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#### 1. PURPOSE

The purpose of this activity is to develop a representative "limiting" axial burnup profile for pressurized water reactors (PWRs), which would encompass the isotopic axial variations caused by different assembly irradiation histories, and produce conservative isotopics with respect to criticality. The effect that the low burnup regions near the ends of spent fuel have on system reactivity is termed the "end-effect". This calculation will quantify the end-effects associated with Pressurized Water Reactor (PWR) fuel assemblies emplaced in a hypothetical 21 PWR waste package. The scope of this calculation covers an initial enrichment range of 3.0 through 5.0 wt% U-235 and a burnup range of 10 through 50 GWd/MTU.

This activity supports the validation of the process for ensuring conservative generation of spent fuel isotopics with respect to criticality safety applications, and the use of burnup credit for commercial spent nuclear fuel. The intended use of these results will be in the development of PWR waste package loading curves, and applications involving burnup credit.

Limitations of this evaluation are that the limiting profiles are only confirmed for use with the B&W 15x15 fuel assembly design. However, this assembly design is considered bounding of all other typical commercial PWR fuel assembly designs.

This calculation is subject to the Quality Assurance Requirements and Description (QARD) because this activity supports investigations of items or barriers on the Q-list (YMP 2001).

#### 2. METHOD

A bounding burnup profile is defined as one that would maximize fuel assembly reactivity. Thus, a truly bounding profile for typical light water reactors would be where the fuel has not been irradiated, which is referred to as the "fresh fuel" assumption. This "fresh fuel" assumption is very conservative in calculations of criticality potential. As fuel is burned in a reactor, the burnup of the fuel becomes distributed axially and the reactivity of the fuel decreases. The profile of this axial distribution attains a flattened cosine shape with time, although the exact profile will vary with operating history and other effects unique to the individual reactor and fuel assembly. The cosine shape is representative of typical burnup profiles, which shows that the ends of the fuel are less burned than the central region. An axial profile database (Cacciapouti and Van Volkinburg 1997) composed of various PWR fuel assembly designs, which include variations in enrichment, burnup, and burnable absorbers, will be used to determine the limiting axial profile(s).

The process for testing if a selected profile is conservative will be made by comparing  $k_{eff}$  results using the limiting profile(s) against the mean assembly profile(s). Prior studies in this area (DeHart 1996, p. 88) have indicated that a single-zone profile is conservative when using fission product isotopes until a certain burnup point where the axially varying profile becomes more conservative. This analysis will also determine where the cross-over point is.

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## 3. ASSUMPTIONS

- 3.1 It was assumed that the use of the Babcock & Wilcox 15x15 MK-B2 fuel assembly design for burnup profile comparisons is indicative of all assemblies. The rationale for this assumption is that for the purpose of  $\Delta k_{eff}$  evaluations, different assembly designs will have slightly different nominal depletion parameters which have an effect on spectrum, but the relative effect on the  $\Delta k_{eff}$  values using those different parameters is negligible. This is because the difference in the keff values are based on the difference in the axial burnup profile. This assumption is used in Section 5.
- 3.2 It was assumed that the B&W 15x15 Mk-B2 assembly design is the most limiting PWR fuel assembly design. The basis for this assumption is that a previous analysis for the BR-100 transportation cask established the B&W 15x15 fuel assembly as one of the most reactive fuel assembly designs (p. II 6-6, B&W Fuel Company 1991). The B&W 15x15 design contains larger radius fuel pellets than the Westinghouse 17x17 OFA assembly design which makes the fuel irradiation of the B&W assembly design less efficient in utilizing all the fuel over time. This effect should leave higher fissile material content at discharge than the Westinghouse assembly design. This assumption was used in Section 5.
- 3.3 Since the zinc cross section libraries are unavailable, it was assumed that representing the zinc material composition in aluminum 6061 as aluminum would maintain the same neutronic characteristics. The rationale for this assumption is that the nuclear cross-sections for these two elements are similar. This assumption was used in Section 5.3.1.

# 4. USE OF COMPUTER SOFTWARE AND MODELS

## 4.1 MCNP

The baselined MCNP code (CRWMS M&O 1998a) was used to calculate the neutron multiplication factor for the various spent fuel compositions. The software specifications are as follows:

- Software Title: MCNP
- Version/Revision Number: Version 4B2LV
- Status/Operating System: Qualified/HP-UX B.10.20
- Software Tracking Number: 30033 V4B2LV (Computer Software Configuration Item Number)
- Computer Type: Hewlett Packard 9000 Series Workstations
- Computer Processing Unit number: 700887

The input and output files for the MCNP calculations are contained on a compact disc attachment to this calculation report (Attachment III) as described in Sections 5 and 8, such that an independent repetition of the software use may be performed.

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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 references Briesmeister (1997) and CRWMS M&O (1998b), and (3) obtained from Software Configuration Management in accordance with appropriate procedures.

# 4.2 SCALE

The SAS2H control module of the baselined modular code system SCALE Version 4.4a (CRWMS M&O 2000a) 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 9000 Series Workstations
- Computer Processing Unit number: 700887.

The input and output files for the various SAS2H calculations are contained on a compact disc attachment to this calculation report (Attachment III) as described in Sections 5 and 8, such that an independent repetition of the software use may be performed. The SAS2H code sequence of SCALE that was used is (1) appropriate for the application of commercial fuel assembly depletion, (2) used only within the range of validation as documented in *Users Manual for SCALE-4.4A* (CRWMS M&O 2000b) and *Validation Test Report (VTR) for SCALE-4.4A* (CRWMS M&O 2000c), and (3) obtained from Software Configuration Management in accordance with appropriate procedures.

# 4.3 FT71V01

The baselined FT71V01 code (BSC 2001a) was used for post-processing the binary files generated from SCALE (CRWMS M&O 2000a) into ASCII format. The software specifications are as follows:

- Program Name: FT71V01
- Version/Revision Number: Version 01
- Status/Operating System: Qualified/HP-UX B.10.20
- Software Tracking Number: 10493-01-00
- Computer Type: HP 9000 Series Workstations
- CPU number: 700887

This software application reads the binary files written to the ft71f001 file by ORIGEN-S and processes them into an ASCII format. The binary files that are read and the ASCII text files that it generates are provided on a compact disc attachment to this calculation report (Attachment III) as described in Sections 5 and 8, such that an independent repetition of the software use may be

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performed. The FT71V01 software used was: (1) appropriate for the conversion of binary to ASCII format, (2) used only within the range of validation as documented throughout BSC (2001a), and (3) obtained from Software Configuration Management in accordance with appropriate procedures.

#### 5. CALCULATION

The method of calculation is based upon the calculation of isotopic constituents of irradiated fuel using the SAS2H sequence of the SCALE computer code system, which are then used as irradiated fuel assembly input to MCNP for  $k_{eff}$  evaluations of different fuel assembly axial burnup profiles. The initial enrichments evaluated in this report cover a range of 3.0 through 5.0 wt% U-235, with burnups ranging from 10 GWd/MTU through 50 GWd/MTU. Decay time information is available on the Attachment CD for times up to 100,000 years to facilitate future analyses. Each of the MCNP evaluations was performed in a representative waste package environment with isotopic compositions corresponding to a 5-year decay time. The 5-year decay time is based on the minimum cooling time required for the fuel assemblies to be classified as standard fuel (10 CFR 961.11).

The base assembly design for the burnup profile evaluations is the B&W 15x15 fuel assembly design. Fuel assembly dimensions correspond to the MK-B2 design that are presented in Table 1.

Description	Value
Number of unit cells in assembly	225
Number of fuel rods in assembly	208
Number of guide tubes in assembly	16
Rod pitch in assembly (cm)	1.44272
Fuel pellet diameter (cm)	0.93980
Fuel rod cladding outer diameter (cm)	1.09220
Fuel rod cladding inner diameter (cm)	0.95758
Guide tube outer diameter (cm)	1.34620
Guide tube inner diameter (cm)	1.26492
Instrument tube outer diameter (cm)	1.38193
Instrument tube inner diameter (cm)	1.12014
Assembly pitch (cm)	21.81098

Table 1. B&W 15x15 MK-B2 Assembly Design Parameters

Source: Punatar 2001, pp. 2-5 and 3-1

# 5.1 SAS2H

# 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 2000b.

- BONAMI applies the Bondarenko method of resonance self-shielding to nuclides for which Bondarenko data is 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, it 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 pellet, gap, and clad 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 (BPRs), 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 CRWMS M&O (2000b, Section S2.2.3.1, Volume 1).

Calculation

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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 time-dependent cross sections by SAS2H is documented in CRWMS M&O (2000b, Section S2.2.4, Volume 1).

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 (CRWMS M&O 2000b, p. S2.2.5).

A B&W 15x15 assembly design was used as the base assembly for the calculations in this report. The fuel assembly Path B model dimensions are presented in Table 2.

Equations 1 through 10 were utilized in the Path B model development calculations presented in Table 2. The number of significant figures reported from Equations 1 through 10 are a product of the calculation and should not be interpreted as reflecting an excessively high level of accuracy.

Description	Value	Equation Utilized	
Fuel-to-moderator volume ratio	0.53386	7	
Moderator unit volume in central unit cell of Path B model (cm <sup>2</sup> )	1.91476	8	
Fuel unit volume in fuel rod unit cell (cm <sup>2</sup> )	0.69368	9	
Moderator unit volume in fuel rod unit cell (cm <sup>2</sup> )	1.14454	10	
Number of fuel rod unit cells that must be represented	10 26740	6	
in the homogenized zone of the Path B model	12.30/42	0	
Path B Unit Cell Zone Radii			
Water filled guide tube (R1)	0.63246	1	
Guide tube (R2)	0.67310	2	
Guide tube unit cell moderator (R3)	0.81397	3	
Homogenized region (R4)	2.97599	4	
Moderator in the assembly-to-assembly gap (R5)	2.99939	5	

# Table 2. SAS2H Path B Unit Cell Model Dimension Calculations for<br/>B&W 15x15 Mk-B2 Assembly Type

Equations 1 through 5 were derived based on conservation of area. All distance dimensions are in centimeters. All area dimensions are in square centimeters. All other parameters are

dimensionless. For Equations 7 through 10 the following is a description of the symbol meanings:

*F/M Ratio* = fuel-to-moderator ratio; # = number; *FR* = fuel rods; *FP* = fuel pellet; *P* = rod pitch; *OD* = outer diameter; *GT* = guide tube; *IT* = instrument tube; *ID* = inner diameter; *CRMA* = central region moderator area; *FA* = fuel area; *MA* = moderator area; *x* refers to the number of assembly fuel pin lattice cells that must be represented in the Path B model homogenized region to preserve the fuel-to-moderator unit volume ratio

$$R1 = \frac{GT ID}{2}$$
(Eq. 1)

$$R2 = \frac{GTOD}{2}$$
(Eq. 2)

$$R3 = \frac{P}{\sqrt{\pi}}$$
(Eq. 3)

$$R4 = \sqrt{\frac{x(P)^2}{\pi} + (R3)^2}$$
 (Eq. 4)

where

x is calculated using Equation 6

$$R5 = \begin{cases} \left(\frac{(x+1)}{\# Assembly \ Lattice \ Unit \ Cells}\right)^{*} \\ \left[ (Assembly \ Pitch)^{2} - (P)^{2} * \\ (\# \ Assembly \ Lattice \ Unit \ Cells) \end{bmatrix}^{*} \left(\frac{1}{\pi}\right) + (R4)^{2} \end{cases}$$
(Eq. 5)

$$x = \frac{\left(\frac{F}{M}Ratio\right)(CRMA)}{FA - \left(\frac{F}{M}Ratio\right)(MA)}$$
(Eq. 6)

where

the variables are calculated using Equations 7 through 10

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$$\frac{F}{M} Ratio = \frac{(\# FR)\left(\frac{\pi}{4}\right)(FP \ Diameter)^2}{\left(\# FR\right)\left[P^2 - (FR \ Clad \ OD)^2\left(\frac{\pi}{4}\right)\right] + \left(\# \ GTs\right)\left[P^2 - (GT \ OD)^2\left(\frac{\pi}{4}\right) + (GT \ ID)^2\left(\frac{\pi}{4}\right)\right] + \left[P^2 - (IT \ OD)^2\left(\frac{\pi}{4}\right) + (IT \ ID)^2\left(\frac{\pi}{4}\right)\right] + \left[P^2 - (IT \ OD)^2\left(\frac{\pi}{4}\right) + (IT \ ID)^2\left(\frac{\pi}{4}\right)\right]$$
(Eq. 7)

Equation 7 is based on the GTs and IT being filled with water with no instrument nor burnable poison rods inserted in the respective tubes.

$$CRMA = P^{2} - \left(\frac{\pi}{4}\right) \left[ (GT \ OD)^{2} - (GT \ ID)^{2} + (Inserted \ Rod \ Clad \ OD)^{2} \right]$$
(Eq. 8)

$$FA = \left(Fuel \ Pellet \ OD\right)^2 \left(\frac{\pi}{4}\right)$$
(Eq. 9)

$$MA = P^{2} - \left(FR \ Clad \ OD\right)^{2} \left(\frac{\pi}{4}\right)$$
 (Eq. 10)

#### 5.1.2 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 U-234, U-235, U-236, and U-238. For fresh fuel SAS2H cases, a number of additional isotopes are specified in trace amounts in the fuel composition to assure that their buildup and decay is tracked during the depletion calculation. Table 1 contains a listing of the trace isotopes, which are specified as each having a concentration of 1E-21 atoms/b-cm in the fresh fuel composition.

Table 3. Trace Isotopes Specified in Fresh Fuel Compositions

Kr-83	Kr-85	Sr-90	Y-89	Mo-95	Zr-93	Zr-94
Zr-95	Nb-94	Tc-99	Rh-103	Rh-105	Ru-101	Ru-106
Pd-105	Pd-108	Ag-109	Sb-124	Xe-131	Xe-132	Xe-135
Xe-136	Cs-134	Cs-135	Cs-137	Ba-136	La-139	Ce-144
Nd-143	Nd-145	Pm-147	Pm-148	Nd-147	Sm-147	Sm-149
Sm-150	Sm-151	Sm-152	Gd-155	Eu-153	Eu-154	Eu-155

The fresh fuel compositions for each uranium-235 enrichment used in this evaluation are specified in Table 4, and were calculated using Equation 11 (Bowman et al. 1995, p. 20) for each isotope based on the U-235 wt%.

Enrichment (wt% U-235)	Wt% U-234	Wt% U-235	Wt% U-236	Wt% U-238		
3.0	0.0254	3.0000	0.0138	96.9608		
4.0	0.0347	4.0000	0.0184	95.9469		
5.0	0.0442	5.0000	0.0230	94.9328		
Density <sup>a</sup> = 10.230 g/cm <sup>3</sup>						

Table 4	SAS2H F	Fresh F	Fuel	Comr	ositions
	0/ 102111	100111	uoi	COULT	000100110

NOTE: <sup>a</sup> Calculated by dividing fuel mass by fuel volume where a uranium mass of 468.62 kg was used with a fuel height of 360.162 cm, and a pellet radius of 0.9398 cm (Punatar 2001, pp. 2-5 and 3-1).

 $U^{234} wt\% = (0.007731) * (U^{235} wt\%)^{1.0837}$ 

$$U^{236} wt\% = (0.0046) * (U^{235} wt\%)$$
 (Eq. 11)

$$U^{238}$$
 wt% = 100 -  $U^{234}$  wt% -  $U^{235}$  wt% -  $U^{236}$  wt%

The fuel rod cladding for the representative assembly design was made up of Zircaloy-4 and the spacer grids of Inconel 718. The fuel rod cladding material composition was given a base temperature of 640 K. The spacer grids were homogenized over the active fuel length with a volume fraction of 0.00576 (Punatar 2001, Table 2-3 and Figure 2-3) and given a base temperature corresponding to the nominal moderator temperature. The Zircaloy-4 cladding specifications used in the SAS2H input are presented in Table 5, and the material specification for Inconel 718 is specified in Table 6.

Table 5.	SAS2H	Zircaloy-4	Composition
----------	-------	------------	-------------

Element	Composition ID <sup>a</sup>	Wt%
Cr	24000	0.10
Fe	26000	0.21
0	8016	0.125
Sn	50000	1.45
Zr	40000	98.115
	Density <sup>b</sup> = $6.56 \text{ g/cm}^3$	

Source: ASTM B 811-90 1991, p. 2, Table 2

NOTES: <sup>a</sup> ID = identifier

<sup>b</sup> From ASM International 1990, p. 666, Table 6.

Element Composition ID<sup>a</sup> Wt% Element **Composition ID** Wt% С 6012 0.040 28000 52.5 Ni Si 14000 0.180 Ti 22000 0.90 S 16000 0.008 AI 13027 0.50 Cr 24000 19.0 Nb 41093 5.13 42000 Mn 25055 0.18 Мо 3.05 Fe 26000 18.5  $Density^{b} = 8.19 \text{ g/cm}^{3}$ 

Table 6. SAS2H Inconel 718 Material Composition

Source: Lynch 1989, p. 496

NOTES: <sup>a</sup> ID = identifier

<sup>b</sup> Converted from a reference value of 0.296 lb/cm<sup>3</sup>.

#### 5.2 **BURNUP PROFILES**

As fuel is burned in a reactor, the burnup of the fuel becomes distributed axially and the reactivity of the fuel decreases. The profile of this axial distribution attains a flattened cosine shape with time, although the exact profile will vary significantly with operating history and other effects unique to the individual reactor and fuel assembly. The cosine shape is representative of typical burnup profiles, which shows that the ends of the fuel are less burned than the central region. The ends of the fuel can create positive reactivity relative to the central region, hence the term "end-effects". To develop a representative burnup profile, which would encompass the isotopic axial variations caused by different assembly irradiation histories, requires the development of a "limiting" axial profile that takes credit for fuel burnup.

Several variations in profiles are evaluated in this document. Each of the multi-zone profiles are developed from an axial profile database composed for various PWR fuel assembly designs, which included variations in enrichment, burnup, and burnable absorbers (Cacciapouti and Von Volkinburg 1997). Due to the various assembly designs contained in the database, four profile sets were evaluated. The profile sets are as follows, and are described in more detail in Attachment I:

- (A) Profile Set One based on using all fuel assemblies from the database with the exception of the assemblies that did not contain information for all 18 axial nodes
- (B) Profile Set Two based on using all fuel assemblies from the database with the exception of the assemblies that contained nonuniform axial loadings (i.e., axial blanket fuel) or other characteristics (i.e., partially loaded shield assemblies, missing information), that would make their use in a limiting profile analysis inappropriate
- (C) Profile Set Three based on using only the B&W 15x15 fuel assemblies from the database

The profile sets contain the following assembly burnup profiles:

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- (A) Single zone profile representing the assembly average burnup with nominal depletion history parameters
- (B) An 18 zone profile representing the assembly average burnup with nominal depletion history parameters
- (C) A seven zone profile representing the assembly average burnup with nominal depletion history parameters

Each of the multi-zone profiles is based on dividing the assemblies into burnup groups based on average burnup, for all fuel types and essentially all assemblies from the database. Burnup groups were used because the "end-effects" become more pronounced as burnup increases. Some assemblies from the database were excluded because certain types of fuel assemblies contain nonuniform axial loadings or other characteristics (e.g., axial blanket fuel, missing information) that would make their use in a limiting profile analysis inappropriate. The development of the set of profiles is discussed in Attachment I. The burnup groups used are as follows:

**Burnup Range** 

Group	(GWd/MTU)
1	10 ≤ x < 15
2	15 ≤ x < 20
3	20 ≤ x < 25
4	$25 \le x \le 30$
5	$30 \le x < 35$
6	$35 \le x \le 40$
7	40 ≤ x < 45
8	$45 \le x$

## 5.2.1 Operating History Specifications

The following parameters are nominal for PWR fuel assemblies. They provide the nominal parameter set to be used as the baseline for comparison for the determination of the conservatism of the limiting axial profile. These representative parameters are taken from Summary Report of Commercial Reactor Criticality Data for Crystal River Unit 3 (Punatar 2001) for Crystal River Unit 3:

- Fuel temperature = 861.3 K (Punatar 2001, Table 4-9, node 9, statepoint 7)
- Moderator temperature = 579.8 K (calculated based on a specific power of 0.0225 ft<sup>3</sup>/lbm for assembly A8, node 9 statepoint 7, at an operating pressure of 2200 psia (Punatar 2001, Table 2-2), and CRWMS M&O (2000b, Table S2.5.2)
- Average specific power = 31.249 MW/MTU (Punatar 2001, Table 4-9, node 9, statepoint 7)

Moderator boron concentration values as a function of effective full power days are tabulated in Table 7 and illustrated in Figure 1. Boron concentration information from cycles 7, 9, and 10 for Crystal River Unit 3 were used. These cycles were selected because they cover the number of

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days required to reach a burnup of 50 GWd/MTU at the nominal specific power over 3 cycles of irradiation. This boron letdown information corresponds to the actual depletion history of fuel assembly G27a from Crystal River Unit 3 (Punatar 2001, Table 4-114). The SAS2H time step and boron letdown input parameter information is provided in Table 8 and were interpolated from the nominal values specified in Table 7.

Cycle 7		Сус	Cycle 9		le 10
EFPD	ppmB	EFPD	ppmB	EFPD	ppmB
10	1500	10	1690	25	1726
25	1445	25	1610	50	1653
50	1410	50	1550	75	1579
75	1360	75	1500	100	1505
100	1305	100	1445	125	1431
125	1245	125	1380	150	1358
150	1175	150	1310	175	1284
175	1100	175	1225	200	1210
200	1025	200	1160	225	1136
225	950	225	1090	250	1063
250	880	250	1015	275	989
275	790	275	930	300	915
300	725	300	870	325	841
325	660	325	780	350	768
350	575	350	700	375	694
375	500	375	625	400	620
400	435	400	550	425	546
425	375	425	475	450	473
450	290	450	395	475	399
475	215	475	310	500	325
497.9	150	500	250	525	251
		525	185	550	178
		550	130	575	104
		557.2	120	592.8	30

	<b>_</b>		<u> </u>		
Table 7.	Boron Letdown	Information for	<sup>.</sup> Crvstal River	· Unit 3 Cvcle	es 7, 9, and 10
				•••••••	

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Figure 1	Nominal	Boron	Letdown	Curve
Figure I.	nominai	DUIUII	Leiuowii	Curve

	10 GWd/MTU		20 GWd/MTU			30 GWd/MTU		
Step Length (EFPD) <sup>ª</sup>	Conc. (ppmB) <sup>b</sup>	BFRAC <sup>℃</sup>	Step Length (EFPD)	Conc. (ppmB)	BFRAC	Step Length (EFPD)	Conc. (ppmB)	BFRAC
64.0020	1435.2	1.0000	71.1290	1430.2	1.0000	71.1290	1430.2	1.0000
64.0020	1313.8	0.9154	71.1290	1288.9	0.9012	71.1290	1288.9	0.9012
64.0020	1145.0	0.7978	71.1290	1091.5	0.7632	71.1290	1091.5	0.7632
64.0020	953.0	0.6640	71.1290	882.9	0.6173	71.1290	882.9	0.6173
64.0020	756.2	0.5269	71.1290	672.8	0.4704	71.1290	672.8	0.4704
			71.1290	457.9	0.3201	71.1290	457.9	0.3201
			71.1290	253.0	0.1769	71.1290	253.0	0.1769
			71.0600	1584.7	1.1080	77.0218	1577.6	1.1030
			71.0600	1197.9	0.8375	77.0218	1404.6	0.9821
						77.0218	1179.4	0.8246
						77.0218	948.4	0.6631
						77.0218	710.9	0.4971
						77.0218	479.1	0.3350
4	40 GWd/MTU			50 GWd/MTU				
Step			Step					
Length	Conc.		Length	Conc.				
(EFPD)	(ppmB)	BFRAC	(EFPD)	(ppmB)	BFRAC			
71.1290	1430.2	1.0000	71.1290	1430.2	1.0000			
71.1290	1288.9	0.9012	71.1290	1288.9	0.9012			
71.1290	1091.5	0.7632	71.1290	1091.5	0.7632			

0					
Step Length (EFPD)	Conc. (ppmB)	BFRAC	Step Length (EFPD)	Conc. (ppmB)	BFRAC
71.1290	882.9	0.6173	71.1290	882.9	0.6173
71.1290	672.8	0.4704	71.1290	672.8	0.4704
71.1290	457.9	0.3201	71.1290	457.9	0.3201
71.1290	253.0	0.1769	71.1290	253.0	0.1769
79.6000	1574.5	1.1009	79.6000	1574.5	1.1009
79.6000	1394.6	0.9751	79.6000	1394.6	0.9751
79.6000	1162.6	0.8129	79.6000	1162.6	0.8129
79.6000	921.4	0.6442	79.6000	921.4	0.6442
79.6000	675.4	0.4722	79.6000	675.4	0.4722
79.6000	434.0	0.3035	79.6000	434.0	0.3035
79.6000	204.8	0.1432	79.6000	204.8	0.1432
74.9800	1689.5	1.1813	77.8500	1685.3	1.1784
74.9800	1468.1	1.0265	77.8500	1455.3	1.0176
74.9800	1247.1	0.8720	77.8500	1225.9	0.8572
			77.8500	996.5	0.6967
			77.8500	767.1	0.5363
			77.8500	536.6	0.3752
			77.8500	307.2	0.2148

Table 8. Time Step and Boron Letdown Information

NOTES: <sup>a</sup> effective full-power days (based on mass loading of 0.468620 MTU and average specific power) <sup>b</sup> parts per million boron by mass

<sup>°</sup> BFRAC represents SAS2H input parameter value

Based on the burnup profiles, each assembly node can have a different burnup based on the profile utilized. In determining the corresponding power and step length parameters for the input files, an assembly average specific power of 31.249 MW/MTU was used. This value was used to determine the time necessary to irradiate the assembly to a specific assembly average burnup, so that all nodes had the same irradiation time, by dividing the assembly average burnup by the specific power.

In SAS2H, the duration of a depletion calculation can be separated into a number of time steps of variable length in order to update the cross section libraries as fuel isotopics change. The duration of each time step was specified such that a maximum of 80 days of irradiation was not exceeded between cross section updates. The SAS2H calculations in this calculation utilized one cross section update per irradiation step. Therefore, the maximum duration of any time step in any irradiation layout of this calculation did not exceed 80 days.

Using the calculated time of irradiation and dividing it into  $\leq 80$  day step lengths, along with the required nodal burnup, the power per node per time step is then calculated using Equation 12.

$$Power = 31.249 \frac{MW}{MTU} * 0.468620 MTU * \frac{nodel}{360.172} * PF$$
(Eq. 12)

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Dogo	20	of $11$	
rage	20	0141	

where	
-------	--

0.468620 MTU	= the loading for the B&W MK-B2 assembly design (Punatar 2001,
	Table 3-1) (see Assumption 3.2)
PF	= the nodal burnup profile factor from Attachment I
31.249 MW/MTU	= the specific power
nodel	= the length of the axial node (corresponds to 20.0096 cm for all nodes
	except node four in the 7 node limiting axial profiles, which is
	240.115 cm, based on a total fuel length of 360.172 cm)

The corresponding nodal powers for each of the cases is provided in the SAS2H input files listed in Attachment III.

## 5.3 MCNP

MCNP is a general purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport, including the capability to calculate eigenvalues for critical systems. The code treats an arbitrary three dimensional configuration of materials in geometric cells bounded by first- and second- degree surfaces and fourth-degree elliptical tori (Ref. 7.4, p. ix). The Monte Carlo method is used to duplicate theoretically a statistical process. The individual probabilistic events that comprise a process are simulated sequentially. The probability distributions governing these events are statistically sampled to describe the total phenomenon (Briesmeister 1997, p. 1-3).

In order to quantify the overall effect that the differences in burnup profiles have on system reactivity, MCNP calculations were performed to calculate the effective neutron multiplication factor ( $k_{eff}$ ) that results from using the different sets of profiles and provide a comparison in terms of  $\Delta k_{eff}$ . The MCNP calculations were performed in a representative waste package configuration. The MCNP virtual model of the 21-PWR waste package follows the same description as that in Attachment III. The waste package was modeled in MCNP as containing 21 SNF assemblies with fully flooded conditions in order to maximize reactivity. Since the borated steel hardens the spectrum in the waste package for the intact configuration, assembly – to – assembly interaction is limited, therefore an alternative configuration where the boron was removed from the basket was also evaluated. The general assembly design parameters for the representative fuel assembly were presented in Table 1.

#### 5.3.1 MCNP Material Specifications

The spent fuel isotopes used in the MCNP cases correspond to those from the SAS2H calculations. Isotopes were extracted from the SAS2H outputs, combined with the initial oxygen mass and renormalized to the total mass in terms of weight percents. The values from the SAS2H calculations are given in units of mols, which were converted to units of grams using Equation 14. In order to keep changes in reactivity limited to variations from isotopic concentrations, the MCNP density input for each spent fuel composition was kept constant at the initial fuel density of 10.230 g/cm<sup>3</sup>. Equations 11 and 13 through 16 were used for determining

the initial oxygen mass. Each depleted fuel composition is listed in the MCNP input files contained on a compact disc attachment (Attachment III) in terms of ZAIDs and weight percents, and can be verified by visual inspection from the SAS2H output files along with the equations provided. The SAS2H output files for each calculation are contained on the compact disc attachment (Attachment III).

$$O \text{ Mass in } UO_2 = \begin{pmatrix} O \text{ Mass} / \\ mol \text{ } UO_2 \\ \hline U \text{ Mass} / \\ mol \text{ } UO_2 \end{pmatrix} (U \text{ Mass in } UO_2)$$
(Eq. 13)

*mols Isotope*<sub>i</sub> 
$$*A_i$$
 (Eq. 14)

where

i is the particular isotope

A is the atomic mass value from Audi and Wapstra (1995) U Mass / mol UO2 is calculated as shown in Equation 15 O Mass / mol UO2 is calculated as shown in Equation 16

$$\frac{U Mass}{mol UO_2} = \begin{bmatrix} (A)(U^{234}wt\%) + (A)(U^{235}wt\%) + \\ (A)(U^{236}wt\%) + (A)(U^{238}wt\%) \end{bmatrix} (0.01)$$
(Eq. 15)

where the weight percentages of the uranium isotopes ( $U^{234}$ ,  $U^{236}$ , and  $U^{238}$ ) in uranium for a given initial enrichment were calculated using Equation 11.

$$\frac{O Mass}{mol UO_2} = (2)(A \text{ for oxygen})$$
(Eq. 16)

The waste package representation for the MCNP calculations follows the description as that shown in Attachment III. The outer barrier of the waste package was represented as SB-575 N06022, which is a specific type of nickel-based alloy as described in Table 9. 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 10. The fuel basket plates were represented as Neutronit A978 with 1.62 wt% boron as described in Table 11, and the thermal shunts were represented as SB-209 A96061 T4 (aluminum 6061) as described in Table 12. The basket side and corner guides, and the basket stiffeners were represented as Grade 70 A 516 carbon steel as described in Table 13. Stiffeners were placed equidistant along the length of the basket in eight axial locations.

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 17 and 18. The atomic mass values and atom percent of natural element values for these calculations are from Parrington et al. (1996).

$$WF_{i} = \frac{A_{i}(At\%_{i})}{\sum_{i=1}^{I} A_{i}(At\%_{i})}$$
(Eq. 17)

where

 $WF_i$  = the weight fraction of isotope<sub>i</sub> in the natural element  $A_i$  = the atomic mass of isotope<sub>i</sub>

At%i = the atom percent of isotope<sub>i</sub> in the natural element

I = the total number of isotopes in the natural element

$$Wt\%_i = WF_i(E_{wt\%}) \tag{Eq. 18}$$

where

 $Wt\%_i$  = the weight percent of isotope<sub>i</sub> in the material composition

 $WF_i$  = the weight fraction of isotope<sub>i</sub> from Equation 17

 $E_{wt\%}$  = the referenced weight percent of the element in the material composition

Element/			Flement/		
Licitiona		\A/40/	Lotono		14/40/
isotope	ZAID	<b>VV</b> 1%	isotope	ZAID	<b>VV</b> 1%
C-nat	6000.50c	0.0150	Co-59	27059.50c	2.5000
Mn-55	25055.50c	0.5000	W-182	74182.55c	0.7877
Si-nat	14000.50c	0.0800	W-183	74183.55c	0.4278
Cr-50	24050.60c	0.8879	W-184	74184.55c	0.9209
Cr-52	24052.60c	17.7863	W-186	74186.55c	0.8636
Cr-53	24053.60c	2.0554	V	23000.50c	0.3500
Cr-54	24054.60c	0.5202	Fe-54	26054.60c	0.2260
Ni-58	28058.60c	36.8024	Fe-56	26056.60c	3.6759
Ni-60	28060.60c	14.6621	Fe-57	26057.60c	0.0865
Ni-61	28061.60c	0.6481	Fe-58	26058.60c	0.0116
Ni-62	28062.60c	2.0975	S-32	16032.50c	0.0200
Ni-64	28064.60c	0.5547	P-31	15031.50c	0.0200
Mo-nat	42000.50c	13.5000	Den	sity = 8.69 g/cm <sup>3</sup>	

Table 9.	SB-575	N06022	Material	Composition
				••••••••••••••••••••••••••••••••••••••

Source: DTN: MO0003RIB00071.000

NOTE: <sup>a</sup> ZAID = MCNP material identifier

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

#### Table 10. Material Specifications for SS316NG

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

NOTE: <sup>a</sup> ZAID = MCNP material identifier

#### Table 11. Material Specifications for Neutronit A978 with 1.62 wt% Boron

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

Source: DTN: MO0109RIB00049.001; Audi and Wapstra 1995

NOTE: <sup>a</sup> ZAID = MCNP material identifier

Table 12	Material S	Specifications	for	AI 6061
		specifications	101	

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

Source: DTN: MO9906RIB00048.000

NOTES: <sup>a</sup> ZAID = MCNP material identifier

<sup>b</sup> Zn cross-section data unavailable, therefore it was substituted as AI-27 (See assumption 3.3)

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

Table 13. Grade 70 A516 Carbon Steel Composition

Source: DTN: MO0003RIB00072.000

NOTE: <sup>a</sup> ZAID = MCNP material identifier

The cladding composition was Zircaloy-4 as presented in Table 14 and the spacer grids were Inconel 718 as presented in Table 15. Table 16 presents the component material volume fractions for the upper and lower end-fitting regions and Table 18 presents the upper and lower fuel rod plenum material volume fractions for the B&W 15x15 assembly design. Table 17 presents the upper and lower end-fitting homogenized material compositions and Table 19 presents the upper and lower fuel rod plenum homogenized material compositions for the B&W 15x15 assembly design.

Table 14.	Zircaloy-4	Material	Composition
-----------	------------	----------	-------------

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

Source: ASTM B 811-90 1991, p. 2, Table 2

NOTES: <sup>a</sup> ZAID = MCNP material identifier. <sup>b</sup> From ASM International 1990, p. 666, Table 6.

Element/Isotope	ZAID <sup>a</sup>	Wt%	Element/Isotope	ZAID	Wt%
C-nat	6000.50c	0.0400	Fe-58	26058.60c	0.0537
Si-nat	14000.50c	0.1800	Ni-58	28058.60c	35.2846
S-32	16032.50c	0.0080	Ni-60	28060.60c	14.0574
Cr-50	24050.60c	0.7940	Ni-61	28061.60c	0.6214
Cr-52	24052.60c	15.9050	Ni-62	28062.60c	2.0110
Cr-53	24053.60c	1.8380	Ni-64	28064.60c	0.5319
Cr-54	24054.60c	0.4652	Ti-nat	22000.50c	0.9001
Mn-55	25055.50c	0.1800	AI-27	13027.50c	0.5001

Table 15. Inconel 718 Material Composition

Element/Isotope	ZAID <sup>a</sup>	Wt%	Element/Isotope	ZAID	Wt%
Fe-54	26054.60c	1.0454	Nb-93 <sup>b</sup>	41093.50c	5.1306
Fe-56	26056.60c	17.0031	Mo-nat	42000.50c	3.0504
Fe-57	26057.60c	0.3999	Dens	ity = 8.19 g/cm <sup>3</sup>	

#### Table 15. Inconel 718 Material Composition

Source: Lynch 1989, p. 496

NOTES: <sup>a</sup> ZAID = MCNP material identifier. <sup>b</sup> Reference identifies this material

Reference identifies this material as "columbium," which is actually the element niobium.

# Table 16. End-Fitting Component Material Volume Fractions for Babcock & Wilcox 15x15 Assembly Design

Assembly Design	Stainless Steel Type 304	Inconel	Zircaloy-4	Moderator
Upper End-Fitting	0.2756	0.0441	0.0081	0.6722
Lower End-Fitting	0.1656	0.0306	0.0125	0.7913

Source: Punatar 2001, Section 2

# Table 17. End-Fitting Homogenized Material Compositions for Babcock & Wilcox 15×15 Assembly Design

Element/ Isotope	ZAID <sup>a</sup>	Upper End-Fitting Wt%	Lower End-Fitting Wt%
C-nat	6000.50c	0.0245	0.0203
N-14	7014.50c	0.0668	0.0539
Si-nat	14000.50c	0.5210	0.4229
P-31	15031.50c	0.0301	0.0243
S-32	16032.50c	0.0209	0.0170
Cr-50	24050.60c	0.6181	0.5098
Cr-52	24052.60c	12.3822	10.2114
Cr-53	24053.60c	1.4309	1.1800
Cr-54	24054.60c	0.3622	0.2987
Mn-55	25055.50c	1.3563	1.0968
Fe-54	26054.60c	2.6847	2.1808
Fe-56	26056.60c	43.6633	35.4677
Fe-57	26057.60c	1.0269	0.8342
Fe-58	26058.60c	0.1380	0.1121
Ni-58	28058.60c	8.3820	7.2490
Ni-60	28060.60c	3.3394	2.8880
Ni-61	28061.60c	0.1476	0.1277
Ni-62	28062.60c	0.4777	0.4132
Ni-64	28064.60c	0.1263	0.1093

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# Table 17. End-Fitting Homogenized Material Compositions for Babcock & Wilcox 15×15 Assembly Design

Element/ Isotope	ZAID <sup>a</sup>	Upper End-Fitting Wt%	Lower End-Fitting Wt%
H-1	1001.50c	2.2972	3.6312
O-16	8016.50c	18.2314	28.8196
AI-27	13027.50c	0.0552	0.0514
Ti-nat	22000.50c	0.0993	0.0925
Nb-93	41093.50c	0.5659	0.5272
Mo-nat	42000.50c	0.3364	0.3135
Zr-nat	40000.60c	1.5920	3.2990
Sn-nat	50000.35c	0.0235	0.0488
Densit	y (g/cm <sup>3</sup> )	3.2748	2.4388

NOTE: <sup>a</sup> ZAID = MCNP material identifier.

#### Table 18. Fuel Rod Plenum Material Volume Fractions

Assembly Design	Plenum Location	Type 304 Stainless Steel	Gas (modeled as void)	Zircaloy-4
Babcock & Wilcox 15×15	Upper	0.0811	0.7793	0.1396
	Lower	0.1569	0.5973	0.2458

Source: Punatar 2001, Section 2

NOTE: Volume fractions are renormalized to exclude the cladding, which is modeled explicitly in the input.

# Table 19. Fuel Rod Plenum Homogenized Material Compositions for Babcock & Wilcox 15×15Assembly Design

		Wt% of Element/Isotope in Material Composition		
Element/Isotope	ZAID <sup>a</sup>	Upper Fuel Rod Plenum	Lower Fuel Rod Plenum	
C-nat	6000.50c	0.0124	0.0131	
N-14	7014.50c	0.0413	0.0436	
Si-nat	14000.50c	0.3096	0.3270	
P-31	15031.50c	0.0186	0.0196	
S-32	16032.50c	0.0124	0.0131	
Cr-50	24050.60c	0.3302	0.3485	
Cr-52	24052.60c	6.6148	6.9806	
Cr-53	24053.60c	0.7644	0.8067	
Cr-54	24054.60c	0.1935	0.2042	
Mn-55	25055.50c	0.8257	0.8720	
Fe-54	26054.60c	1.5943	1.6829	
Fe-56	26056.60c	25.9299	27.3712	
Fe-57	26057.60c	0.6099	0.6438	

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 Table 19. Fuel Rod Plenum Homogenized Material Compositions for Babcock & Wilcox 15×15

 Assembly Design

		Wt% of Element/Isotope in Material Composition			
Element/Isotope	ZAID <sup>a</sup>	Upper Fuel Rod Plenum	Lower Fuel Rod Plenum		
Fe-58	26058.60c	0.0820	0.0865		
Ni-58	28058.60c	2.7744	2.9298		
Ni-60	28060.60c	1.1053	1.1672		
Ni-61	28061.60c	0.0489	0.0516		
Ni-62	28062.60c	0.1581	0.1670		
Ni-64	28064.60c	0.0418	0.0442		
O-16	8016.50c	0.0734	0.0705		
Zr-nat	40000.60c	57.6077	55.3392		
Sn-nat	50000.35c	0.8514	0.8178		
Density	/ (g/cm <sup>3</sup> )	1.5597	2.8583		

NOTE: <sup>a</sup> ZAID = MCNP material identifier.

The waste package was represented in a fully flooded condition with normal water at  $1.0 \text{ g/cm}^3$  density.

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#### 6. **RESULTS**

The PWR assembly axial profile results are presented in this section. Several different profile sets were evaluated. Profile sets were categorized into three groups as described in Attachment I.

In order to quantify the overall effect that the differences between the burnup profiles 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. The  $k_{eff}$  results represent the average combined collision, absorption, and track-length estimator from the MCNP calculations. The standard deviation ( $\sigma$ ) represents the standard deviation of  $k_{eff}$  about the average combined collision, and track-length estimate due to the Monte Carlo calculation statistics.

The MCNP input and output files for the cases used in this evaluation are presented in electronic format on a compact disc attachment to this calculation report (Attachment III).

In the following illustrations of the results (Figures 2 through 10) the 1 Node profile results come from a flat axial burnup profile, the 18 Node profile results were generated from an 18 node mean axial burnup profile, and the 7 Node profile results correspond to a statistically derived axial burnup profile.

All outputs are reasonable compared to the inputs and the results of this calculation are suitable for their intended use.

#### 6.1 **PROFILE SET ONE**

The  $k_{eff}$  results for cases that were generated based on profile set one are presented here. Table 20 presents the  $k_{eff}$  results for one, seven, and 18 axial zone representations presented in Attachment I. Graphical illustrations are presented in Figures 2 to 4, along with transition points of where the seven-zone profile set becomes more conservative over the single-zone profile.

Initial		1 Node		7 No	odes	18 Nodes	
Enrichment (wt% U-235)	Burnup (GWd/MTU)	k <sub>eff</sub>	sigma	k <sub>eff</sub>	sigma	k <sub>eff</sub>	sigma
3.0	10	0.95834	0.00051	0.95306	0.0005	0.95189	0.00052
	20	0.87872	0.00049	0.88877	0.00052	0.87343	0.00055
	30	0.8071	0.00045	0.81448	0.0005	0.80908	0.00045
	40	0.75189	0.00047	0.79423	0.00051	0.75314	0.00049
	50	0.70024	0.00045	0.76493	0.00046	0.70512	0.00047
4.0	10	1.03186	0.00051	1.02419	0.00059	1.02488	0.00049
	20	0.95669	0.0005	0.96225	0.00056	0.95133	0.00052
	30	0.88744	0.00056	0.89343	0.00056	0.88512	0.00052
	40	0.82476	0.0005	0.86352	0.00052	0.82745	0.00046
	50	0.76402	0.00045	0.8346	0.00051	0.77424	0.00049
5.0	10	1.08585	0.00056	1.07649	0.00058	1.07826	0.00054
	20	1.01682	0.00057	1.0155	0.00057	1.01052	0.00054
	30	0.95271	0.00055	0.95194	0.00052	0.94891	0.00053
	40	0.89193	0.00056	0.92251	0.00055	0.8914	0.00051
	50	0.82952	0.00047	0.89052	0.00055	0.83718	0.00057

#### Table 20. Results Using Profile Set One with Nominal Depletion Parameters



Figure 2. Results for Profile Set One with Initial Enrichment of 3.0 Wt% U-235

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Figure 3. Results for Profile Set One with Initial Enrichment of 4.0 Wt% U-235



Figure 4. Results for Profile Set One with Initial Enrichment of 5.0 Wt% U-235

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#### 6.2 **PROFILE SET TWO**

The  $k_{eff}$  results for cases that were generated based on profile set one are presented here. Table 21 presents the  $k_{eff}$  results for one, seven, and 18 axial zone representations presented in Attachment I. Graphical illustrations are presented in Figures 5 to 7, along with transition points of where the seven-zone profile set becomes more conservative over the single-zone profile.

Initial		1 N	ode	7 Nodes		18 Nodes	
Enrichment (wt% U-235)	Burnup (GWd/MTU)	k <sub>eff</sub>	sigma	k <sub>eff</sub>	sigma	k <sub>eff</sub>	sigma
3.0	10	0.95834	0.00051	0.95231	0.00054	0.9526	0.00053
	20	0.87872	0.00049	0.88407	0.00053	0.87477	0.00049
	30	0.8071	0.00045	0.82071	0.00051	0.80803	0.00048
	40	0.75189	0.00047	0.76083	0.00051	0.7528	0.00048
	50	0.70024	0.00045	0.72201	0.00048	0.70246	0.00044
4.0	10	1.03186	0.00051	1.02399	0.00058	1.02592	0.00054
	20	0.95669	0.0005	0.95706	0.00055	0.94991	0.00059
	30	0.88744	0.00056	0.89702	0.00055	0.8858	0.00054
	40	0.82476	0.0005	0.83332	0.00056	0.8267	0.00051
	50	0.76402	0.00045	0.79227	0.00053	0.76958	0.00052
5.0	10	1.08585	0.00056	1.07754	0.00054	1.07849	0.00056
	20	1.01682	0.00057	1.0116	0.00062	1.00952	0.00055
	30	0.95271	0.00055	0.95492	0.00057	0.9486	0.00058
	40	0.89193	0.00056	0.89617	0.00053	0.88987	0.00054
	50	0.82952	0.00047	0.85558	0.00054	0.83327	0.00052

Table 21. Results Using Profile Set Two with Nominal Depletion Parameters



Figure 5. Results for Profile Set Two with Initial Enrichment of 3.0 Wt% U-235



Figure 6. Results for Profile Set Two with Initial Enrichment of 4.0 Wt% U-235

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#### 6.3 PROFILE SET THREE

The  $k_{eff}$  results for cases that were generated based on profile set three are presented here. Table 22 presents the  $k_{eff}$  results for one, seven, and 18 axial zone representations presented in Attachment I. Graphical illustrations are presented in Figures 8 to 10, along with transition points of where the seven-zone profile set becomes more conservative over the single-zone profile.



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Initial		1 N	ode	7 No	odes	18 Nodes	
Enrichment (wt% U-235)	Burnup (GWd/MTU)	k <sub>eff</sub>	sigma	k <sub>eff</sub>	sigma	k <sub>eff</sub>	sigma
3.0	10	0.95834	0.00051	0.95293	0.00053	0.95245	0.00052
	20	0.87872	0.00049	0.88391	0.00058	0.87439	0.00054
	30	0.8071	0.00045	0.82715	0.00045	0.80868	0.0005
	40	0.75189	0.00047	0.76708	0.00051	0.75357	0.0005
	50	0.70024	0.00045	0.71844	0.00046	0.70353	0.00044
4.0	10	1.03186	0.00051	1.02426	0.00053	1.02576	0.00058
	20	0.95669	0.0005	0.95832	0.00049	0.95021	0.00053
	30	0.88744	0.00056	0.90198	0.00057	0.88537	0.0005
	40	0.82476	0.0005	0.84079	0.00052	0.82755	0.00048
	50	0.76402	0.00045	0.78922	0.00053	0.77126	0.0005
5.0	10	1.08585	0.00056	1.07753	0.00056	1.07882	0.00056
	20	1.01682	0.00057	1.01391	0.00055	1.01121	0.0005
	30	0.95271	0.00055	0.96032	0.0006	0.94782	0.00058
	40	0.89193	0.00056	0.90316	0.00052	0.8911	0.00056
	50	0.82952	0.00047	0.85043	0.00056	0.83572	0.00056

#### Table 22. Results Using Profile Set Three with Nominal Depletion Parameters



Figure 8. Results for Profile Set Three with Initial Enrichment of 3.0 Wt% U-235

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**Calculation** 



Figure 9. Results for Profile Set Three with Initial Enrichment of 4.0 Wt% U-235



Figure 10. Results for Profile Set Three with Initial Enrichment of 5.0 Wt% U-235

#### 6.4 **PROFILE SET FOUR**

MCNP cases were not run for these sets of profiles because there is nothing in the profiles that would change the behavior of the results from the previous profile sets. The profiles that compose this set were part of the profiles used in profile sets one and two so they have not been excluded from evaluation. Also, the B&W 15x15 assembly design is considered to be the most limiting fuel assembly design (see Assumption 3.2), which would envelop results generated with this profile set.

#### 6.5 PROFILE SET COMPARISON

A comparison of the statistically derived axial burnup profiles (seven-zone profile) was performed for each of the evaluated profile sets (i.e., one, two, and three). The results are presented in Figures 11, 12, and 13, for 3.0, 4.0, and 5.0 wt% U-235 initial enriched fuel, respectively. Profile Set One results were generated from using nearly all assembly profiles in the statistical analysis, Profile Set Two results were generated from assemblies that did not contain axial blanket or zoned fuel assembly profiles, and Profile Set Three results were generated using only B&W 15x15 fuel assembly profiles.

As can be seen in the figures, the choice of profile is relatively even at lower burnups. As the burnup increases Profile Set One becomes more deviant, most likely due to the presence of axially zoned fuel assemblies, but Profile Sets Two and Three behave well. The Profile Set Three results tend to produce a slightly higher  $k_{eff}$  value than the Profile Set Two results until almost 50 GWd/MTU. This is most likely an artifact of the limited number of assemblies in the database with burnups greater than 45 GWd/MTU (provides only a 62.4 percent confidence level of covering 95 percent of the population [See Attachment III]). Since the B&W 15x15 fuel assembly design is considered bounding of the other fuel assembly designs, it is recommended that the Profile Set Three profiles be used when the B&W 15x15 assembly design is the representative spent fuel assembly for burnup credit applications. It should also be noted that an additional comparison may be beneficial where burnup groups 7 and 8 are combined to develop a profile for burnups in excess of 40 GWd/MTU.

**Calculation** 







Figure 12. 4.0 Wt% U-235 Initial Enrichment Seven-Zone Profile Comparison



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Figure 13. 5.0 Wt% U-235 Initial Enrichment Seven-Zone Profile Comparison

#### 6.6 SENSITIVITY TO NEUTRON ABSORBING ENVIRONMENT

A set of cases were evaluated to observe the effects (if any) of an axially zoned profile versus a single zone profile in an environment where a strong thermal neutron absorber was present. The MCNP representation was performed for an assembly with an initial enrichment of 4.0 wt% U-235 for a burnup range of 10 to 50 GWd/MTU. The axially zoned profile selected for comparison was the profile set two, seven-zone profile. The results are presented in Table 23.

	1 Fuel	Zone	7 Fuel Zones		
Burnup (GWd/MTU)	k <sub>eff</sub>	sigma	k <sub>eff</sub>	sigma	
10	1.12672	0.00057	1.13414	0.00048	
20	1.05413	0.0005	1.05235	0.00049	
30	0.98543	0.0005	0.97603	0.00052	
40	0.9164	0.00052	0.90648	0.00045	
50	0.87118	0.00045	0.83976	0.00046	

Table 23.	Results of	Sensitivity to	Strong	Neutron	Absorber
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#### 8. ATTACHMENTS

Table 24 presents the attachment specifications for this calculation file. The contents of Attachment II are provided electronically on an attachment CD to this calculation file (Attachment III).

Attachment #	# of Pages	Description			
Ι	25	Axial Burnup Profiles			
	3	Listing of contents on Attachment III			
Ш	N/A	Compact Disc attachment containing information listed in Attachment II			

#### Table 24. Attachment Listing

**Page I-1** of 25

# **Attachment I: Axial Burnup Profiles**

#### I. AXIAL BURNUP PROFILE DEVELOPMENT

The profiles were developed based on using a statistical approach for selecting limiting values. The axial profile database lists normalized factors for 18 axial nodes. The number of axial zones was reduced from 18 used in the axial profile database (Cacciapouti and Van Volkinburg, 1997) to seven. Using a seven-zone scheme is based on a study performed by Oak Ridge National Laboratories where they investigated various axial zoning schemes and determined that a sevenaxial-zone model was sufficient (DeHart 1996, p. 84). The limiting axial profiles were developed from the axial profile database (Cacciapouti and Van Volkinburg, 1997) by dividing the assemblies into burnup groups based on average burnup, for all fuel types and essentially all assemblies from the database. Certain types of fuel assemblies that contained nonuniform axial loadings or other characteristics i.e., axial blanket fuel, that would make their use in a limiting profile analysis inappropriate, were excluded, as well as any assemblies that did not have information for all 18 axial zones. The excluded assembly sets are provided in the spreadsheet attachments under the tab "Omitted" in spreadsheets profile set1.xls and profile set2.xls in Attachment III. Limiting axial profiles were developed for a set of eight burnup ranges. In general, for a particular burnup range, the highest reactivity would be found at the top and bottom of an assembly where the fuel is the least burned. Therefore, in selecting the nodal values for the limiting profiles, the lower limit values for each of the top and bottom 3 nodes, respectively, within a given burnup range, were assigned to the burnup profile. The values for the central node of each limiting profile were selected by renormalizing them so that the average burnup of the assembly would remain constant using Equation 19.

Formula for 7 node normalization technique:

$$pf = \frac{1 - \sum_{j=1}^{6} a_j b_j}{1 - \sum_{j=1}^{6} b_j}$$
(Eq. 19)

where

pf = the central zone profile normalization factor

 $a_i$  = profile normalization factor

 $b_i = axial length$ 

When selecting profile normalization factors, the data are treated as a random sample of data (profile normalization factors) from the burnup range population of interest and straightforward statistical techniques are applied to determine the limiting profile factor (i.e. lower limit). Using a statistical process requires determining if the sample population is normally distributed. When a normal distribution is observed, the normal distribution tolerance-limit (NDTL) method is used, and when the sample population is not normally distributed, the distribution-free tolerance-

limit (DFTL) method is used. The two methods are described below. For each of the profile data sets, the Shapiro-Wilk test for normality was used.

# NDTL Method

The NDTL method is used for conditions in which the profile normalization factors are sufficient in number and scope to determine reasonable justification of normality.

Given that the profile normalization factors are shown to be normally distributed, the lower limit factors can be calculated as illustrated in Equation 20.

Lower Limit = 
$$\beta$$
ave - K<sub>b</sub> $\sigma$  (Eq. 20)

where

 $\beta_{ave}$  = the mean value of the profile normalization factor values

- K<sub>b</sub> = a multiplier from statistical tables for one-sided tolerance limits for normal distributions (taken from Odeh and Owen [1980, pp. 30-33])
- $\sigma_{\Delta k_{eff}}$  = the standard deviation associated with the selected profile normalization factor values as shown in Equation 21

$$\sigma_{\Delta k_{eff}} = \sqrt{\sum_{j=1}^{n} \frac{(x_j - \overline{x})^2}{n - 1}}$$
(Eq. 21)

where

 $x_j$  = profile normalization factor

 $\overline{x}$  = the sample mean

n = the sample population

#### **DFTL Method**

The DFTL method applies when the data set does not pass the test for normality. This approach establishes a lower limit through the use of distribution-free statistical tolerance limit methods. The requirement for applying distribution-free methods to establish a statistical tolerance limit is that the data be from a random sample from a continuous distribution. The methods are described in Natrella (1963, pp. 1-14, 1-15, 2-15); and Hogg and Craig (1966, pp. 182-185).

Applying this method is straightforward when the resulting indices for the sample size, confidence level, and the portion of the population to be covered are included in published tables (Natrella 1963, Table A-31). In this case, one uses the table for the appropriate values for confidence, population coverage, and sample size and obtains an index value, which is applied to the ranked (sorted) values of the profile normalization factors. For instance, if the sample size is 100 and a 95/95 percent lower tolerance limit is desired, the index is 2. This means that the second smallest observation serves as the 95/95 percent lower one-sided tolerance limit.

For this method, the number of observations must be sufficient to accommodate the desired confidence level and portion of the population to be covered. For instance, if normality is not justified, and the number of observations is fewer than 59, one cannot make a 95 percent confidence statement about 95 percent of the population being above the smallest observed value. Such a limit would be close to, but not quite, a 95/95 percent lower tolerance limit because at least one of the statement descriptors would not be strictly met.

#### I.1 PROFILE SET ONE

Profile set one was based on using all fuel assemblies from the database with the exception of the assemblies that did not contain information for all 18 axial nodes. This profile set includes assemblies with nonuniform axial enrichments (axial blanket fuel assemblies) and partially loaded shield assemblies. The profiles used for this set are provided in a spreadsheet (*profile\_set1.xls*) contained on the attachment CD (Attachment III) along with a listing of the profiles that were omitted.

The profile sample set numbers and associated index values are illustrated in Table 25 for profile set one. And the calculated limiting profile factors are provided in Table 26.

Burnup Range (GWd/MTU)	Ν	Index	Notes
10 ≤ x < 15	306	9	All nodes not normally distributed
15 ≤ x < 20	636	22	All nodes not normally distributed
20 ≤ x < 25	471	15	All nodes not normally distributed
25 ≤ x < 30	366	11	All nodes not normally distributed
30 ≤ x < 35	488	16	Node 5 normally distributed, all others distribution-free
35 ≤ x < 40	379	12	All nodes not normally distributed
40 ≤ x < 45	230	6	All nodes not normally distributed
45 < x	128	2	Nodes 2 and 5 normally distributed, all others distribution-free

 Table 25. Profile Set One Sample Population Indices

NOTE: Indices were interpolated from Natrella (1963, Table A-31)

Table 26.	Seven-Node Limiting	Axial Profiles b	v Burnup Gi	roup for Profile	Set One
10010 20.		<i>i</i> wiai i i onico b	y Dunnup Oi		001 0110

	Group 1 <sup>b</sup>	Group 2 <sup>b</sup>	Group 3 <sup>b</sup>	Group 4 <sup>b</sup>	Group 5 <sup>b</sup>	Group 6 <sup>b</sup>	Group 7 <sup>b</sup>	Group 8 <sup>b</sup>
Axial Pos. <sup>a</sup>	10 ≤ x < 15	15 ≤ x < 20	20 ≤ x < 25	25 ≤ x < 30	30 ≤ x < 35	35 ≤ x < 40	40 ≤ x < 45	45 ≤ x
0.028	0.239	0.316	0.544	0.602	0.558	0.313	0.318	0.328
0.083	0.784	0.861	0.885	0.921	0.905	0.912	0.918	0.924
0.139	0.952	1.001	1.015	1.055	1.024	1.026	1.024	1.021
0.194 – 0.806	1.187	1.158	1.115	1.094	1.104	1.137	1.136	1.137
0.861	0.882	0.918	0.951	0.995	0.979	0.986	0.987	0.989
0.917	0.665	0.715	0.782	0.807	0.819	0.828	0.824	0.816
0.972	0.237	0.290	0.440	0.486	0.471	0.293	0.293	0.283

NOTES: <sup>a</sup> Axial Pos. is percent of core height from bottom to top <sup>b</sup> Burnup ranges are in units of GWd/MTU

For comparative purposes, mean profiles were determined from the profile set one-database assemblies and are provided in Table 27.

	Group 1 <sup>b</sup>	Group 2 <sup>b</sup>	Group 3 <sup>b</sup>	Group 4 <sup>b</sup>	Group 5 <sup>b</sup>	Group 6 <sup>b</sup>	Group 7 <sup>b</sup>	Group 8 <sup>b</sup>
Axial Pos. <sup>a</sup>	10 ≤ x < 15	15 ≤ x < 20	20 ≤ x < 25	25 ≤ x < 30	30 ≤ x < 35	35 ≤ x < 40	40 ≤ x < 45	45 ≤ x
0.028	0.573	0.619	0.638	0.607	0.643	0.639	0.651	0.653
0.083	0.901	0.927	0.938	0.930	0.934	0.938	0.943	0.944
0.139	1.048	1.053	1.054	1.050	1.044	1.045	1.046	1.045
0.194	1.094	1.092	1.085	1.085	1.076	1.076	1.074	1.073
0.25	1.112	1.102	1.092	1.094	1.086	1.086	1.083	1.081
0.306	1.110	1.098	1.087	1.091	1.084	1.084	1.081	1.079
0.361	1.113	1.095	1.085	1.089	1.082	1.082	1.080	1.079
0.417	1.115	1.093	1.083	1.087	1.080	1.079	1.078	1.076
0.472	1.114	1.090	1.081	1.085	1.078	1.076	1.074	1.072
0.528	1.118	1.091	1.084	1.088	1.078	1.077	1.075	1.073
0.583	1.115	1.090	1.082	1.087	1.077	1.075	1.072	1.070
0.639	1.113	1.089	1.083	1.088	1.077	1.076	1.071	1.070
0.694	1.105	1.085	1.080	1.086	1.076	1.074	1.070	1.069
0.75	1.084	1.073	1.070	1.077	1.068	1.067	1.063	1.062
0.806	1.046	1.047	1.049	1.056	1.052	1.053	1.050	1.050
0.861	0.960	0.981	0.990	0.997	1.003	1.005	1.005	1.008
0.917	0.788	0.832	0.850	0.854	0.873	0.880	0.883	0.890
0.972	0.489	0.540	0.568	0.546	0.589	0.589	0.601	0.608

Table 27	18 Node Mean	Axial Profiles	by Burnup	Group for	r Profile Set One
10010 27.	TO NOUC MICAN	Avial 1 Tomes	by Durnup	Oroup io	

NOTES: <sup>a</sup> Axial Pos. is percent of core height from bottom to top <sup>b</sup> Burnup ranges are in units of GWd/MTU **Page I-4** of 25

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Figure 14. Burnup Group One ( $10 \le x < 15$ ) Profile Set One Profiles



Figure 15. Burnup Group Two ( $15 \le x < 20$ ) Profile Set One Profiles

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Figure 16. Burnup Group Three ( $20 \le x < 25$ ) Profile Set One Profiles



Figure 17. Burnup Group Four ( $25 \le x < 30$ ) Profile Set One Profiles





Figure 18. Burnup Group Five  $(30 \le x < 35)$  Profile Set One Profiles



Figure 19. Burnup Group Six ( $35 \le x < 40$ ) Profile Set One Profiles

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Figure 20. Burnup Group Seven ( $40 \le x < 45$ ) Profile Set One Profiles



Figure 21. Burnup Group Eight ( $45 \le x$ ) Profile Set One Profiles

#### I.2 PROFILE SET TWO

Profile set two was based on using all fuel assemblies from the database with the exception of the assemblies that contained nonuniform axial loadings (i.e., axial blanket fuel) or other characteristics (i.e., partially loaded shield assemblies, missing information), that would make their use in a limiting profile analysis inappropriate. The profiles used for this set are provided in a spreadsheet attachment (*profile\_set2.xls*) contained on the attachment CD (Attachment III) along with a listing of the profiles that were omitted.

The profile sample set numbers and associated index values are illustrated in Table 28 for profile set two. And the calculated limiting profile factors are provided in Table 29.

Burnup Range (GWd/MTU)	Ν	Index	Notes
10 ≤ x < 15	295	8	All nodes not normally distributed
15 ≤ x < 20	603	21	All nodes not normally distributed
20 ≤ x < 25	457	15	All nodes not normally distributed
25 ≤ x < 30	332	10	Node 1 normally distributed, all others distribution-free
30 ≤ x < 35	475	16	Node 5 normally distributed, all others distribution-free
35 ≤ x < 40	343	10	All nodes not normally distributed
40 ≤ x < 45	212	5	Nodes 2 and 5 normally distributed, all others distribution-free
45 ≤ x	115	2	Node 5 normally distributed, all others distribution-free

T-1-1- 00	Duefle Oat To		
i able 28.	Profile Set IV	vo Sample Po	pulation indices

NOTE: Indices were interpolated from Natrella (1963, Table A-31)

Table 20	Soven Nede Limiting	Avial Drafiles by		up for Drofilo Sot Two
Table 29.	Seven-Noue Limiting	Axial FIUIIIes D	у Битпир Стс	up for Frome Set I wo

	Group 1 <sup>♭</sup>	Group 2 <sup>b</sup>	Group 3 <sup>b</sup>	Group 4 <sup>b</sup>	Group 5 <sup>b</sup>	Group 6 <sup>b</sup>	Group 7 <sup>b</sup>	Group 8 <sup>b</sup>
Axial Pos. <sup>a</sup>	10 ≤ x < 15	15 ≤ x < 20	20 ≤ x < 25	25 ≤ x < 30	30 ≤ x < 35	35 ≤ x < 40	40 ≤ x < 45	45 ≤ x
0.028	0.502	0.550	0.574	0.583	0.602	0.622	0.618	0.574
0.083	0.784	0.861	0.885	0.900	0.907	0.914	0.925	0.917
0.139	0.950	1.001	1.015	1.017	1.024	1.026	1.024	1.021
0.194 – 0.806	1.153	1.128	1.107	1.107	1.098	1.088	1.090	1.096
0.861	0.881	0.916	0.952	0.962	0.979	0.985	0.986	0.991
0.917	0.664	0.714	0.792	0.778	0.820	0.847	0.840	0.832
0.972	0.380	0.416	0.494	0.479	0.495	0.554	0.524	0.515

NOTES: <sup>a</sup> Axial Pos. is percent of core height from bottom to top <sup>b</sup> Burnup ranges are in units of GWd/MTU

For comparative purposes, mean profiles were determined from the profile set two-database assemblies and are provided in Table 30.

	Group 1 <sup>b</sup>	Group 2 <sup>b</sup>	Group 3 <sup>b</sup>	Group 4 <sup>b</sup>	Group 5 <sup>b</sup>	Group 6 <sup>b</sup>	Group 7 <sup>b</sup>	Group 8 <sup>b</sup>
Axial Pos. <sup>a</sup>	10 ≤ x < 15	15 ≤ x < 20	20 ≤ x < 25	25 ≤ x < 30	30 ≤ x < 35	35 ≤ x < 40	40 ≤ x < 45	45 ≤ x
0.028	0.584	0.631	0.646	0.637	0.652	0.666	0.678	0.682
0.083	0.903	0.928	0.939	0.931	0.934	0.939	0.944	0.944
0.139	1.048	1.052	1.053	1.047	1.043	1.043	1.043	1.040
0.194	1.094	1.090	1.083	1.080	1.075	1.072	1.069	1.065
0.25	1.111	1.100	1.090	1.089	1.084	1.081	1.078	1.074
0.306	1.108	1.096	1.085	1.085	1.083	1.079	1.076	1.072
0.361	1.111	1.093	1.083	1.083	1.081	1.077	1.075	1.072
0.417	1.112	1.091	1.082	1.082	1.078	1.074	1.073	1.070
0.472	1.111	1.088	1.080	1.080	1.076	1.071	1.069	1.066
0.528	1.116	1.090	1.083	1.083	1.077	1.072	1.070	1.068
0.583	1.113	1.088	1.081	1.083	1.076	1.070	1.067	1.065
0.639	1.111	1.088	1.082	1.084	1.076	1.071	1.067	1.066
0.694	1.104	1.084	1.079	1.082	1.074	1.070	1.066	1.065
0.75	1.082	1.071	1.069	1.073	1.067	1.063	1.059	1.059
0.806	1.044	1.046	1.049	1.054	1.051	1.049	1.047	1.048
0.861	0.959	0.981	0.991	0.997	1.003	1.004	1.005	1.010
0.917	0.789	0.833	0.851	0.857	0.873	0.882	0.886	0.896
0.972	0.498	0.551	0.576	0.573	0.596	0.614	0.627	0.638

Table 30. 18 Node Mean Axial Profiles by Burnup Group for Profile Set Two

NOTES: <sup>a</sup> Axial Pos. is percent of core height from bottom to top <sup>b</sup> Burnup ranges are in units of GWd/MTU



Figure 22. Burnup Group One ( $10 \le x < 15$ ) Profile Set Two Profiles

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Figure 23. Burnup Group Two ( $15 \le x < 20$ ) Profile Set Two Profiles



Figure 24. Burnup Group Three ( $20 \le x \le 25$ ) Profile Set Two Profiles

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Figure 26. Burnup Group Five  $(30 \le x < 35)$  Profile Set Two Profiles

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Figure 28. Burnup Group Seven ( $40 \le x < 45$ ) Profile Set Two Profiles



Figure 29. Burnup Group Eight ( $45 \le x$ ) Profile Set Two Profiles

## I.3 PROFILE SET THREE

Profile set three was based on using only the B&W 15x15 fuel assemblies from the database. The profiles used for this set are provided in a spreadsheet attachment (*profile\_set3.xls*) contained on the attachment CD (Attachment III). This set of fuel assemblies was selected to be evaluated separately due to observations of the axial profile database indicating that the majority of the lower profile factor datapoints within the database come from B&W 15x15 fuel assembly designs.

The profile sample set numbers and associated index values are illustrated in Table 31 for profile set three. And the calculated limiting profile factors are provided in Table 32.

Burnup Range (GWd/MTU) Index<sup>a</sup> Ν Notes 130 All nodes not normally distributed 10 ≤ x < 15 3 All nodes not normally distributed 301 9 15 ≤ x < 20 20 ≤ x < 25 214 5 All nodes not normally distributed  $25 \le x \le 30$ 161 3 All nodes not normally distributed 199 All nodes not normally distributed  $30 \le x < 35$ 4  $35 \le x < 40$ 141 3 All nodes not normally distributed 40 ≤ x < 45 61 1 Nodes 2 and 5 normally distributed, all others distribution-free 42<sup>b</sup> 1 Nodes 2 and 5 normally distributed, all others distribution-free 45 ≤ x

#### Table 31. Profile Set Three Sample Population Indices

NOTES: <sup>a</sup> Indices were interpolated from Natrella (1963, Table A-31)

<sup>b</sup> Sample size was insufficient for 95/95 confidence level. Sample size of 42 provides 62.4 percent confidence that 95 percent of the population is above the lowest value (Natrella 1963, Table A-32)

Table 32. Seven-Node Limiting Axial Profiles by Burnup Group for Profile Set Three

	Group 1 <sup>b</sup>	Group 2 <sup>b</sup>	Group 3 <sup>b</sup>	Group 4 <sup>b</sup>	Group 5 <sup>♭</sup>	Group 6 <sup>b</sup>	Group 7 <sup>b</sup>	Group 8 <sup>b</sup>
Axial Pos. <sup>a</sup>	10 ≤ x < 15	15 ≤ x < 20	20 ≤ x < 25	25 ≤ x < 30	30 ≤ x < 35	35 ≤ x < 40	40 ≤ x < 45	45 ≤ x
0.028	0.497	0.554	0.525	0.587	0.599	0.619	0.635	0.640
0.083	0.837	0.882	0.882	0.903	0.907	0.914	0.923	0.926
0.139	1.009	1.021	0.986	1.016	1.028	1.027	1.024	1.023
0.194 – 0.806	1.150	1.126	1.122	1.113	1.104	1.094	1.094	1.086
0.861	0.859	0.920	0.934	0.950	0.971	0.988	0.991	0.998
0.917	0.664	0.694	0.766	0.738	0.778	0.822	0.800	0.841
0.972	0.333	0.416	0.440	0.454	0.471	0.506	0.502	0.541

NOTES: <sup>a</sup> Axial Pos. is percent of core height from bottom to top <sup>b</sup> Burnup ranges are in units of GWd/MTU

For comparative purposes, mean profiles were determined from the profile set three-database assemblies and are provided in Table 33.

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	Group 1 <sup>♭</sup>	Group 2 <sup>b</sup>	Group 3 <sup>b</sup>	Group 4 <sup>b</sup>	Group 5 <sup>b</sup>	Group 6 <sup>b</sup>	Group 7 <sup>b</sup>	Group 8 <sup>b</sup>
Axial Pos. <sup>a</sup>	10 ≤ x < 15	15 ≤ x < 20	20 ≤ x < 25	25 ≤ x < 30	30 ≤ x < 35	35 ≤ x < 40	40 ≤ x < 45	45 ≤ x
0.028	0.594	0.630	0.630	0.634	0.642	0.658	0.673	0.692
0.083	0.929	0.932	0.935	0.933	0.933	0.935	0.942	0.946
0.139	1.069	1.057	1.055	1.050	1.046	1.043	1.043	1.040
0.194	1.099	1.092	1.086	1.083	1.081	1.077	1.074	1.069
0.25	1.096	1.096	1.088	1.086	1.089	1.085	1.082	1.076
0.306	1.090	1.091	1.082	1.081	1.087	1.084	1.082	1.076
0.361	1.086	1.085	1.077	1.076	1.082	1.078	1.076	1.072
0.417	1.092	1.083	1.078	1.076	1.079	1.073	1.072	1.067
0.472	1.101	1.085	1.082	1.078	1.078	1.071	1.070	1.066
0.528	1.110	1.088	1.087	1.083	1.078	1.071	1.069	1.065
0.583	1.115	1.091	1.092	1.087	1.080	1.072	1.069	1.065
0.639	1.115	1.093	1.094	1.090	1.081	1.074	1.069	1.065
0.694	1.110	1.090	1.092	1.089	1.080	1.074	1.069	1.064
0.75	1.093	1.079	1.083	1.081	1.073	1.068	1.064	1.060
0.806	1.054	1.052	1.058	1.060	1.055	1.053	1.051	1.049
0.861	0.969	0.986	0.993	1.000	1.003	1.006	1.008	1.011
0.917	0.793	0.832	0.842	0.853	0.865	0.880	0.883	0.894
0.972	0.486	0.537	0.549	0.560	0.570	0.597	0.605	0.623

Table 33. 18 Node Mean Axial Profiles by Burnup Group for Profile Set Three

NOTES: <sup>a</sup> Axial Pos. is percent of core height from bottom to top <sup>b</sup> Burnup ranges are in units of GWd/MTU



Figure 30. Burnup Group One ( $10 \le x < 15$ ) Profile Set Three Profiles

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Axial Height Fraction
7 Node Bounding — 18 Node Mean

Figure 31. Burnup Group Two ( $15 \le x < 20$ ) Profile Set Three Profiles



Figure 32. Burnup Group Three ( $20 \le x < 25$ ) Profile Set Three Profiles

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Figure 34. Burnup Group Five  $(30 \le x < 35)$  Profile Set Three Profiles

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Figure 36. Burnup Group Seven ( $40 \le x < 45$ ) Profile Set Three Profiles



Figure 37. Burnup Group Eight ( $45 \le x$ ) Profile Set Three Profiles

#### I.4 PROFILE SET FOUR

Profile set four was based on using only the Westinghouse 17x17 fuel assemblies from the database. The profiles used for this set are provided in a spreadsheet attachment (*profile\_set4.xls*) contained on the attachment CD (Attachment III).

The profile sample set numbers and associated index values are illustrated in Table 34 for profile set four, and the calculated limiting profile factors are provided in Table 35.

Burnup Range (GWd/MTU)	Ν	Index <sup>a</sup>	Notes
$10 \le x \le 15$	72	1	All nodes not normally distributed
15 < x ≤ 20	174	4	Node 3 normally distributed, all others distribution-free
20 < x ≤ 25	137	3	Node 5 normally distributed, all others distribution-free
25 < x ≤ 30	116	2	Nodes 2 and 5 normally distributed, all others distribution-free
30 < x ≤ 35	119	2	Nodes 3, 5, and 6 normally distributed, all others distribution- free
35 < x ≤ 40	113	2	Node 5 normally distributed, all others distribution-free
40 < x ≤ 45	99	2	Node 5 normally distributed, all others distribution-free
45 < x ≤ 50	49 <sup>b</sup>	1	Node 5 normally distributed, all others distribution-free

Table 34. Profile Set Four Sample Population Indices

NOTES: <sup>a</sup> Indices were interpolated from Natrella (1963, Table A-31)

<sup>b</sup> Sample size was insufficient for 95/95 confidence level. Sample size of 49 provides 70.8 percent confidence that 95 percent of the population is above the lowest value (Natrella 1963, Table A-32)

	Group 1 <sup>b</sup>	Group 2 <sup>b</sup>	Group 3 <sup>b</sup>	Group 4 <sup>b</sup>	Group 5 <sup>b</sup>	Group 6 <sup>b</sup>	Group 7 <sup>b</sup>	Group 8 <sup>b</sup>
Axial Pos. <sup>a</sup>	10 ≤ x ≤ 15	15 < x ≤ 20	20 < x ≤ 25	25 < x ≤ 30	30 < x ≤ 35	35 < x ≤ 40	40 < x ≤ 45	45 < x ≤ 50
0.028	0.266	0.285	0.291	0.311	0.558	0.309	0.316	0.327
0.083	0.846	0.859	0.885	0.901	0.912	0.912	0.917	0.917
0.139	1.024	1.031	1.018	1.027	1.028	1.026	1.032	1.032
0.194 – 0.806	1.182	1.166	1.155	1.147	1.099	1.143	1.139	1.139
0.861	0.880	0.906	0.957	0.961	0.974	0.980	0.984	0.983
0.917	0.575	0.691	0.747	0.778	0.835	0.799	0.813	0.800
0.972	0.225	0.229	0.243	0.260	0.508	0.260	0.273	0.269

Table 35. Seven-Node Limiting Axial Profiles by Burnup Group for Profile Set Four

NOTES: <sup>a</sup> Axial Pos. is percent of core height from bottom to top <sup>b</sup> Burnup ranges are in units of GWd/MTU

For comparative purposes, mean profiles were determined from the profile set four-database assemblies and are provided in Table 36.

	Group 1 <sup>♭</sup>	Group 2 <sup>b</sup>	Group 3 <sup>b</sup>	Group 4 <sup>b</sup>	Group 5 <sup>b</sup>	Group 6 <sup>b</sup>	Group 7 <sup>b</sup>	Group 8 <sup>b</sup>
Axial Pos. <sup>a</sup>	10 ≤ x ≤ 15	15 < x ≤ 20	20 < x ≤ 25	25 < x ≤ 30	30 < x ≤ 35	35 < x ≤ 40	40 < x ≤ 45	45 < x ≤ 50
0.028	0.567	0.627	0.633	0.606	0.666	0.643	0.643	0.596
0.083	0.897	0.932	0.943	0.933	0.939	0.941	0.944	0.942
0.139	1.055	1.062	1.060	1.056	1.050	1.052	1.054	1.059
0.194	1.103	1.098	1.088	1.090	1.076	1.078	1.078	1.086
0.25	1.140	1.115	1.104	1.104	1.087	1.090	1.089	1.098
0.306	1.127	1.108	1.093	1.098	1.082	1.084	1.083	1.091
0.361	1.139	1.109	1.097	1.100	1.084	1.087	1.086	1.094
0.417	1.134	1.104	1.093	1.096	1.082	1.084	1.083	1.091
0.472	1.115	1.094	1.081	1.087	1.076	1.077	1.076	1.083
0.528	1.122	1.095	1.085	1.090	1.078	1.080	1.079	1.086
0.583	1.105	1.086	1.075	1.083	1.072	1.074	1.073	1.080
0.639	1.104	1.083	1.076	1.082	1.072	1.074	1.072	1.078
0.694	1.097	1.077	1.073	1.079	1.070	1.073	1.070	1.077
0.75	1.067	1.058	1.059	1.066	1.059	1.062	1.059	1.065
0.806	1.036	1.034	1.043	1.048	1.045	1.049	1.047	1.053
0.861	0.946	0.966	0.986	0.987	0.996	0.999	1.000	1.002
0.917	0.765	0.813	0.844	0.843	0.865	0.867	0.871	0.868
0.972	0.477	0.536	0.562	0.540	0.602	0.585	0.591	0.552

Table 36. 18 Node Mean Axial Profiles by Burnup Group for Profile Set Four

NOTES: <sup>a</sup> Axial Pos. is percent of core height from bottom to top <sup>b</sup> Burnup ranges are in units of GWd/MTU Page I-21 of 25

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Figure 38. Burnup Group One ( $10 \le x < 15$ ) Profile Set Four Profiles



Figure 39. Burnup Group Two ( $15 \le x < 20$ ) Profile Set Four Profiles





Figure 40. Burnup Group Three ( $20 \le x < 25$ ) Profile Set Four Profiles



Figure 41. Burnup Group Four ( $25 \le x < 30$ ) Profile Set Four Profiles



Figure 42. Burnup Group Five  $(30 \le x < 35)$  Profile Set Four Profiles



Figure 43. Burnup Group Six ( $35 \le x < 40$ ) Profile Set Four Profiles

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Figure 44. Burnup Group Seven ( $40 \le x < 45$ ) Profile Set Four Profiles



Figure 45. Burnup Group Eight ( $45 \le x$ ) Profile Set Four Profiles

# Attachment II: Attachment CD File Listing

This attachment contains a listing and description of the files contained on the attachment CD of this report (Attachment III). The CD was written using ROXIO Easy CD Creator 5 Basic installed on CRWMS M&O tag number 150527 central processing unit, and can be viewed on most standard CD-ROM drives. The zip archive was created using WINZIP 8.1. The file attributes on the CD are as follows:

<u>Filename</u>	<u>File Size (bytes)</u>	File Date	<u>File Time</u>	Description
21PWRWP.pdf <sup>a</sup>	447,274	9/16/2003	08:15a	Preliminary drawing of Repository Design Waste Package Project 21-PWR Waste Package with Absorber Plates
cases.zip	269,093,276	9/17/2003	01:45p	Archive containing SCALE, MCNP, and FT71V01 files
profile_set1.xls	7,458,816	9/12/2003	01:35p	Excel spreadsheet containing profile set 1 information
profile_set2.xls	6,194,176	9/12/2003	10:58a	Excel spreadsheet containing profile set 2 information
profile_set3.xls	2,114,048	9/12/2003	11:10a	Excel spreadsheet containing profile set 3 information
profile_set4.xls	1,520,640	9/15/2003	08:49a	Excel spreadsheet containing profile set 4 information

Note: <sup>a</sup> Drawing is taken from BSC 2003, which states to use BSC 2001b

There are 34,434 total files (not including folders) contained in a unique directory structure for the archive file. The following extracted directory structure corresponds as follows:

/Documents and Settings/scaglionej/My Documents/PWR Axial Profile/temp/\*: where \* is designated SAS or MCNP to indicate which files are contained within the respective directory

A) Within the SAS directory the naming system is /Nominal/\* where \* is as follows:

1_Node	Indicates single node cases
Profile_Set_1	Indicates cases using Profile Set 1 information
Profile_Set_2	Indicates cases using Profile Set 2 information
Profile_Set_3	Indicates cases using Profile Set 3 information

Within the *1\_Node* subdirectory are folders that use a *X.XatYY* naming system where the X.X represents the initial enrichment in terms of wt% U-235 and YY represents the burnup in terms of GWd/MTU.

Within the *Profile\_Set\_1, 2*, or 3 subdirectories there are folders named 7\_*Node* and 18\_*Node* representing files based on a 7 or 18 axial node representation, respectively.

Within the 7\_*Node* and 18\_*Node* subdirectories, the naming system of the folders follows that of the 1\_*Node* naming system given previously.

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B) Within the MCNP directory are two folders labeled No\_Basket\_Absorber and Nominal

Within the *No\_Basket\_Absorber* subdirectory are folders labeled *1\_Node* and 7\_*Node* corresponding to cases using the single axial fuel node representation or the 7 axial fuel node representation.

Within the Nominal subdirectory are folders labeled as follows:

1_Node	Indicates single node cases
Profile_Set_1	Indicates cases using Profile Set 1 information
Profile_Set_2	Indicates cases using Profile Set 2 information
Profile_Set_3	Indicates cases using Profile Set 3 information

Within the *Profile\_Set\_1, 2,* or 3 subdirectories are folders named 7\_*Node* and 18\_*Node* representing files based on a 7 or 18 axial node representation, respectively.

Upon file extraction, the file naming system corresponds as follows:

#### SAS2H Cases

 $N^*$ .*inp* files are the SAS2H input files, where the  $N^*$  represents the corresponding fuel node (i.e., a number from 1 to 18).

 $N^*.msgs$  files are generated by SAS2H and contain the standard run-time messages associated with the SAS2H calculations, where the  $N^*$  represents the corresponding fuel node (i.e., a number from 1 to 18).

 $N^*.log$  contains an echo of the input and pertinent information extracted from the SAS2H output file prior to discarding, to indicate that the case ran successfully. The  $N^*$  represents the corresponding fuel node (i.e., a number from 1 to 18).

 $ft71f001.N^*$  files are binary files generated by ORIGEN-S for each time step, which were retained, that contain the isotopic concentrations as a function of time. The  $N^*$  represents the corresponding fuel node (i.e., a number from 1 to 18).

ft71-case\*.N\* files are the ASCII files generated by the FT71V01 software for each case and node, where the N\* represents the corresponding fuel node (i.e., a number from 1 to 18) and the case\* represents a particular decay time as listed in Table II-1.

Case #	01	02	03	04	05	06	07	08	09
Decay Time (yrs)	0	5	10	33	100	333	1,000	3,333	5,000
Case #	10	11	12	13	14	15	16	17	18
Decay Time (yrs)	10,000	11,000	12,000	13,000	14,000	15,000	16,000	18,000	20,000
Case #	19	20	21	22	23	24	25	26	
Decay Time (vrs)	22.500	25.000	27.500	30.000	35.000	50.000	75.000	100.000	

Table II-1. Case # and Decay Time Relationships

#### **MCNP** Cases

The extracted MCNP cases have a naming system as E.EBBN where the E.E represents the initial fuel enrichment in wt% U-235 (range from 3.0 to 5.0), the BB represents the burnup in GWd/MTU (range from 10 to 50), and N represents the number of fuel nodes represented (1, 7, or 18). Files without on "o" at the end are input files, and files with an "o" at the end are output files.

## Calculation

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