04	3.66E-04	3.93E-04	3.85E-04	3.27E-04	3.40E-04	3.40E-04
^{134}Cs	6.10E-05	2.92E-05	6.31E-05	7.20E-05	7.13E-05	5.77E-05	5.86E-05	5.88E-05
^{137}Cs	2.06E-03	1.37E-03	2.18E-03	2.32E-03	2.29E-03	1.98E-03	2.04E-03	2.03E-03
^{151}Eu	5.28E-07	3.94E-07	4.79E-07	5.72E-07	4.86E-07	4.73E-07	5.89E-07	6.00E-07
^{153}Eu	2.37E-04	1.42E-04	2.51E-04	2.65E-04	2.58E-04	2.20E-04	2.31E-04	2.30E-04
^{155}Eu	6.61E-06	3.64E-06	6.84E-06	7.49E-06	7.14E-06	6.03E-06	6.45E-06	6.45E-06
^{147}Sm	2.78E-04	2.67E-04	3.00E-04	2.91E-04	2.85E-04	2.87E-04	2.89E-04	2.87E-04
^{149}Sm	2.46E-06	2.18E-06	2.24E-06	2.63E-06	2.40E-06	2.60E-06	2.69E-06	2.75E-06
^{150}Sm	5.26E-04	3.39E-04	5.45E-04	5.91E-04	5.71E-04	5.01E-04	5.26E-04	5.26E-04
^{151}Sm	1.57E-05	1.16E-05	1.43E-05	1.70E-05	1.46E-05	1.42E-05	1.74E-05	1.77E-05
^{152}Sm	2.23E-04	1.63E-04	2.39E-04	2.44E-04	2.46E-04	2.18E-04	2.19E-04	2.18E-04
^{155}Gd	5.70E-06	3.14E-06	5.88E-06	6.45E-06	6.13E-06	5.18E-06	5.58E-06	5.58E-06
^{241}Am	3.50E-04	2.44E-04	3.09E-04	3.64E-04	2.95E-04	2.90E-04	3.79E-04	3.84E-04
^{241m}Am	1.26E-06	9.37E-07	9.90E-07	1.27E-06	8.59E-07	8.99E-07	1.52E-06	1.55E-06
^{243}Am	4.25E-04	1.25E-04	4.43E-04	5.12E-04	4.74E-04	3.29E-04	3.78E-04	3.77E-04
^{237}Np	7.62E-04	4.56E-04	7.70E-04	8.74E-04	7.86E-04	7.07E-04	8.13E-04	8.18E-04
^{95}Mo	1.32E-03	9.59E-04	1.42E-03	1.47E-03	1.46E-03	1.31E-03	1.33E-03	1.33E-03
^{99}Tc	1.38E-03	1.00E-03	1.48E-03	1.53E-03	1.51E-03	1.36E-03	1.39E-03	1.38E-03
^{101}Ru	1.42E-03	9.58E-04	1.52E-03	1.59E-03	1.57E-03	1.37E-03	1.41E-03	1.40E-03
^{103}Rh	7.21E-04	5.42E-04	7.35E-04	7.73E-04	7.27E-04	6.81E-04	7.29E-04	7.28E-04
^{109}Ag	1.82E-04	1.02E-04	1.87E-04	2.02E-04	1.94E-04	1.60E-04	1.73E-04	1.72E-04
^{242}Cm	4.71E-08	2.83E-08	4.62E-08	5.10E-08	4.45E-08	4.32E-08	4.83E-08	4.90E-08
^{243}Cm	9.82E-07	3.76E-07	8.87E-07	1.11E-06	9.33E-07	8.19E-07	9.91E-07	1.01E-06
^{244}Cm	1.99E-04	3.22E-05	1.96E-04	2.63E-04	2.44E-04	1.40E-04	1.68E-04	1.68E-04
^{245}Cm	8.21E-06	1.02E-06	6.73E-06	1.11E-05	8.77E-06	5.17E-06	7.54E-06	7.74E-06

Table 6-2 presents the results in terms of percent difference for the calculated isotopic concentrations compared with the measured results (Table 5-2).

Table 6-2. Assembly YJ1433 Sample Percent Differences

Sample	D8-3D2B	D8-4G3	D9-1D2	D9 2D2	D9 4D4	D9-4G1E1	H5-3A1C	H5-3A1G
Node	15	23	6	11	18	22	15	16
Isotope	(Calculated Concentration – Measured Concentration) x 100/Measured Concentration							
^{234}U	-7.42	1.29	-2.46	-4.58	-9.08	-7.70	-4.15	-4.18
^{235}U	-38.29	-24.06	25.07	8.82	-37.71	-28.20	-14.78	-13.97
^{236}U	-2.49	-0.48	1.92	2.65	2.09	2.60	-0.94	-0.87
^{238}Pu	1.43	-26.51	6.86	4.77	-15.10	-14.99	-8.79	-7.94
^{239}Pu	-11.15	-24.83	9.69	3.68	-21.40	-21.08	-13.45	-12.61
^{240}Pu	-4.36	-9.15	6.73	5.41	-2.40	-0.61	-4.82	-4.45
^{241}Pu	-8.47	-24.75	6.69	1.08	-22.65	-22.43	-10.29	-9.08
^{242}Pu	26.02	0.81	4.32	5.53	8.91	3.71	14.98	16.01
^{143}Nd	1.81	-1.76	17.36	12.49	-5.83	-2.60	2.67	3.34
^{145}Nd	11.07	5.39	6.10	5.92	5.20	5.05	6.22	5.97
^{146}Nd	13.67	3.25	4.98	5.48	6.52	5.14	4.42	5.05
^{148}Nd	11.06	2.56	4.45	4.56	4.14	3.32	4.09	4.23
^{150}Nd	12.60	0.85	7.05	6.68	5.48	3.69	4.77	5.26
^{134}Cs	6.17	-12.86	7.08	0.38	-1.25	1.99	-6.14	-5.27
^{137}Cs	9.75	1.61	9.55	6.62	9.30	11.13	4.24	4.60
^{151}Eu	10.62	-8.73	40.03	41.64	10.99	4.64	13.44	14.05
^{153}Eu	22.21	1.03	20.23	20.06	19.85	9.35	17.11	16.76
^{155}Eu	-16.92	-32.15	-14.57	-16.91	-18.27	-24.57	-20.45	-20.34
^{147}Sm	-3.55	3.42	1.86	-1.82	-1.71	-4.11	-1.72	-2.58
^{149}Sm	-8.41	-24.92	33.99	11.94	-14.44	-15.57	-8.47	-6.67
^{150}Sm	9.32	1.64	9.52	7.22	5.12	2.19	3.68	4.34
^{151}Sm	16.04	-5.42	41.50	37.36	7.96	4.97	12.84	15.72
^{152}Sm	46.44	35.72	33.68	38.76	48.12	38.11	46.94	47.24
^{155}Gd	-52.11	-67.61	-24.62	-26.59	-33.28	-33.56	-35.12	-30.99
^{241}Am	-10.07	-23.16	9.22	11.64	-22.54	-21.54	-7.02	-7.23
^{241m}Am	6.60	-19.25	48.26	55.83	-13.22	-15.18	7.19	6.32
^{243}Am	40.41	-3.71	22.30	30.55	13.12	9.33	27.68	26.81
^{237}Np	-3.74	-15.62	0.35	-2.91	-11.25	-13.96	-5.47	-5.46
^{95}Mo	3.72	-3.51	-1.04	3.47	6.37	2.97	3.81	3.58
^{99}Tc	8.87	0.17	6.35	12.66	8.18	17.11	13.64	17.20
^{101}Ru	11.07	0.23	1.11	5.44	7.09	2.97	6.51	3.13
^{103}Rh	-3.23	-10.73	1.78	1.88	-9.12	-8.15	-3.34	-7.10
^{109}Ag	13.10	-7.30	28.02	31.71	24.95	32.60	28.78	14.01
^{242}Cm	-4.01	-24.12	23.20	35.45	-15.68	-22.24	0.34	14.86
^{243}Cm	-14.65	-41.90	4.53	-1.57	-31.90	-32.31	-20.11	-22.32
^{244}Cm	27.45	-30.14	8.31	19.07	0.45	-7.46	3.40	3.16
^{245}Cm	-35.88	-69.04	-29.19	-27.70	-53.86	-54.28	-50.70	-49.38

6.2 MCNP CALCULATION RESULTS

The results of MCNP runs using standard fuel rods with the fresh fuel compositions from Table 5-7 are presented in Table 6-3.

Table 6-3. MCNP Results for Fresh Nuclear Fuel

Pin Type Filling the Waste Package	^{235}U (Wt%)	k_{eff}	σ	AENCF
D8	3.60 (with 5.0 wt% Gd_2O_3)	0.17581	0.00014	0.827
D9	3.95	0.91651	0.00068	0.163

Table 6-4 presents the MCNP results for each of the spent nuclear fuel samples.

Table 6-4. MCNP Results for Spent Nuclear Fuel Samples

Sample #	Sample ID	RCA[a]			Operating History[b]			Delta (Operating History - RCA)[c]	
		k_{eff}	σ	AENCF	k_{eff}	σ	AENCF	Δk_{eff}	σ[d]
1	D8–3D2B	0.55913	0.00052	0.304	0.51709	0.00045	0.330	-0.04204	0.00069
2	D8–4G3	0.63515	0.00052	0.259	0.57645	0.00049	0.279	-0.05870	0.00071
3	D9–1D2	0.46612	0.00044	0.369	0.48665	0.00041	0.351	0.02053	0.00060
4	D9–2D2	0.50712	0.00047	0.339	0.51048	0.00043	0.335	0.00336	0.00064
5	D9–4D4	0.53262	0.00049	0.324	0.46549	0.00041	0.361	-0.06713	0.00064
6	D9–4G1E1	0.56781	0.00048	0.299	0.50364	0.00048	0.331	-0.06417	0.00068
7	H5–3A1C	0.58889	0.00047	0.290	0.5552	0.00042	0.305	-0.03369	0.00063
8	H5–3A1G	0.59134	0.00051	0.291	0.55936	0.00050	0.304	-0.03198	0.00071

NOTES: [a] Results based on measured compositions of spent nuclear fuel samples.
[b] Results based on SAS2H calculated compositions using reactor operating history information adjusted to yield the sample measured burnup.
[c] Values reported were calculated from MCNP reported values which lists results out to five significant digits, therefore computing delta values from table values will introduce some roundoff error.
[d] Delta σ value equals the square root of the sum of the squared σ values for RCAs and operating history.

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7.4 SOFTWARE CODES

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CRWMS M&O 2000. *Software Code: SCALE.* V4.4A. HP. 10129-4.4A-00.

8. ATTACHMENTS

Table 8-1 presents the attachment specifications for this calculation file. The contents of Attachment II are provided electronically on an attachment CD to this calculation file. A listing of the contents of the CD is provided in hard-copy form for Attachment II in the attachments to this calculation file.

Table 8.1. Attachment Listing

Attachment #	# of Pages	Description
I	23 HRR 08/25/03	44-BWR Waste Package Configurations for Site Recommendation Sketch
II	12 HRR 08/26/03	Excel spreadsheet, SAS2H input files, SAS2H outputs, MCNP inputs, and MCNP outputs
III	N/A	Compact Disc attachment containing information listed in Attachment II

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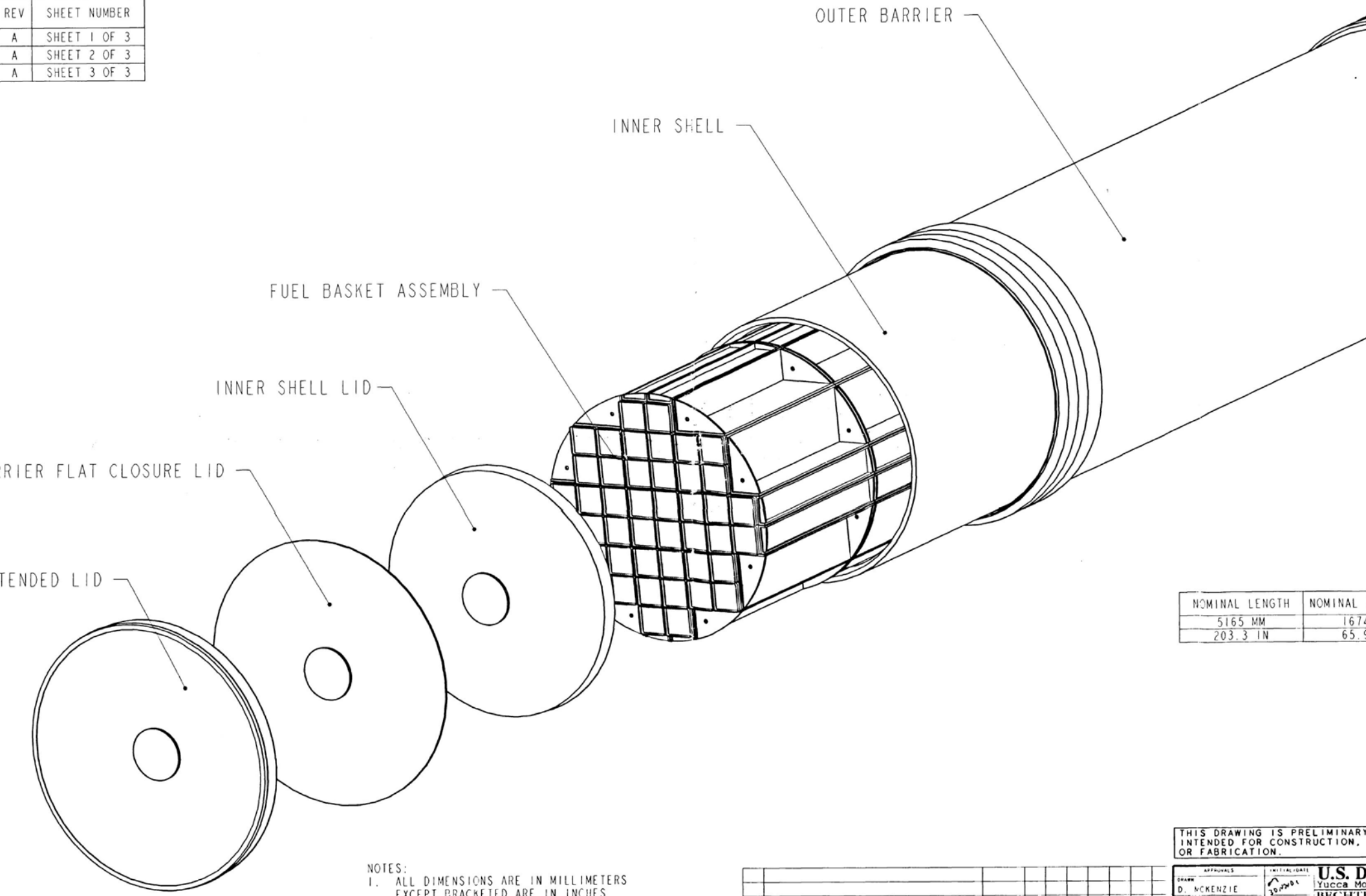
A	SHEET 1 OF 3
A	SHEET 2 OF 3
A	SHEET 3 OF 3



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203.3 IN	65.9

NOTES:
1. ALL DIMENSIONS ARE IN MILLIMETERS EXCEPT BRACKETED ARE IN INCHES
2. ALL MASSES ARE ROUNDED UP TO THE NEAREST THOUSAND
3. DO NOT SCALE FROM DRAWING
4. OUTER BARRIER AND INNER SHELL

THIS DRAWING IS PRELIMINARY INTENDED FOR CONSTRUCTION, OR FABRICATION.

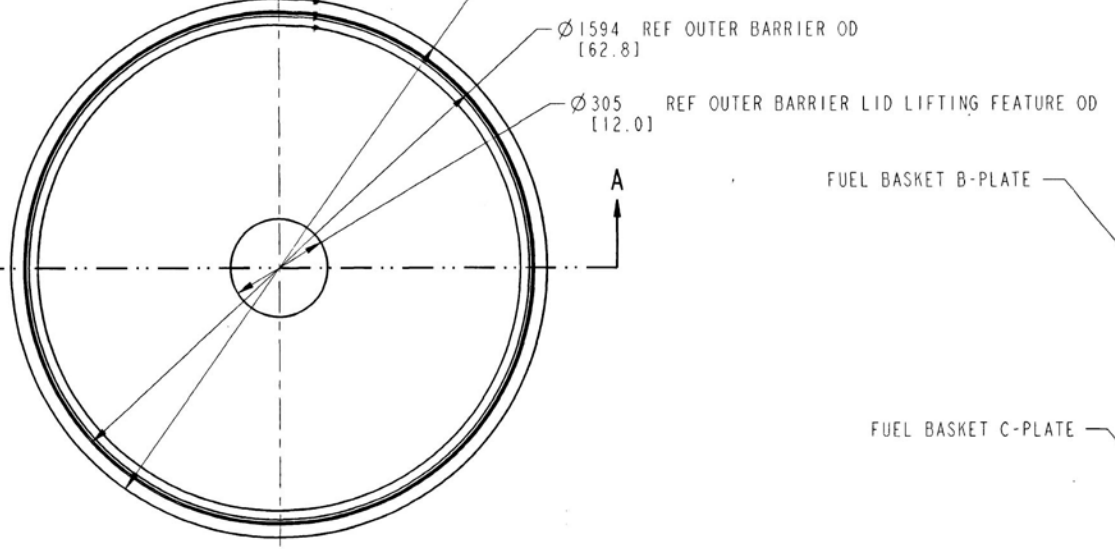
REV	DESCRIPTION									
A	ISSUED FOR SR BASELINE	11/30/01								

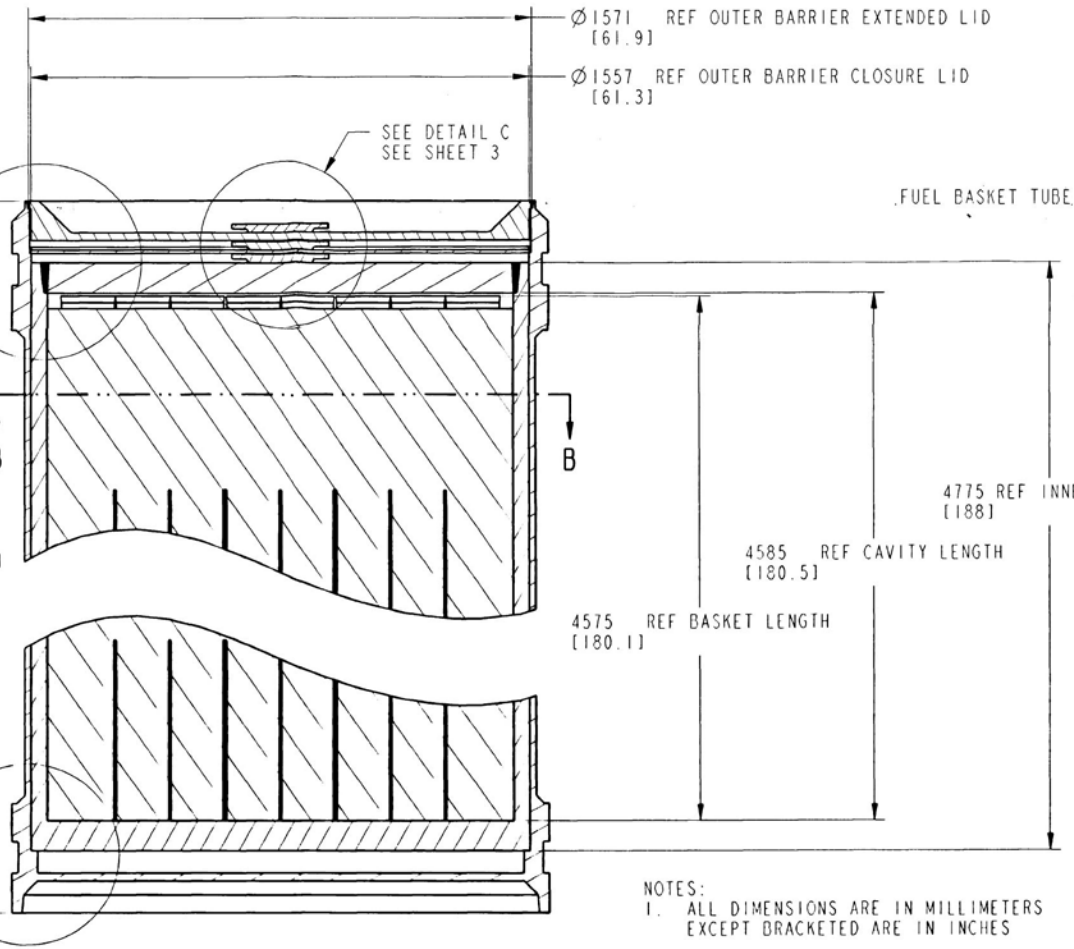
APPROVALS	INITIAL/DATE
DRAWN D. MCKENZIE	11/30/01
ORIGINATOR D. MCKENZIE	11/30/01
CHECKED T. SCHMITT	TS 11/30/01
VERIFICATION N/A	
DESIGN LEAD ENGINEER S. BENNETT	SMB 11/30/01
QUALITY ENGINEERING REP. D. TUNNEY	DT 11/30/01

U.S. D
Yucca Mo
BECHTT
SAIC

WA
44

SIZE D





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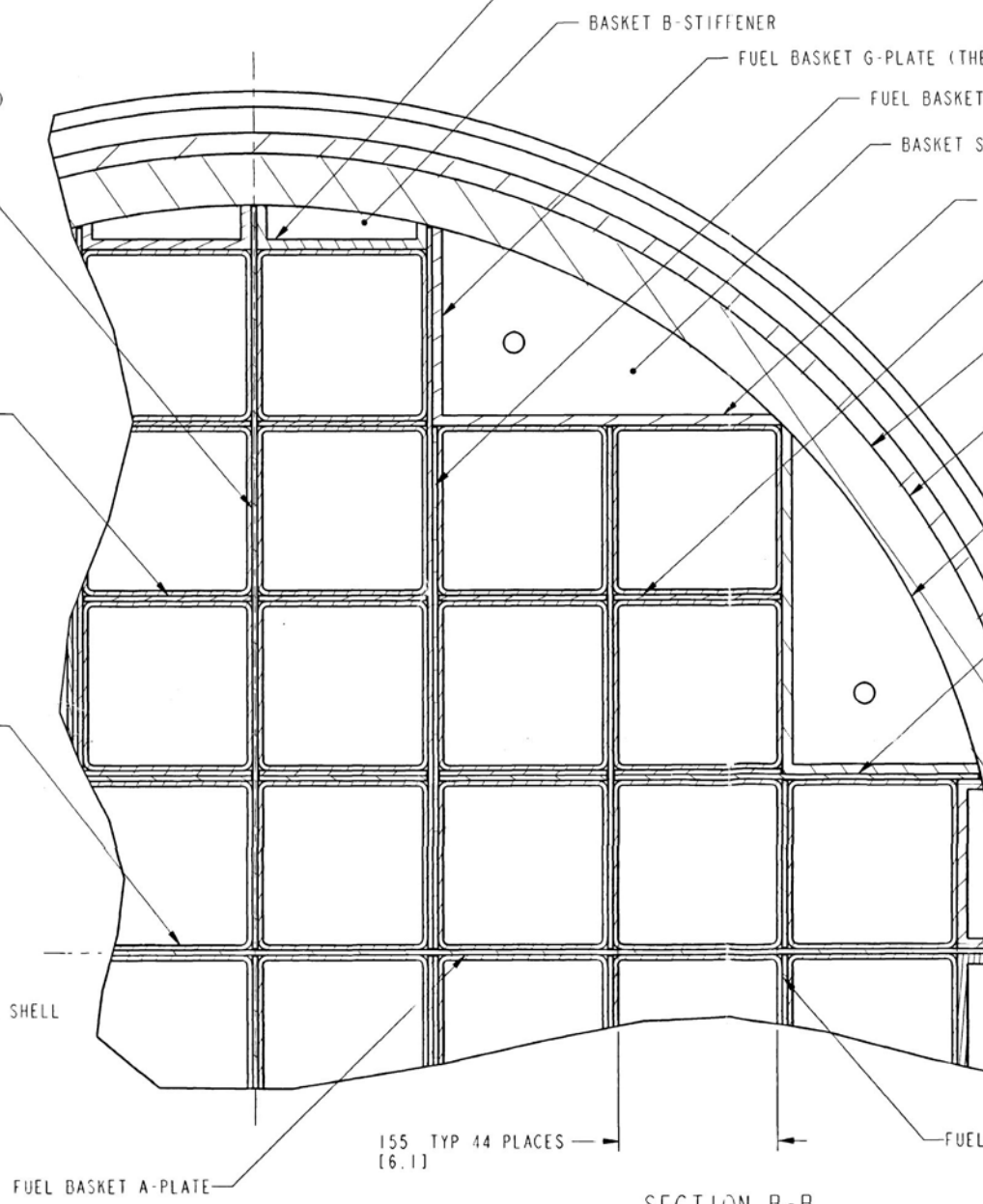

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SCALE 1:3

NOTES:
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2. ALL MASSES ARE ROUNDED UP TO THE NEAREST THOUSAND
3. DO NOT SCALE FROM DRAWING
4. OUTER BARRIER AND INNER SHELL

THIS DRAWING IS PRELIMINARY
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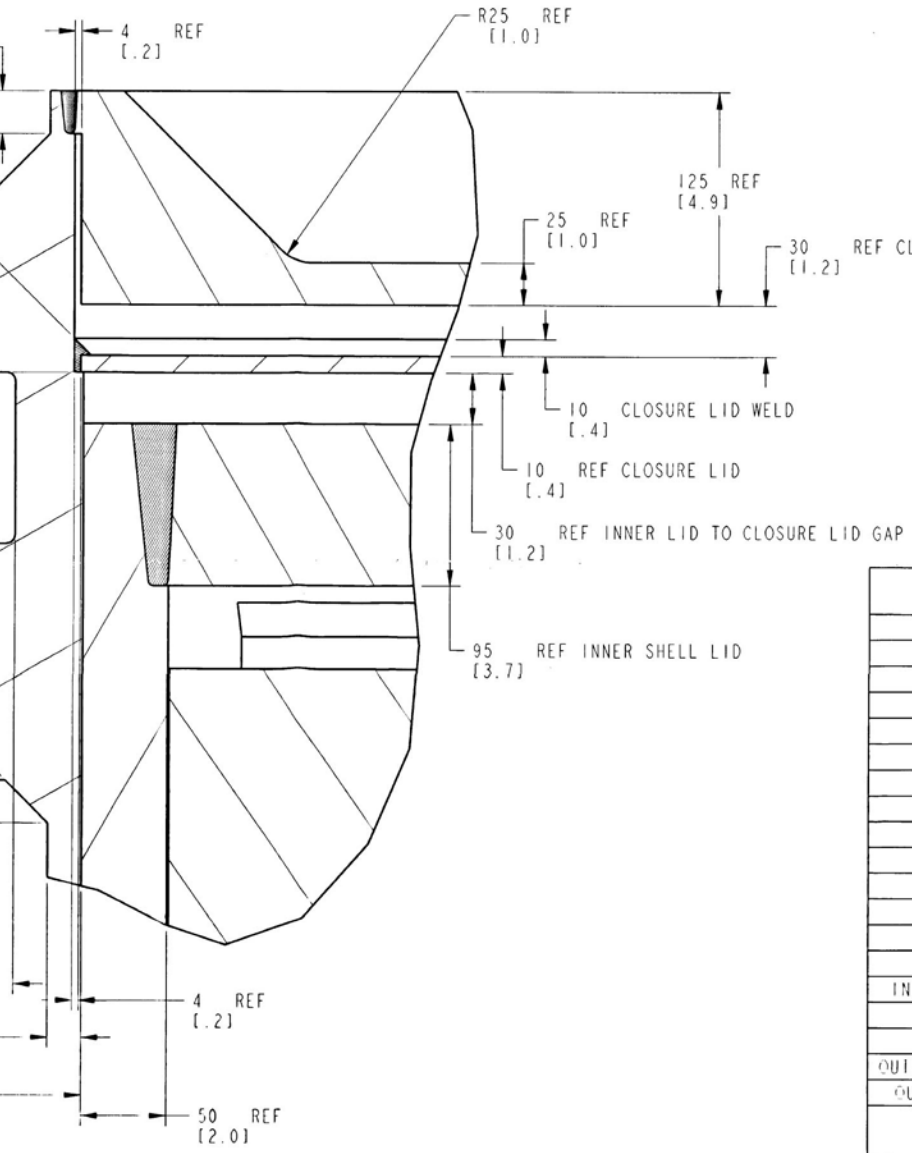
REV	DESCRIPTION								
A	ISSUED FOR SR BASELINE	11/30/01							

APPROVALS	INITIAL/DATE
DRAWN D. MCKENZIE	11/30/01
ORIGINATOR D. MCKENZIE	11/30/01
CHECKED T. SCHMITT	11/30/01
VERIF CATION N/A	
DESIGN LEAD ENGINEER S. BENNETT	11/30/01
QUALITY ENGINEERING REP. D. TUNNEY	11/30/01

U.S. D
Yucca Mou
BECHTE
SAIC COMPANY

WAS
44

SIZE D



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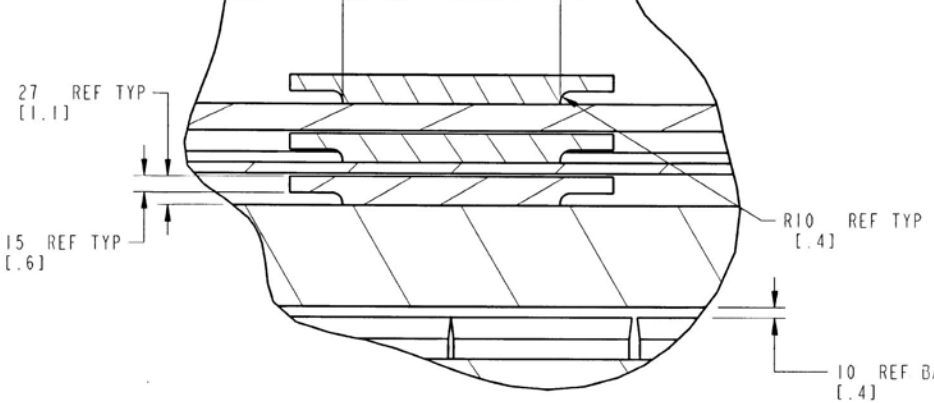
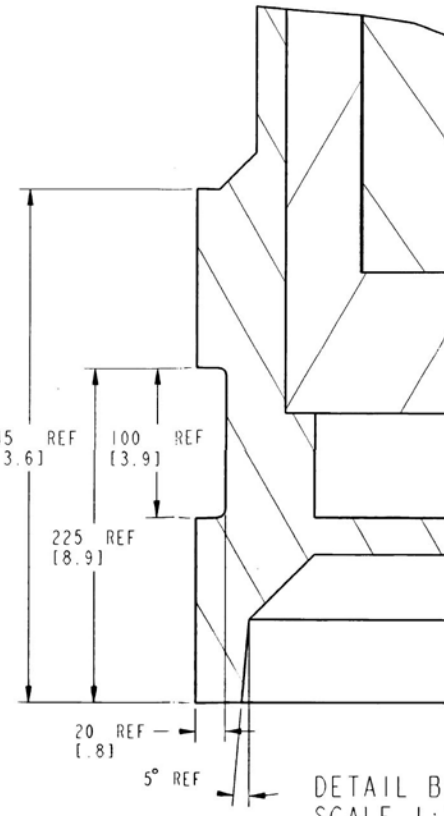


DETAIL C
SCALE 1:3



DETAIL B
SCALE 1:

COMPONENT	MATERIAL	MASS	QTY RQD
BASKET B-SIDEGUIDE	SA-516 K02700	-	32
BASKET B-STIFFENER	SA-516 K02700	-	64
BASKET CORNERGUIDE	SA-516 K02700	-	32
BASKET STIFFENER	SA-516 K02700	-	64
FUEL BASKET A-PLATE	NEUTRONIT A 978	-	4
FUEL BASKET B-PLATE	NEUTRONIT A 978	-	4
FUEL BASKET C-PLATE	NEUTRONIT A 978	-	16
FUEL BASKET D-PLATE	NEUTRONIT A 978	-	16
FUEL BASKET E-PLATE	NEUTRONIT A 978	-	16
FUEL BASKET F-PLATE	SB-209 A96061 T4	-	8
FUEL BASKET G-PLATE	SB-209 A96061 T4	-	8
FUEL BASKET TUBE	SA-516 K02700		44
INNER SHELL	SA-240 S31600	-	1
INNER SHELL LID	SA-240 S31600	-	1
INNER SHELL LID LIFTING FEATURE	SA-240 S31600	-	1
OUTER BARRIER	SA-575 N06022	-	1
OUTER BARRIER EXTENDED LID	SA-575 N06022	-	1
OUTER BARRIER LID LIFTING FEATURE	SA-575 N06022	-	2
OUTER BARRIER FLAT CLOSURE LID	SA-575 N06022	-	1
WASTE PACKAGE ASSEMBLY	-	27000 KG	1
	-	60000 LB	1
WP ASSEMBLY WITH SNF	-	43000 KG	1
	-	95000 LB	1

NOTES:
1. ALL DIMENSIONS ARE IN MILLIMETERS EXCEPT BRACKETED ARE IN INCHES
2. ALL MASSES ARE ROUNDED UP TO THE NEAREST THOUSAND
3. DO NOT SCALE FROM DRAWING
4. OUTER BARRIER AND INNER SHELL HAVE RADIAL GAP OF 0 TO 4 MM REF

THIS DRAWING IS PRELIMINARY INTENDED FOR CONSTRUCTION, P OR FABRICATION.

REV	DESCRIPTION	DATE
A	ISSUED FOR SR BASELINE	11/30/01

APPROVALS	INITIAL/DATE
DRAWN: D. MCKENZIE	11/30/01
ORIGINATOR: D. MCKENZIE	11/30/01
CHECKED: T. SCHMITT	11/30/01
VERIFICATION: N/A	
DESIGN LEAD ENGINEER: S. BENNETT	11/30/01
QUALITY ENGINEERING REP: D. TUNNEY	11/30/01
PROJECT MANAGER	

U.S. DE
Yucca Mou
BECHTEL
SAIC

WAS
44-

SIZE D

ATTACHMENT II

This attachment contains a listing and description of the zip file contained on Attachment III, the CD of this calculation. The CD was written using the Hewlett Packard (HP) CD-Writer Plus model 7200e external CD-rewritable drive for personal computers, and the zip archive was created using WINZIP 8.1. The zip file attributes on the CD are as follows:

Archive Filename	File Size (bytes)	File Date	File Time
att.zip	5,056,040	07-28-2003	4:17p

There are 78 total files contained in the root directory. Upon file extraction, the file naming system corresponds as follows for the SAS2H cases, and as listed in Table II-1 for the MCNP cases.

- *N*.inp* files are the SAS2H input files.
- *N*.msgs* files contain the standard run-time messages associated with the SAS2H calculations (these are generated by SAS2H).
- *ft72f001.N** files are temporary ASCII files generated by SAS2H, which must be retained, that contain the isotopic concentrations as a function of time (the actual SAS2H output file contains a large amount of information that is not needed for this calculation, therefore it is discarded, but the temporary files SAS2H creates are retained).
- *act_N*.mass* files contain the extracted actinide isotopes from the *ft72f001.N** files and provides them in units of grams.
- *fp_N*.mass files* contain the extracted fission product isotopes from the *ft72f001.N** files and provides them in units of grams.

Table II-1. Sample and MCNP Filename Identification

File Name[a]	Sample ID	Comments
1m	D8–3D2B	Cases for samples from assembly YJ1433 radiochemical assay measured isotopic concentrations.
2m	D8–4G3	
3m	D9–1D2	
4m	D9–2D2	
5m	D9–4D4	
6m	D9–4G1E1	
7m	H5–3A1C	
8m	H5–3A1G	
1c	D8–3D2B	Cases for samples from assembly YJ1433 using operating history information adjusted to sample measured burnup in SAS2H to generate isotopic concentrations.
2c	D8–4G3	
3c	D9–1D2	
4c	D9–2D2	
5c	D9–4D4	
6c	D9–4G1E1	
7c	H5–3A1C	
8c	H5–3A1G	
1f	Representative for pin D8	Cases with fresh fuel in the same geometric configuration as the rest of the cases.
2f	Representative for pins D9 and H5	

NOTE: [a] Input files have an "i" at the end of the file name, and output files have an "io" at the end of the file name.

LGS1RCA.xls is an Excel spreadsheet that contains design parameters and operation information (limited to cycles 5, 6, and 7) for Limerick Unit 1 BWR core and YJ1433 fuel assembly.