OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
CALCULATION COVER SHEET

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9. Remarks

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1. PURPOSE

The objective of this calculation is to compute gamma and neutron dose rates in order to determine the maximum radiolytic production of nitric acid and other chemical species inside the 21-PWR (pressurized-water reactor) waste package (WP). The scope of this calculation is limited to the time period between 5,000 and 100,000 years after emplacement. The information provided by the sketches attached to this calculation is that of the potential design for the type of WP considered in this calculation.

The results of this calculation will be used to evaluate nitric acid corrosion of fuel cladding from radiolysis in the 21-PWR WP. This calculation was performed in accordance with the *Technical Work Plan for: Waste Package Design Description for LA* (Civilian Radioactive Waste Management System (CRWMS) Management and Operating Contractor (M&O) 2000a). AP-3.12Q, *Calculations*, is used to perform the calculation and develop the document. This calculation is associated with the total system performance assessment (TSPA) of which the spent fuel cladding integrity is to be evaluated.

2. METHOD

The integrity of the cladding material of PWR spent nuclear fuel (SNF) is one of the issues of the TSPA for the site recommendation (SR) study. It is recognized that chemical species produced by ionizing radiation (radiolysis) can have adverse effect on the fuel cladding by nitric acid corrosion. Nitric acid is produced in an irradiated air-water vapor system when the hydroxyl radicals, generated from water vapor, convert nitrogen dioxides, formed by radiolytic reaction between nitrogen and oxygen, to nitric acids. Prior to waste package failure, radiolysis effect is insignificant because of the absence of water and air in the waste package. Therefore, it is only after waste package failure that radiation-enhanced corrosion of fuel cladding can occur. Typically, the time of waste package failure is expected to be 10,000 years or more after emplacement.

Although radiolytic production of individual chemical species depends on the radiation environment, the chemical components present, and the physical conditions of the environment (temperature, pressure, and relative humidity), the yield of a chemical species is characterized by a single parameter, G value (Reed and Van Konyneburg, 1991). The G value represents the number of molecules of a chemical species produced per 100 eV of radiation energy absorbed in the ambient environment; it has the dimensions of (molecules/100 eV).

In this calculation, it is assumed that the 21-PWR waste package has failed, and air and water are present for the time period between 10,000 and 100,000 years after emplacement (Assumption 3.1). For the failed waste package, the maximum amount of nitric acid production is determined by the total radiation dose absorbed by the moist air in the waste package. For the 21-PWR WP loaded with the average SNF (Assumption 3.2), the dose rates outside the fuel rods are calculated at time steps within this time period. Then, the rate of nitric acid production is determined for each time step based on the dose rate and the G value of unity. Finally, the total maximum amount of nitric acid production between 10,000 to 100,000 years is obtained by integrating the production rates over this time period. The average PWR SNF has the following characteristics: 4.0-wt% initial ^{235}U, 48-GWd/MTU burnup, and 21-year decay time (Assumption 3.2).

Scoping dose rate calculations is performed for a PWR fuel rod using a one-dimensional cylindrical geometry of the SAS1 module of the SCALE code system (Oak Ridge National Laboratory (ORNL) 1997). Then, three-dimensional Monte Carlo calculations of the dose rates inside the 21-PWR WP for time steps between 5,000 to 100,000 years are carried out using the MCNP program (Briesmeister 1997).

All electronic data are stored on unrewritable compact disk(s) and the control of the electronic management of data is accomplished in accordance with the methods specified in the *Technical Work Plan for: Waste Package Design Description for LA* (CRWMS M&O 2000a).

3. ASSUMPTIONS

3.1 The 21-PWR WP is assumed to fail, and air and water are present in the WP for the time period between 10,000 and 100,000 years after emplacement. The rational for this assumption is that air and water must be present for radiolysis to take place and that the earliest possible first breach time for a waste package is about 10,000 years (CRWMS M&O 2000c, p. 80). This assumption is used in Section 5.

3.2 The PWR SNF having 4.0-wt% initial ^{235}U, 48-GWd/MTU burnup, and 21-year decay time is assumed to be the SNF with average characteristics. The rational for this assumption is that the source term for the SNF with these characteristics generates conservative (higher) radiation dose rates for an average PWR SNF (CRWMS M&O 2000b, Assumption 3.2). This assumption is used in Section 5.

3.3 The chemical composition of the SNF is assumed to be the same as that of the fresh fuel. The rational for this assumption is that small weight variations of the elements do not affect the accuracy of the gamma dose results, as long as the total weight is maintained. Also, using fresh fuel for SNF results in conservative (higher) neutron dose rates. This assumption is used in Section 5.

3.4 The non-fuel material compositions used in this calculation have elements with allowable ranges of weight percentages. For elements with weight percent range, the midpoint value is used, and the weight percent of the most abundant element is adjusted. The rationale for this assumption is that small weight variations for the affected elements do not affect the accuracy of dose results, as long as the total weight is maintained. This assumption is used throughout Section 5.

3.5 The basket assembly, the trunnion collar sleeves, the extended outer shell lid, the lifting features of the upper shell lids, and the bottom support ring in the 21-PWR WP are not included in the geometry of the MCNP calculations. The rational for this assumption is that excluding the basket assembly and the components yields higher (conservative) radiation dose rate. This assumption is used in Section 5.

3.6 For each PWR SNF assembly, the following items in the active fuel region are not included in the MCNP calculations: the guide tubes, instrument tube, incore-spacers, and grid supports. The rational for this assumption is the same as that for Assumption 3.5. This assumption is used in Section 5.

3.7 For each PWR SNF assembly, the materials in each of the following regions are homogenized within the lateral boundaries of the assembly: the plenum region, top end-fitting region, and bottom end-fitting region. The rational for this assumption is that the study of source geometry effect (CRWMS M&O 1998b) on the surface dose rates for a 21-PWR WP has shown that the detailed representation of each assembly and each assemblies homogenized inside its transverse dimensions give essentially the same results. This assumption is used in Section 5.

3.8 It is assumed that the temperature and pressure inside the failed 21-PWR WP for the time period between 10,000 and 100,000 years are 25 °C and one atmosphere, respectively. The rational for this assumption is that the density of moist air in the WP is needed to calculate the energy absorbed in moist air for radiolysis evaluation. Since the density of moist air is inversely proportional to the temperature, the assumed ambient temperature of 25 °C would yield higher absorbed energy, and provide more conservative (higher) radiolysis effect. This assumption is used in Section 5.5.

3.9 It is assumed that the entire cavity within the active fuel region of the WP is subjected to the same radiation dose rate as the space in each fuel cell. The rational for this assumption is that for the purpose of evaluating radiolysis effects this assumption will lead to higher (more conservative) nitric acid production within the WP. This assumption is used in Section 5.5.

3.10 It is assumed that the G value for nitrogen dioxide production by gamma radiation is 1.5 molecules/100 eV. The rational for this assumption is that the G values between 0.5 to 1.5 molecules/100 eV have been observed in the long-term and lower dose rate gamma studies (Reed and Van Konynenburg 1991, p. 1399). Since this calculation is for long-term and low gamma irradiation conditions, G value of 1.5 is conservative by producing the highest of nitric acid. This assumption is used in Section 5.5.

3.11 It is assumed that the internal configuration of the 21-PWR WP remains intact for the time period between 5,000 and 100,000 years after emplacement. The rational for this assumption is that the intact configuration leads to higher (conservative) radiolytic production of chemical species due to higher dose rate in the moist air in the WP. This assumption is used in Section 5.5.

4. USE OF COMPUTER SOFTWARE AND MODELS

4.1 SOFTWARE

4.1.1 SCALE 4.3

The SAS1 analysis sequence of the SCALE 4.3 computer code system is used to calculate neutron and gamma fluxes on the surface of a fuel rod for dose rate evaluation.

- Program Name: SCALE
- Version/Revision number: Version 4.3 (addendum)
- Computer Software Configuration Item (CSCI) Number: 30011 V4.3 (addendum) (CRWMS M&O 1997a and CRWMS M&O 1999a)
- Computer Type: HP 9000/700 Series workstation
- This software was previously obtained from Software Configuration Management (SCM) in accordance with appropriate procedures
- Computer Processing Unit Name and Yucca Mountain Project (YMP) Tag Number: 'Bloom,' YMP Tag 700887.

The SAS1 sequence of the SCALE 4.3 computer code system is an appropriate tool to determine the dose rate on and near the side of a cylindrical body. The software is appropriate to estimate the dose rate outside a fuel rod and is used within the range of validation as described in the qualification document.

The input file for each computer calculation is echoed in the output file of the calculation. The output files are described in Section 8.

4.1.2 MCNP 4B2LV

The MCNP 4B2LV computer code is used to calculate gamma fluxes inside the WP for dose rate evaluations. The software is appropriate to determine the dose rate within a waste package and is used within the range of validation as described in the qualification document.

- Program Name: MCNP
- Version/Revision number: Version 4B2
- CSCI Number: 30033 V4B2LV (CRWMS M&O 1998a)
- Computer Type: HP 9000/700 Series workstation
- This software was previously obtained from SCM in accordance with appropriate procedures
- Computer Processing Unit Name and YMP Tag Number: 'Bloom,' YMP Tag 700887.

The input file for each computer calculation is echoed in the output file of the calculation. The output files are described in Section 8.

4.1.3 MICROSOFT EXCEL 97 SR-2

Microsoft EXCEL 97 SR-2 was used for graphic representation and simple arithmetical manipulations in this document. Microsoft EXCEL 97 SR-2 is exempt software application in accordance with AP-SI.1Q, Section 2.1.

4.2 MODELS

No models are used in this calculation.

5. CALCULATION

This section provides the radiation source terms, the geometry of the 21-PWR WP, and the chemical compositions of the materials used in the SAS1 and MCNP calculations. The WP consists of the 21-PWR disposal container, 21 PWR SNF assemblies, and a basket assembly. Sketch SK-0175 REV 02 that is included in Attachment I describes the geometry and material specifications of the 21-PWR disposal container.

The number of digits in the values cited herein may be the result of a calculation or may reflect the input from another source; consequently, the number of digits should not be interpreted as an indication of accuracy.

5.1 21-PWR DISPOSAL CONTAINER

The 21-PWR disposal container primary consists of an inner reinforcement cylindrical shell, an outer shell, top and bottom inner shell lids, a bottom outer-shell lid, two top outer shell lids, upper and lower trunnion collar sleeves, and the basket assembly. The details of geometry and material specifications of the 21-PWR disposal container are described in sketch SK-0175 REV 02. The basket assembly, the trunnion collar sleeves, the extended outer shell lid, the extended lid reinforcement ring, the lifting features of the upper shell lids, and the bottom support ring are not represented in the MCNP calculations (Assumption 3.5). Table 1 presents the geometry and material specifications of the 21-PWR disposal container that are represented in the MCNP calculations.

The chemical compositions and the associated atom densities of SB-575 N06022 and SA-240 S31600 are given in Tables 2 and 3, respectively. For elements with weight percent range, the midpoint value is used, and the weight percent of the most abundant element is adjusted (Assumption 3.4).

The atom densities (AD) of the element/isotope contents, in atoms/b·cm are calculated according to the following equation:

$$\text{AD } (atoms/b \cdot cm) = \frac{\text{material density}(g/cm^3) * \text{weight fraction}_{\text{isotope}} * \text{N}_\text{A}\,(atoms/mole)}{10^{24}\,(b/cm^2) * \text{atomic mass}_{\text{isotope}}\,(g/mole)}$$

In the above equation, N_A is the Avogadro constant, whose value is 6.0221367E+23 atoms per mole (Parrington et al. 1996, page 59).

Table 1. Geometry and Material Specifications for the 21-PWR Disposal Container

Component	Material	Characteristic	Dimension (mm)
Inner shell	SA-240 S31600	Thickness	50
Top and bottom Inner lids	SA-240 S31600	Thickness	95
Outer shell	SB-575 N06022	Thickness	20
Top and bottom outer lids	SB-575 N06022	Thickness	25
Closure lid to outer lid gap	Void	Thickness	30
Closure lid	SB-575 N06022	Thickness	10
Inner lid to closure lid gap	Void	Thickness	30
Bottom outer lid to inner lid gap	Void	Thickness	70
Fuel basket tube	SA-516 K02700[a]	Thickness	5
		Inner transverse dimension	226.4
Cavity	Void	Length	4,585
		Inner diameter	1,424

NOTE: [a]Represented as void in MCNP calculations (Assumption 3.5).

Table 2. Chemical Composition of SB-575 N06022

Element[a]	Weight Percent Range[a]	Weight Percent Used	Atomic Mass[b] (g/mole)	Atom Density (atoms/b•cm)
C	0.015 (max)	0.015	12.0107	6.5357E-05
Mn	0.50 (max)	0.5	54.93805	4.7629E-04
Si	0.08 (max)	0.08	28.0855	1.4907E-04
Cr	20.00-22.50	21.25	51.9961	2.1387E-02
Mo	12.5-14.5	13.5	95.94	7.3638E-03
Co	2.50 (max)	2.5	58.9332	2.2200E-03
W	2.5-3.5	3	183.84	8.5399E-04
V	0.35 (max)	0.35	50.9415	3.5956E-04
Fe	2.0-6.0	4	55.845	3.7484E-03
P	0.02 (max)	0.02	30.97376	3.3791E-05
S	0.02 (max)	0.02	32.066	3.2640E-05
Ni	Balance	54.765	58.6934	4.8830E-02
Total		100		8.6374E-02
Density = 8.69 g/cm³				

SOURCE: [a]ASTM (American Society for Testing and Materials) B 575-97, *Standard Specification for Low-Carbon Nickel-Molybdenum-Chromium, Low-Carbon Nickel-Chromium-Molybdenum, Low-Carbon Nickel-Chromium-Molybdenum-Copper and Low-Carbon Nickel-Chromium-Molybdenum-Tungsten Alloy Plate, Sheet, and Strip,* p. 2.
[b]Parrington et al. 1996.

NOTE: SA-575 identical with ASTM Specification B 575-97 (ASME 1998, p. 759).

Table 3. Chemical Composition of SA-240 S31600

Element	Weight Percent Range[a]	Weight Percent Used	Atomic Mass[c] (g/mole)	Atom Density (atoms/b•cm)
Carbon	0.08 (max)	0.08	12.0107	3.2009E-04
Mn	2.00 (max)	2	54.93805	1.7495E-03
P	0.045 (max)	0.045	30.97376	6.9819E-05
S	0.030 (max)	0.03	32.066	4.4960E-05
Si	0.75 (max)	0.75	28.0855	1.2833E-03
Cr	16.00-18.00	17	51.9961	1.5712E-02
Ni	10.00-14.00	12	58.6934	9.8253E-03
Mo	2.00-3.00	2.5	95.94	1.2523E-03
N	0.10 (max)	0.1	14.00674	3.4310E-04
Fe	Balance	65.495	55.845	5.6361E-02
Total		100		8.6961E-02
Density[b] = 7.98 g/cm^3				

SOURCE: [a] ASTM A 240/A 240M-97a, *Standard Specification for Heat-Resisting Chromium and Chromium-Nickel Stainless Steel Plate, Sheet, and Strip for Pressure Vessels*, p. 2.
[b] ASTM G 1-90, *Standard Practice for Preparing, Cleaning, and Evaluating Corrosion Test Specimens*, p. 7.
[c]Parrington et al. 1996.
NOTE: SA-240 identical with ASTM Specification A 240-97a (ASME 1998, p. 363).

5.2 PWR SNF ASSEMBLIES

The PWR SNF assembly used in this calculation is a Babcock and Wilcox (B&W) 15x15 PWR SNF assembly. The mechanical design parameters for a B&W 15x15 PWR fuel assembly are obtained from (CRWMS M&O 2000b, Table 7). Table 4 presents these parameters.

Fresh fuel is assumed for the PWR SNF (Assumption 3.3). To be consistent with the values used in the source term calculations, the mass of uranium and uranium dioxide for each assembly are obtained from CRWMS M&O (1999, Attachment I, p. I-1) instead of using the values in Table 4. The composition of fresh fuel is presented in Table 5. The composition of Zircalloy-4 is given in Table 6. For elements with weight percent range, the midpoint value is used, and the weight percent of the most abundant element is adjusted (Assumption 3.4).

In MCNP calculations, each PWR SNF assembly axially consists of four regions: the bottom end-fitting region, active fuel region, plenum region, and top end-fitting region. Except for the active fuel region, each assembly region is homogenized inside its volume (see Figures 1 through 3), resulting in a uniform distribution of the region contents inside each region volume (Assumption 3.7). For the active fuel region, the content of each cell in the assembly is represented explicitly, but the guide tubes, instrument tube, incore-spacers, and grid supports are not included (Assumption 3.6). The chemical compositions and the associated atomic densities of the three non-fuel regions of each PWR assembly are obtained from CRWMS M&O (2000b, Attachment II) and presented in Tables 7, 8, and 9.

Table 4. Mechanical Design Parameters of B&W 15x15 Mark B Fuel Assembly[a]

Design Component	Material	Zone	Characteristic	Value
Assembly	N/A (Not Applicable)	N/A	Width	8.536 in. (21.68144 cm)
			Length	165.625 in. (420.6875 cm)
Fuel pin	N/A	In core	Number per assembly	208
			Length	153.68 in. (390.3472 cm)
Fuel pellets	UO_2	Active fuel	Mass/pin	5.58 lb. (2.53105 kg)
			Mass U/assembly	0.46363 metric tons
			Diameter	0.3686 in. (0.93624 cm)
			Stack length	141.8 in. (360.172 cm)
Cladding	Zircaloy-4	In core	Thickness	0.0265 in. (0.06731 cm)
			Fuel-clad gap	0.0042 in. (0.010668 cm)
Top nozzle	SS CF3M	Top	Mass/assembly	7.48 kg
Bottom nozzle	SS CF3M	Bottom	Mass/assembly	8.16 kg
Guide tube	Zircaloy-4	In core	Mass/assembly	8.0 kg
Instrument tube	Zircaloy-4	In core	Mass/assembly	0.64 kg
Spacer-plenum	Inconel-718	Plenum	Mass/assembly	1.04 kg
Spacer-bottom	Inconel-718	Bottom	Mass/assembly	1.3 kg
Spacer-incore	Inconel-718	In core	Mass/assembly	4.9 kg
Spring retainer	SS CF3M	Top	Mass/assembly	0.91 kg
Holding spring	Inconel-718	Top	Mass/assembly	1.8 kg
Upper end plug	SS 304	Top	Mass/assembly	0.06 kg
Upper nut	SS 304L	Top	Mass/assembly	0.51 kg
Lower nut	SS 304	Bottom	Mass/assembly	0.15 kg
Grid supports	Zircaloy-4	In core	Mass/assembly	0.64 kg
Plenum spring	SS 302	Plenum	Mass/assembly	0.042 lb. (0.01905 kg)
Plenum region	-	-	Length[b]	30.1752 cm
Bottom end-fitting	-	-	Length[c]	4 in. (10.16 cm)

SOURCE: [a]CRWMS M&O 2000b, Table 7.
NOTES: [b]Calculated: fuel pin length – fuel pellet length = 390.3472 cm – 360.172 cm.
[c]A bottom end-fitting region of 4-in. length provides conservative (higher) dose rates for bottom region of the WP.

Table 5. Chemical Composition of Fresh PWR Fuel

Isotope	Isotopic Mass[a] (g/mole)	Wt% of U[b]	Wt. Portion of UO_2	Wt. Fraction of UO_2	Atom Density (atoms/b•cm)
U-235	235.043922	4.0000	0.0400	0.0352	9.4426E-04
U-234	234.040945	0.0347	0.0003	0.0003	8.2334E-06
U-236	236.045561	0.0184	0.0002	0.0002	4.3252E-06
U-238	238.050785	95.9469	0.9595	0.8443	2.2364E-02
O	15.9994	-	0.1364	0.1200	4.7289E-02
Total	-	-	1.1364[c]	1.0000	7.0609E-02
Density[d] = 10.47 g/cm^3					

SOURCE: [a]Parrington et al. 1996.
[b]CRWMS M&O 2000b, Table II-5.
[c]CRWMS M&O 1999b, Attachment I, p. I-1. Mass of UO_2/mass of U = 539.77/475 = 1.1364.
[d]CRWMS M&O 1999b, Attachment I, p. I-1.

Table 6. Chemical Composition of Zircalloy-4

Element	Weight Percent Range[a]	Weight Percent Used	Atomic Mass[c] (g/mole)	Atom Density (atoms/b•cm)
Sn	1.20-1.70	1.45	118.71	4.8254E-04
Fe	0.18-0.24	0.21	55.845	1.4856E-04
Cr	0.07-0.13	0.115	51.9961	8.7374E-05
O	0.09-0.16	0.125	15.9994	3.0865E-04
Fe + Cr	0.28-0.37	0.325	-	-
Zr	Balance	98.1	91.224	4.2483E-02
Total	-	100	-	4.3510E-02
Density[b] = 6.56 g/cm^3				

SOURCE: [a]ASTM B 811-90, *Standard Specification for Wrought Zirconium Alloy Seamless Tubes for Nuclear Reactor Fuel Cladding,* Table 2.
[b]ASM International 1990, p. 666.
[c]Parrington et al. 1996.

Table 7. Chemical Composition of the Bottom End-Fitting Region[a]

Element/Isotope	Mass (g)	Nuclide Identification[c]	Atomic Mass[b] (g/mole)	Atom Density (atoms/b•cm)
C	3.608	6000.01p	12.0107	3.7877E-05
Mn	129.95	25055.01p	54.93805	2.9825E-04
P	0.2625	15031.01p	30.97376	1.0686E-06
S	0.24	16000.01p	32.066	9.4373E-07
Si	169.25	14000.01p	28.0855	7.5985E-04
Cr	1825.9	24000.01p	51.9961	4.4278E-03
Ni	1499.375	28000.01p	58.6934	3.2211E-03
N	0.15	7014.01p	14.003074	1.3507E-06
Fe	5635.8115	26000.01p	55.845	1.2725E-02
Mo	243.65	42000.01p	95.94	3.2022E-04
Nb	66.625	41093.01p	92.90638	9.0422E-05
Ti	11.7	22000.01p	47.867	3.0820E-05
Al	6.5	13027.01p	26.98154	3.0376E-05
Co	13	27059.01p	58.9332	2.7814E-05
Cu	3.9	29000.01p	63.546	7.7385E-06
B	0.078	N/A	10.811	9.0972E-07
^{10}B (19.9 at%)	N/A	5010.01p	N/A	1.8103E-07
^{11}B (80.1 at%)	N/A	5011.01p	N/A	7.2869E-07
Total	9610	N/A	N/A	2.1981E-02

SOURCE: [a]CRWMS M&O 2000b, Attachment II, Table II-3.
[b]Parrington et al. 1996.
[c]Briesmeister 1997, Appendix G.

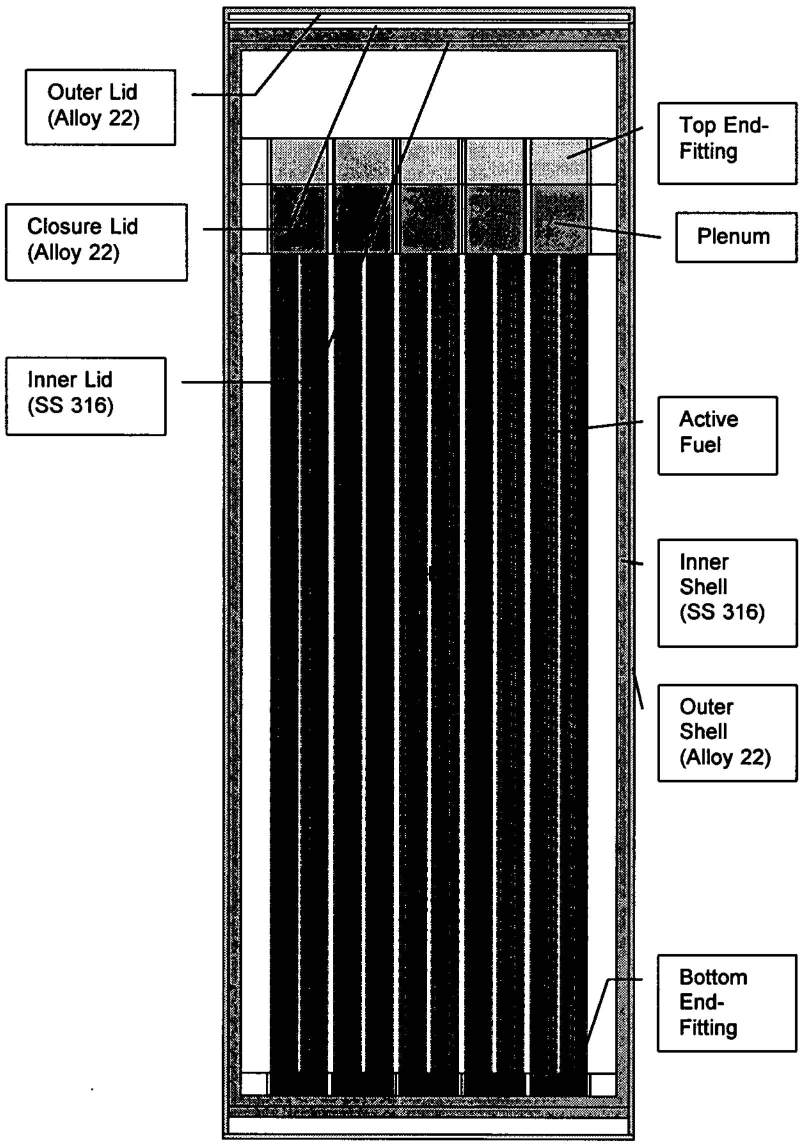

Figure 1. Source Region Representation in MCNP Calculations

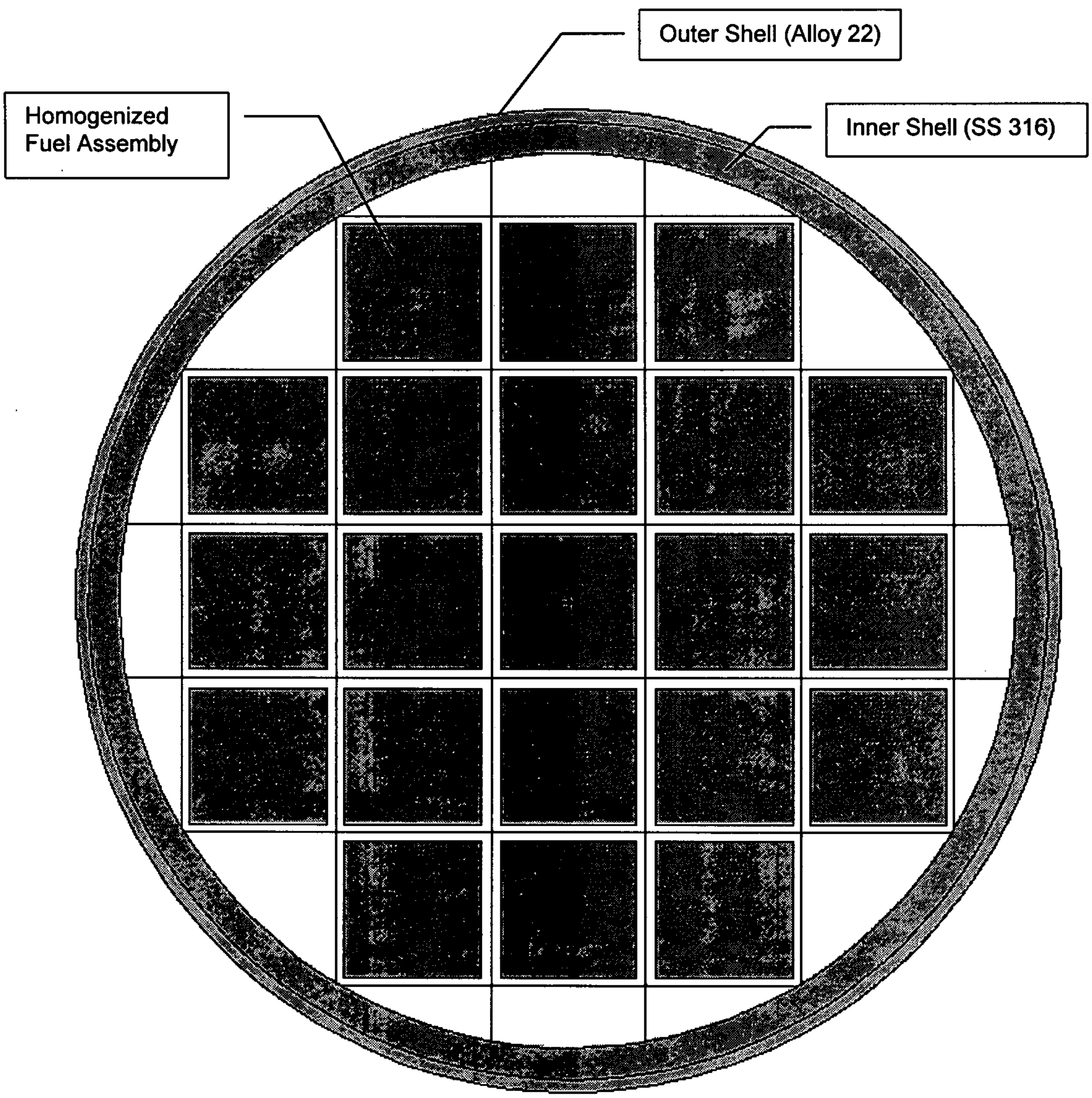

Figure 2. Lateral View of the WP Plenum Region in MCNP Calculations

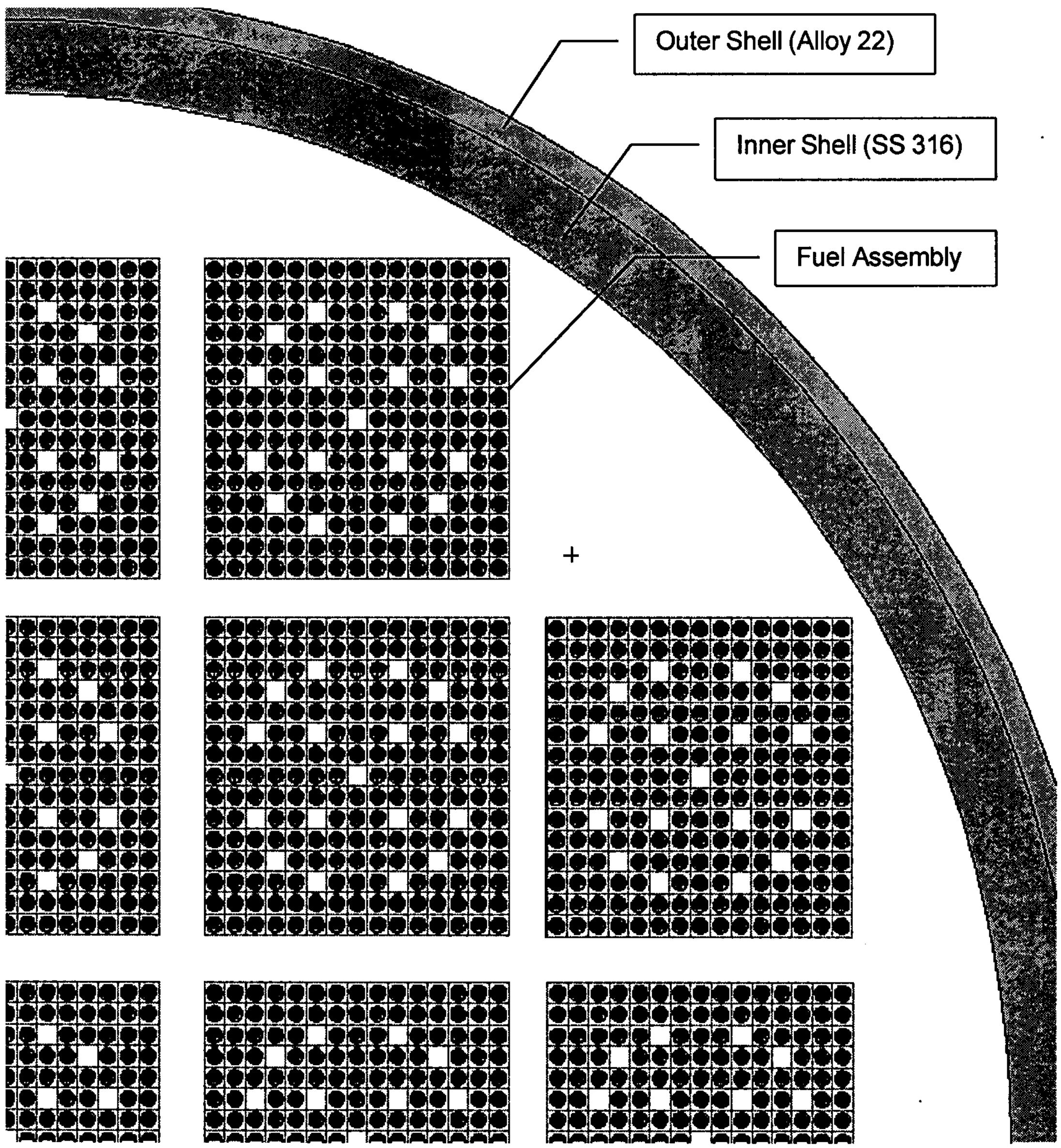

Figure 3. Partial Lateral View of the WP Active Fuel Region in MCNP Calculations

Table 8. Chemical Composition of the Plenum Region[a]

Element/Isotope	Mass (g)	Nuclide Identification[c]	Atomic Mass[b] (g/mole)	Atom Density (atoms/b•cm)
Ni	537.3145	28000.01p	58.6934	3.8865E-04
Cr	241.79133	24000.01p	51.9961	1.9742E-04
Fe	218.6757	26000.01p	55.845	1.6624E-04
Nb	53.3	41093.01p	92.90638	2.4356E-05
Mo	31.72	42000.01p	95.94	1.4036E-05
Ti	9.36	22000.01p	47.867	8.3016E-06
Al	5.2	13027.01p	26.981538	8.1820E-06
Co	10.4	27059.01p	58.9332	7.4920E-06
Mn	4.021	25055.01p	54.938049	3.1073E-06
Si	3.782875	14000.01p	28.0855	5.7183E-06
Cu	3.12	29000.01p	63.546	2.0844E-06
C	0.860575	6000.01p	12.0107	3.0419E-06
S	0.161715	16000.01p	32.066	2.1411E-07
P	0.1645725	15031.01p	30.973761	2.2557E-07
B	0.0624	N/A	10.811	2.4504E-07
^{10}B (19.9 at%)	N/A	5010.01p	N/A	4.8764E-08
^{11}B (80.1 at%)	N/A	5011.01p	N/A	3.9060E-08
Sn	139.0715	50000.01p	118.71	4.9736E-05
O	11.988922	8016.01p	15.994915	3.1822E-05
Zr	9379.1735	40000.01p	91.224	4.3650E-03
N	0.01905	7014.01p	14.003074	5.7741E-08
Total	N/A	N/A	N/A	5.2757E-03

SOURCE: [a]CRWMS M&O 2000b, Attachment II, Table II-10.
[b]Parrington et al. 1996.
[c]Briesmeister 1997, Appendix G.

Table 9. Chemical Composition of the Top End-Fitting Region[a]

Element/Isotope	Mass (g)	Nuclide Identification[c]	Atomic Mass[b] (g/mole)	Atom Density (atoms/b•cm)
C	4.158	6000.01p	12.0107	2.1977E-05
Mn	143.55	25055.01p	54.93805	1.6587E-04
P	0.5265	15031.01p	30.97376	1.0791E-06
S	0.441	16000.01p	32.066	8.7305E-07
Si	178.525	14000.01p	28.0855	4.0352E-04
Cr	2044.4	24000.01p	51.9961	2.4960E-03
Ni	1822.55	28000.01p	58.6934	1.9712E-03
N[d]	0.57	7014.01p	14.003074	2.5840E-06
Fe	6159.6715	26000.01p	55.845	7.0020E-03
Mo	264.65	42000.01p	95.94	1.7511E-04
Nb	92.25	41093.01p	92.90638	6.3033E-05
Ti	16.2	22000.01p	47.867	2.1485E-05
Al	9	13027.01p	26.98154	2.1175E-05
Co	18	27059.01p	58.9332	1.9389E-05

Cu	5.4	29000.01p	63.546	5.3945E-06
B	0.108	N/A	10.811	6.3417E-07
^{10}B (19.9 at%)	N/A	5010.01p	N/A	1.2620E-07
^{11}B (80.1 at%)	N/A	5011.01p	N/A	5.0797E-07
Total	10760	N/A	N/A	1.2371E-02

SOURCE: [a]CRWMS M&O 2000b, Attachment II, Table II-13.
[b]Parrington et al. 1996.
[c]Briesmeister 1997, Appendix G.

5.3 RADIATION SOURCES

Neutron and gamma radiation sources for the time period between 5,000 and 100,000 years are obtained from CRWMS M&O (1999b, Att. IV), and presented in Tables 10 and 11, respectively. The neutron source spectrum per assembly is presented in seven energy groups, starting from 20 MeV and descending to 0.1 MeV. The total neutron source intensity per assembly, which is the sum of the group spectrum, is also provided. The neutron source density per fuel rod is given in the last column of Table 1. The gamma source spectrum per assembly is provided in 18 energy groups, starting from 0.01 MeV and ascending to 10 MeV. The total gamma source intensity per assembly and the source density per fuel rod are also given. Finally, the total gamma source intensity in the 21-PWR WP is included in the last column of the table.

The neutron and gamma sources per fuel rod are used in the SAS1 calculations, and the total gamma source intensities per waste package are used in MCNP calculations. The neutron and gamma source intensities per volume of a fuel rod are calculated by dividing the source intensities per assembly by the number of rods in an assembly and by the volume of a fuel rod. There are 208 fuel rods in an assembly. The volume of a fuel rod is:

$$\pi D^2 H/4$$
$$= \pi (0.93624)^2(360.172)/4 \text{ cm}^3$$
$$= 247.956 \text{ cm}^3$$

Table 10. Neutron Source Spectra (n/s) of the Average PWR SNF Assembly

Age (Years)	**Upper Energy Boundary (MeV)** 2.00E+01	6.43E+00	3.00E+00	1.85E+00	1.40E+00	9.00E-01	4.00E-01	**Total**	**n/s•cm³ per fuel rod**
5000	5.89E+04	7.16E+05	8.34E+05	4.28E+05	5.62E+05	6.14E+05	1.21E+05	3.33E+06	6.46E+01
7500	4.58E+04	5.65E+05	6.61E+05	3.44E+05	4.49E+05	4.82E+05	9.42E+04	2.64E+06	5.12E+01
10000	3.69E+04	4.57E+05	5.38E+05	2.80E+05	3.64E+05	3.89E+05	7.61E+04	2.14E+06	4.15E+01
15000	2.60E+04	3.23E+05	3.83E+05	1.98E+05	2.57E+05	2.74E+05	5.36E+04	1.51E+06	2.94E+01
20000	2.02E+04	2.51E+05	2.98E+05	1.54E+05	2.00E+05	2.13E+05	4.17E+04	1.18E+06	2.28E+01
25000	1.71E+04	2.12E+05	2.50E+05	1.30E+05	1.69E+05	1.80E+05	3.53E+04	9.93E+05	1.93E+01
30000	1.54E+04	1.89E+05	2.21E+05	1.16E+05	1.52E+05	1.62E+05	3.18E+04	8.87E+05	1.72E+01
35000	1.45E+04	1.75E+05	2.04E+05	1.08E+05	1.42E+05	1.52E+05	2.97E+04	8.25E+05	1.60E+01
40000	1.39E+04	1.67E+05	1.93E+05	1.03E+05	1.35E+05	1.46E+05	2.85E+04	7.86E+05	1.52E+01
45000	1.35E+04	1.61E+05	1.85E+05	9.94E+04	1.31E+05	1.42E+05	2.77E+04	7.60E+05	1.47E+01
50000	1.32E+04	1.57E+05	1.79E+05	9.69E+04	1.29E+05	1.39E+05	2.72E+04	7.41E+05	1.44E+01
55000	1.30E+04	1.54E+05	1.75E+05	9.50E+04	1.26E+05	1.37E+05	2.68E+04	7.27E+05	1.41E+01
60000	1.29E+04	1.51E+05	1.71E+05	9.34E+04	1.25E+05	1.35E+05	2.64E+04	7.15E+05	1.39E+01
65000	1.27E+04	1.49E+05	1.68E+05	9.20E+04	1.23E+05	1.34E+05	2.61E+04	7.05E+05	1.37E+01

70000	1.26E+04	1.47E+05	1.65E+05	9.08E+04	1.22E+05	1.32E+05	2.59E+04	6.95E+05	1.35E+01
75000	1.25E+04	1.45E+05	1.62E+05	8.97E+04	1.20E+05	1.31E+05	2.56E+04	6.86E+05	1.33E+01
80000	1.24E+04	1.43E+05	1.60E+05	8.86E+04	1.19E+05	1.30E+05	2.53E+04	6.78E+05	1.32E+01
85000	1.22E+04	1.41E+05	1.58E+05	8.76E+04	1.18E+05	1.28E+05	2.51E+04	6.70E+05	1.30E+01
90000	1.21E+04	1.40E+05	1.56E+05	8.67E+04	1.17E+05	1.27E+05	2.49E+04	6.64E+05	1.29E+01
95000	1.20E+04	1.38E+05	1.54E+05	8.57E+04	1.16E+05	1.26E+05	2.46E+04	6.56E+05	1.27E+01
100000	1.19E+04	1.37E+05	1.52E+05	8.49E+04	1.14E+05	1.25E+05	2.44E+04	6.49E+05	1.26E+01

Table 11. Gamma Source Spectra (p/s) of the Average PWR SNF Assembly

Age (Years)	**Upper Energy Boundary (MeV)**						
	5.00E-02	1.00E-01	2.00E-01	3.00E-01	4.00E-01	6.00E-01	8.00E-01
5000	7.66E+11	4.38E+11	2.39E+11	1.53E+11	2.98E+10	1.26E+10	5.11E+10
7500	6.21E+11	3.46E+11	1.90E+11	1.22E+11	2.66E+10	1.25E+10	4.94E+10
10000	5.11E+11	2.80E+11	1.51E+11	9.76E+10	2.42E+10	1.23E+10	4.79E+10
15000	3.55E+11	1.88E+11	9.72E+10	6.31E+10	2.10E+10	1.21E+10	4.52E+10
20000	2.58E+11	1.31E+11	6.34E+10	4.18E+10	1.93E+10	1.19E+10	4.29E+10
25000	1.97E+11	9.58E+10	4.24E+10	2.88E+10	1.85E+10	1.18E+10	4.10E+10
30000	1.59E+11	7.39E+10	2.94E+10	2.09E+10	1.83E+10	1.16E+10	3.94E+10
35000	1.33E+11	6.06E+10	2.14E+10	1.62E+10	1.83E+10	1.15E+10	3.80E+10
40000	1.17E+11	5.25E+10	1.65E+10	1.35E+10	1.86E+10	1.14E+10	3.68E+10
45000	1.05E+11	4.77E+10	1.35E+10	1.20E+10	1.90E+10	1.13E+10	3.58E+10
50000	9.76E+10	4.50E+10	1.18E+10	1.13E+10	1.94E+10	1.12E+10	3.49E+10
55000	9.20E+10	4.35E+10	1.09E+10	1.10E+10	1.98E+10	1.11E+10	3.42E+10
60000	8.80E+10	4.28E+10	1.04E+10	1.11E+10	2.03E+10	1.10E+10	3.35E+10
65000	8.50E+10	4.26E+10	1.01E+10	1.12E+10	2.07E+10	1.09E+10	3.29E+10
70000	8.27E+10	4.27E+10	1.01E+10	1.15E+10	2.11E+10	1.08E+10	3.24E+10
75000	8.10E+10	4.29E+10	1.02E+10	1.18E+10	2.15E+10	1.07E+10	3.19E+10
80000	7.97E+10	4.32E+10	1.03E+10	1.21E+10	2.18E+10	1.06E+10	3.15E+10
85000	7.87E+10	4.36E+10	1.04E+10	1.25E+10	2.22E+10	1.06E+10	3.11E+10
90000	7.79E+10	4.40E+10	1.06E+10	1.28E+10	2.25E+10	1.05E+10	3.08E+10
95000	7.73E+10	4.44E+10	1.08E+10	1.31E+10	2.28E+10	1.04E+10	3.04E+10
100000	7.69E+10	4.48E+10	1.10E+10	1.34E+10	2.31E+10	1.03E+10	3.01E+10

Table 11. Gamma Source Spectra (p/s) of the Average PWR SNF Assembly (Continued)

Age (Years)	**Upper Energy Boundary (MeV)**						
	1.00E+00	1.33E+00	1.66E+00	2.00E+00	2.50E+00	3.00E+00	4.00E+00
5000	2.20E+10	7.74E+08	2.50E+08	3.24E+08	1.23E+08	2.39E+06	7.99E+05
7500	2.03E+10	1.06E+09	4.02E+08	5.74E+08	2.18E+08	3.89E+06	1.09E+06
10000	1.88E+10	1.36E+09	5.58E+08	8.30E+08	3.16E+08	5.44E+06	1.41E+06
15000	1.61E+10	1.94E+09	8.65E+08	1.33E+09	5.06E+08	8.51E+06	2.07E+06
20000	1.38E+10	2.48E+09	1.16E+09	1.80E+09	6.87E+08	1.14E+07	2.72E+06
25000	1.20E+10	3.00E+09	1.43E+09	2.25E+09	8.58E+08	1.42E+07	3.35E+06
30000	1.04E+10	3.49E+09	1.70E+09	2.67E+09	1.02E+09	1.68E+07	3.94E+06
35000	9.05E+09	3.94E+09	1.94E+09	3.06E+09	1.17E+09	1.93E+07	4.51E+06
40000	7.94E+09	4.37E+09	2.18E+09	3.43E+09	1.31E+09	2.16E+07	5.04E+06
45000	7.01E+09	4.77E+09	2.39E+09	3.78E+09	1.44E+09	2.38E+07	5.53E+06
50000	6.23E+09	5.15E+09	2.60E+09	4.10E+09	1.57E+09	2.58E+07	6.00E+06
55000	5.58E+09	5.50E+09	2.79E+09	4.41E+09	1.68E+09	2.77E+07	6.43E+06
60000	5.04E+09	5.83E+09	2.97E+09	4.69E+09	1.79E+09	2.95E+07	6.84E+06
65000	4.59E+09	6.13E+09	3.14E+09	4.96E+09	1.89E+09	3.12E+07	7.22E+06
70000	4.22E+09	6.42E+09	3.30E+09	5.20E+09	1.99E+09	3.27E+07	7.58E+06
75000	3.91E+09	6.68E+09	3.45E+09	5.43E+09	2.07E+09	3.42E+07	7.91E+06
80000	3.65E+09	6.93E+09	3.58E+09	5.65E+09	2.16E+09	3.55E+07	8.22E+06

85000	3.43E+09	7.16E+09	3.71E+09	5.85E+09	2.23E+09	3.68E+07	8.51E+06
90000	3.26E+09	7.37E+09	3.83E+09	6.03E+09	2.30E+09	3.79E+07	8.77E+06
95000	3.11E+09	7.57E+09	3.94E+09	6.20E+09	2.37E+09	3.90E+07	9.02E+06
100000	2.99E+09	7.75E+09	4.05E+09	6.36E+09	2.43E+09	4.00E+07	9.24E+06

Table 11. Gamma Source Spectra (p/s) of the Average PWR SNF Assembly (Continued)

Age (Years)	Upper Energy Bound (MeV)				Total	p/s•cm³ per fuel rod	Total per WP
	5.00E+00	6.50E+00	8.00E+00	1.00E+01			
5000	1.14E+05	4.57E+04	8.95E+03	1.90E+03	1.71E+12	3.32E+07	3.60E+13
7500	9.17E+04	3.68E+04	7.20E+03	1.53E+03	1.39E+12	2.70E+07	2.92E+13
10000	7.56E+04	3.03E+04	5.94E+03	1.26E+03	1.15E+12	2.22E+07	2.41E+13
15000	5.55E+04	2.22E+04	4.36E+03	9.24E+02	8.02E+11	1.56E+07	1.68E+13
20000	4.47E+04	1.79E+04	3.51E+03	7.45E+02	5.88E+11	1.14E+07	1.24E+13
25000	3.89E+04	1.56E+04	3.05E+03	6.48E+02	4.55E+11	8.82E+06	9.55E+12
30000	3.56E+04	1.43E+04	2.80E+03	5.93E+02	3.72E+11	7.21E+06	7.81E+12
35000	3.37E+04	1.35E+04	2.65E+03	5.61E+02	3.18E+11	6.17E+06	6.68E+12
40000	3.25E+04	1.30E+04	2.55E+03	5.42E+02	2.86E+11	5.54E+06	6.00E+12
45000	3.17E+04	1.27E+04	2.49E+03	5.29E+02	2.64E+11	5.11E+06	5.54E+12
50000	3.11E+04	1.25E+04	2.45E+03	5.19E+02	2.51E+11	4.86E+06	5.27E+12
55000	3.07E+04	1.23E+04	2.41E+03	5.12E+02	2.42E+11	4.70E+06	5.09E+12
60000	3.03E+04	1.22E+04	2.38E+03	5.06E+02	2.37E+11	4.60E+06	4.99E+12
65000	3.00E+04	1.20E+04	2.36E+03	5.00E+02	2.34E+11	4.54E+06	4.92E+12
70000	2.97E+04	1.19E+04	2.33E+03	4.95E+02	2.32E+11	4.51E+06	4.88E+12
75000	2.94E+04	1.18E+04	2.31E+03	4.90E+02	2.32E+11	4.49E+06	4.86E+12
80000	2.91E+04	1.17E+04	2.29E+03	4.86E+02	2.31E+11	4.48E+06	4.86E+12
85000	2.88E+04	1.16E+04	2.27E+03	4.81E+02	2.32E+11	4.49E+06	4.86E+12
90000	2.85E+04	1.14E+04	2.24E+03	4.77E+02	2.32E+11	4.50E+06	4.87E+12
95000	2.83E+04	1.13E+04	2.22E+03	4.72E+02	2.32E+11	4.51E+06	4.88E+12
100000	2.80E+04	1.12E+04	2.20E+03	4.68E+02	2.33E+11	4.52E+06	4.90E+12

5.4 GAMMA ENERGY ABSORPTION RESPONSE FUNCTIONS

This section compares the gamma energy absorption response function of water computed from the water mass-energy-absorption (MEA) coefficient to that derived from the ANS-6.1.1-1977 flux-to-dose-rate factors (ANSI/ANS-6.1.1-1977). The purpose of this section is to show that using the ANS-6.1.1-1977 flux-to-dose-rate factors leads to higher gamma energy absorption in the 21-PWR WP, which in turn provides higher (more conservative) yield for nitric acid production rate.

For gamma interaction with matter, the amount of energy deposition in a material by gamma rays is characterized by the MEA coefficient of the material. The MEA coefficients for gamma energy from 10 keV to 10 MeV for dry air and water are presented in Table 12 (Chilton et al. 1984). It can be seen from the last column of Table 12 that the MEA coefficient of water is approximately 12% higher than that of air. Therefore, using the water MEA coefficient to determine gamma energy absorption in water-air mixture would give higher (conservative) energy deposition.

Table 13 provides a comparison of the gamma flux-to-energy-absorption response function of water computed from the MEA coefficient of water to that derived from Table 4 of the ANS-6.1.1-1977 flux-to-dose-rate factors. The gamma flux-to-energy-absorption response function for water is obtained by multiplying the water MEA coefficient by 3600 to account for the factor between hour and second. The ANS-6.1.1-1977 gamma flux-to-dose-rate factor is converted to the gamma flux-to-flux-to-dose-rate factors. The gamma flux-to-energy-absorption response function for water is obtained by multiplying the water MEA coefficient by 3600 to account for the factor between hour and second. The ANS-6.1.1-1977 gamma flux-to-dose-rate factor is converted to the gamma flux-to-energy-absorption response function by converting the dose unit from rad to eV/g with the factor 6.2415E+13. This value is obtained from three conversion factors starting from one rad equals 0.01 gray, which is the energy per unit mass of one joule per kilogram imparted to matter by ionizing radiation (Parrington et al 1996, p.58). Since one joule equals $(1.602177E\text{-}19)^{-1}$ eV (Parrington et al 1996, p.58) and one kilogram equals 1000 gram, the product of these two values and 0.01 yields the factor 6.2415E+13.

The response functions are graphically presented in Figure 4 for gamma energy from 10 keV to 10 MeV. It is clear that the ANS-6.1.1-1977 flux-to-dose-rate factor leads to higher gamma energy absorption in the 21-PWR WP, which, in turn, yields higher (more conservative) nitric acid production rate.

Table 12. Mass Energy-Absorption Coefficients of Air and Water

Energy (eV)	Air, Dry		Water		Water/Air Ratio
	$(cm^2\ g^{-1})^a$	$(eV\ cm^2\ g^{-1})^b$	$(cm^2\ g^{-1})^a$	$(eV\ cm^2\ g^{-1})^b$	
1.00E+04	4.57E+00	4.57E+04	4.72E+00	4.72E+04	1.03E+00
1.50E+04	1.25E+00	1.88E+04	1.29E+00	1.94E+04	1.03E+00
2.00E+04	5.01E-01	1.00E+04	5.05E-01	1.01E+04	1.01E+00
3.00E+04	1.39E-01	4.17E+03	1.40E-01	4.20E+03	1.01E+00
4.00E+04	6.16E-02	2.46E+03	6.20E-02	2.48E+03	1.01E+00
5.00E+04	3.74E-02	1.87E+03	3.83E-02	1.92E+03	1.02E+00
6.00E+04	2.83E-02	1.70E+03	2.96E-02	1.78E+03	1.05E+00
8.00E+04	2.31E-02	1.85E+03	2.49E-02	1.99E+03	1.08E+00
1.00E+05	2.27E-02	2.27E+03	2.48E-02	2.48E+03	1.09E+00
1.50E+05	2.47E-02	3.71E+03	2.74E-02	4.11E+03	1.11E+00
2.00E+05	2.65E-02	5.30E+03	2.95E-02	5.90E+03	1.11E+00
3.00E+05	2.87E-02	8.61E+03	3.19E-02	9.57E+03	1.11E+00
4.00E+05	2.94E-02	1.18E+04	3.28E-02	1.31E+04	1.12E+00
5.00E+05	2.98E-02	1.49E+04	3.31E-02	1.66E+04	1.11E+00
6.00E+05	2.95E-02	1.77E+04	3.28E-02	1.97E+04	1.11E+00
8.00E+05	2.87E-02	2.30E+04	3.19E-02	2.55E+04	1.11E+00
1.00E+06	2.78E-02	2.78E+04	3.10E-02	3.10E+04	1.12E+00
1.50E+06	2.54E-02	3.81E+04	2.83E-02	4.25E+04	1.11E+00
2.00E+06	2.34E-02	4.68E+04	2.60E-02	5.20E+04	1.11E+00
3.00E+06	2.05E-02	6.15E+04	2.27E-02	6.81E+04	1.11E+00
4.00E+06	1.87E-02	7.48E+04	2.07E-02	8.28E+04	1.11E+00
5.00E+06	1.74E-02	8.70E+04	1.92E-02	9.60E+04	1.10E+00
6.00E+06	1.65E-02	9.90E+04	1.81E-02	1.09E+05	1.10E+00
8.00E+06	1.53E-02	1.22E+05	1.67E-02	1.34E+05	1.09E+00
1.00E+07	1.46E-02	1.46E+05	1.58E-02	1.58E+05	1.08E+00

SOURCE: [a]Chilton et al. 1984, pp. 424-425
NOTE: [b]MEA coefficient in $(cm^2\ g^{-1})$ multiplied by gamma energy in eV.

Table 13. Comparison of Gamma-Ray Energy-Absorption Response Functions

Energy (eV)	Water Mass Energy-Absorption Coefficient		ANS-6.1.1-1977 Dose Factors[a]	
	eV cm^2 g^{-1}	eV g^{-1} h^{-1}/cm^{-2} s^{-1}	rad h^{-1}/cm^{-2} s^{-1}	eV g^{-1} h^{-1}/cm^{-2} s^{-1}
1.00E+04	4.72E+04	1.70E+08	3.96E-06	2.47E+08
1.50E+04	1.94E+04	6.97E+07	1.95E-06	1.22E+08
2.00E+04	1.01E+04	3.64E+07	1.18E-06	7.37E+07
3.00E+04	4.20E+03	1.51E+07	5.82E-07	3.63E+07
4.00E+04	2.48E+03	8.93E+06	3.61E-07	2.25E+07
5.00E+04	1.92E+03	6.89E+06	2.90E-07	1.81E+07
6.00E+04	1.78E+03	6.39E+06	2.65E-07	1.65E+07
8.00E+04	1.99E+03	7.17E+06	2.61E-07	1.63E+07
1.00E+05	2.48E+03	8.93E+06	2.83E-07	1.77E+07
1.50E+05	4.11E+03	1.48E+07	3.79E-07	2.37E+07
2.00E+05	5.90E+03	2.12E+07	5.01E-07	3.13E+07
3.00E+05	9.57E+03	3.45E+07	7.59E-07	4.74E+07
4.00E+05	1.31E+04	4.72E+07	9.85E-07	6.15E+07
5.00E+05	1.66E+04	5.96E+07	1.17E-06	7.30E+07
6.00E+05	1.97E+04	7.08E+07	1.36E-06	8.49E+07
8.00E+05	2.55E+04	9.19E+07	1.68E-06	1.05E+08
1.00E+06	3.10E+04	1.12E+08	1.98E-06	1.24E+08
1.50E+06	4.25E+04	1.53E+08	2.64E-06	1.64E+08
2.00E+06	5.20E+04	1.87E+08	3.21E-06	2.00E+08
3.00E+06	6.81E+04	2.45E+08	4.19E-06	2.62E+08
4.00E+06	8.28E+04	2.98E+08	5.03E-06	3.14E+08
5.00E+06	9.60E+04	3.46E+08	5.80E-06	3.62E+08
6.00E+06	1.09E+05	3.91E+08	6.56E-06	4.09E+08
8.00E+06	1.34E+05	4.81E+08	8.03E-06	5.01E+08
1.00E+07	1.58E+05	5.69E+08	9.51E-06	5.94E+08

SOURCE: [a]ANSI/ANS-6.1.1-1977, Table 4.

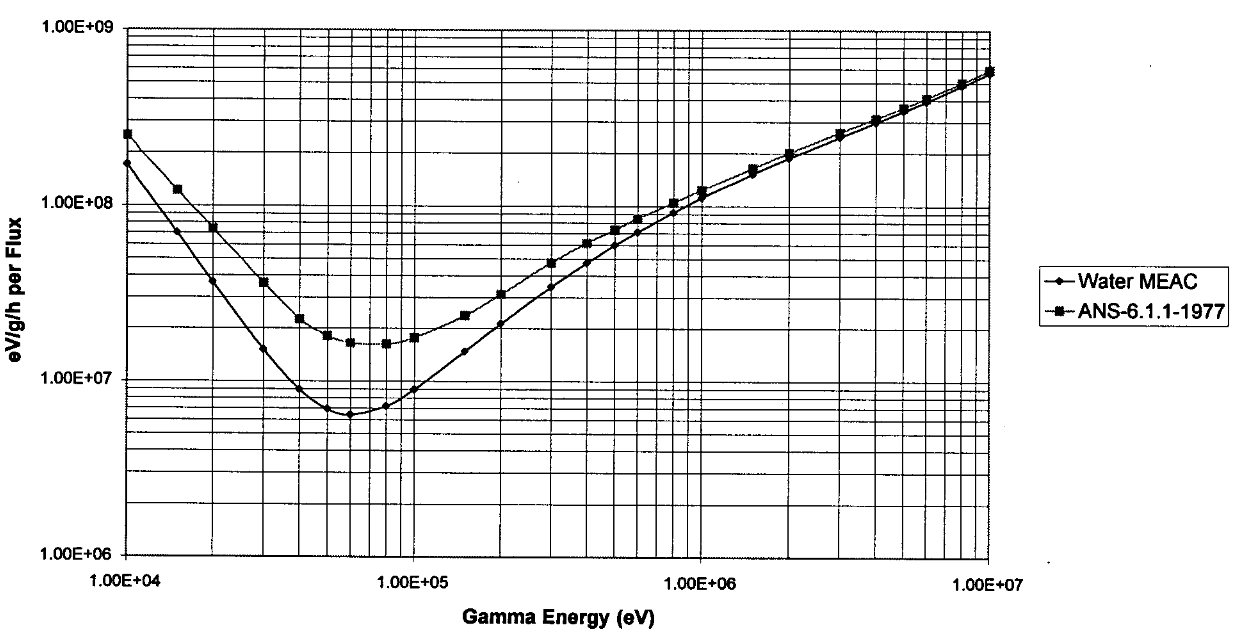

Figure 4. Plot of Gamma-Ray Energy-Absorption Response Functions

5.5 NITRIC ACID PRODUCTION RATE IN THE 21-PWR WP

Radiolytic production of nitric acid by gamma radiation in the failed 21-PWR WP over the time period between 10,000 and 100,000 years can be determined from the dose rates inside the WP, provided that the G value for nitrogen dioxide and the mass of the moist air being irradiated are known. In this calculation, the internal configuration of the 21-PWR WP is assumed to be intact (Assumption 3.11), and the dose rates in the WP at different times are calculated by MCNP. The mass of moist air is computed from the density and volume of the moist air in the WP while the G value of 1.5 is assumed for nitrogen dioxide (Assumption 3.10).

Since it is assumed that the temperature and pressure inside the WP are 25 °C and one atmosphere, respectively (Assumption 3.8), the density of moist air is 1.1845 g/l (Weast 1979, Table IV, p. F-10). Furthermore, based on Assumption 3.9, the volume of the moist air equals to the volume of the WP cavity within the active fuel region subtracted by the volume of the fuel rods.

The volume of the WP cavity in the active fuel region is:

$$\pi\,(71.2)^2(360.172)\ \text{cm}^3$$
$$= 5736.141 \text{ liters.}$$

The volume of fuel rods is:

$$(21)\,(208)\,\pi\,(0.5461)^2(360.172)\ \text{cm}^3$$
$$= 1473.964 \text{ liters.}$$

Therefore, the volume of the moist air is

$$5736.141 - 1473.964$$
$$4262.177 \text{ liters,}$$

and the mass of the moist air is

$$(1.1845\ \text{g/l})\,(4262.177\ \text{l})$$
$$= 5048.549\ \text{g.}$$

The amount of nitric acid produced by gamma radiation per year is calculated as follows:

$$(\text{Dose Rate rad/h})\,(6.2415\text{E}+13\ \text{eV/g/rad})\,(1.5\ \text{molecules/100 eV})\,(5048.549\ \text{g})\,(8760\ \text{h/y})$$
$$= (\text{Dose Rate})\,(4.14\text{E}+19)\ \text{molecules/y.}$$

6. RESULTS

This document may be affected by technical product input information that requires confirmation. Any changes to the document that may occur as a result of completing the confirmation activities will be reflected in subsequent revisions. The status of the technical product input information quality may be confirmed by review of the DIRS database.

6.1 SAS1 DOSE RATES OF A PWR SNF ROD

Dose rates of a PWR SNF rod calculated by the SAS1 module of the SCALE code system are presented in Table 14. Gamma and neutron dose rates are determined on the mid-plane of the fuel rod at the surface and at 0.17 cm from the surface between 5,000 and 100,000 years after emplacement. Gamma dose rate accounts for over 99 percent of the total dose rate. Hence, the dose contribution by neutrons is negligible. Gamma dose rates for the time period between 10,000 and 100,000 years are depicted in Figure 5.

It is noted that the gamma dose rates decrease and then begin to rise after 45,000 years. After examination of the time dependencies of both the concentrations of radionuclides that contribute to the gamma source and the energy-dependent dose rates, it is believed that the dose rate increase is mainly due to the Bi-214 isotope. This isotope, produced from the decay chain of U-234, emits energetic gamma rays with energy ranging from 0.6 to 3 MeV. The dose rate due to the Bi-214 gamma rays increases slowly and eventually dominates the total dose rate after 45,000 years.

Table 14. SAS1 Dose Rates (rem/h) of a PWR SNF Rod

Years after Emplacement	Gamma		Neutron		Total		Gamma Fraction	
	Surface	Outside	Surface	Outside	Surface	Outside	Surface	Outside
5000	0.63816	0.47115	0.00249	0.00184	0.64065	0.47299	0.99611	0.99611
7500	0.60277	0.44513	0.00198	0.00146	0.60475	0.44659	0.99673	0.99673
10000	0.57254	0.42289	0.00160	0.00118	0.57414	0.42407	0.99721	0.99721
15000	0.53258	0.39351	0.00113	0.00084	0.53371	0.39435	0.99787	0.99787
20000	0.50353	0.37214	0.00088	0.00065	0.50441	0.37279	0.99826	0.99826
25000	0.48830	0.36094	0.00074	0.00055	0.48904	0.36149	0.99848	0.99848
30000	0.47885	0.35400	0.00066	0.00049	0.47951	0.35449	0.99862	0.99862
35000	0.47352	0.35009	0.00062	0.00046	0.47414	0.35055	0.99870	0.99870
40000	0.47236	0.34926	0.00059	0.00043	0.47295	0.34969	0.99876	0.99876
45000	0.47259	0.34944	0.00057	0.00042	0.47316	0.34986	0.99880	0.99880
50000	0.47482	0.35110	0.00055	0.00041	0.47537	0.35151	0.99883	0.99883
55000	0.47871	0.35399	0.00054	0.00040	0.47925	0.35439	0.99887	0.99887
60000	0.48253	0.35682	0.00053	0.00040	0.48306	0.35722	0.99889	0.99889
65000	0.48739	0.36043	0.00053	0.00039	0.48792	0.36082	0.99892	0.99892
70000	0.49269	0.36435	0.00052	0.00038	0.49321	0.36473	0.99895	0.99895
75000	0.49696	0.36751	0.00051	0.00038	0.49747	0.36789	0.99897	0.99897
80000	0.50166	0.37100	0.00051	0.00038	0.50217	0.37138	0.99899	0.99899
85000	0.50710	0.37502	0.00050	0.00037	0.50760	0.37539	0.99902	0.99902
90000	0.51212	0.37874	0.00050	0.00037	0.51262	0.37911	0.99903	0.99903
95000	0.51618	0.38175	0.00049	0.00036	0.51667	0.38211	0.99906	0.99906
100000	0.51985	0.38447	0.00048	0.00036	0.52033	0.38483	0.99907	0.99907

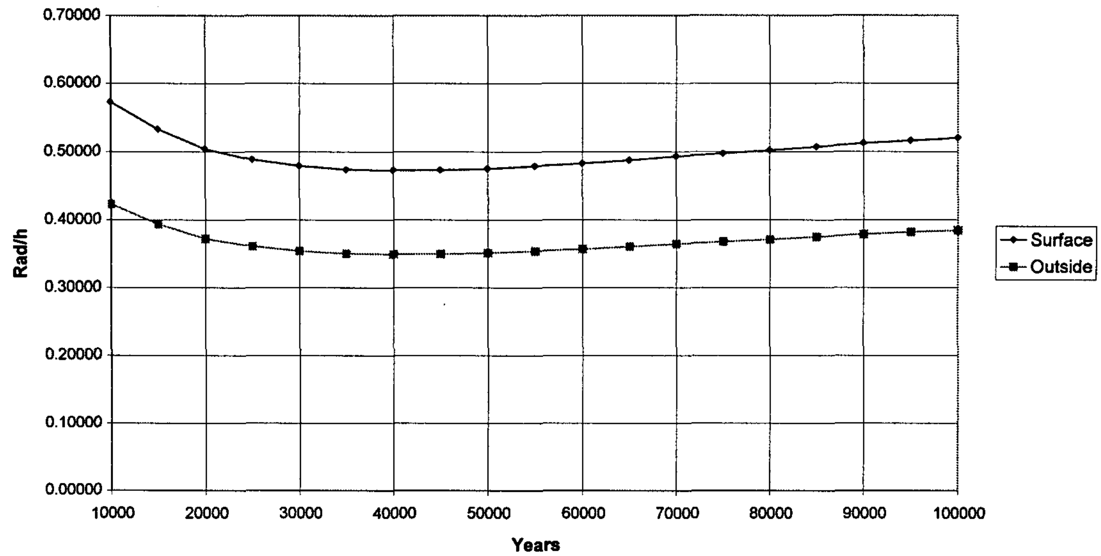

Figure 5. Gamma Dose Rates of a PWR SNF Rod Calculated by SAS1

6.2 MCNP GAMMA DOSE RATES IN THE 21-PWR WP

Gamma dose rates are calculated for three locations in the 21-PWR WP with detailed three-dimensional geometry using MCNP program. Table 15 provides the dose results for the twelve time steps between 5,000 and 100,000 years. For the cavity wall, the dose rates represent the average values over the middle one-third of the active fuel height. For the fuel cells and vacant cells, the dose rates are obtained by tallying inside the respective cells over the active fuel height within the nine central assemblies in the WP. Dose rates for the cavity wall and the fuel cells for the time period between 10,000 and 100,000 years are plotted in Figure 6.

Similar to the SAS1 results, the dose rates start to increase after 30,000 years. Again, this behavior is a result of the gamma rays from the Bi-214 isotope.

Table 15. MCNP Gamma Dose Rates (rad/h) in the 21-PWR WP

Years after Emplacement	Cavity Wall		Fuel Cells		Vacant Cells	
5000	1.5018	0.0460[a]	3.4631	0.0099[a]	3.4655	0.0180[a]
7500	1.4772	0.0423	3.3303	0.0094	3.3611	0.0170
10000	1.4489	0.0396	3.2124	0.0089	3.2408	0.0160
20000	1.3548	0.0319	2.9773	0.0073	3.0182	0.0127
30000	1.3336	0.0260	2.9590	0.0062	3.0322	0.0107
40000	1.3639	0.0224	3.0055	0.0056	3.0320	0.0096
50000	1.3909	0.0203	3.1034	0.0053	3.1366	0.0091
60000	1.4470	0.0194	3.2193	0.0052	3.2376	0.0088
70000	1.4908	0.0188	3.3309	0.0051	3.3399	0.0086
80000	1.5357	0.0186	3.4462	0.0051	3.4525	0.0086
90000	1.5920	0.0186	3.5432	0.0051	3.5602	0.0085
100000	1.6313	0.0185	3.6436	0.0051	3.6622	0.0084

Note: [a]Relative error.

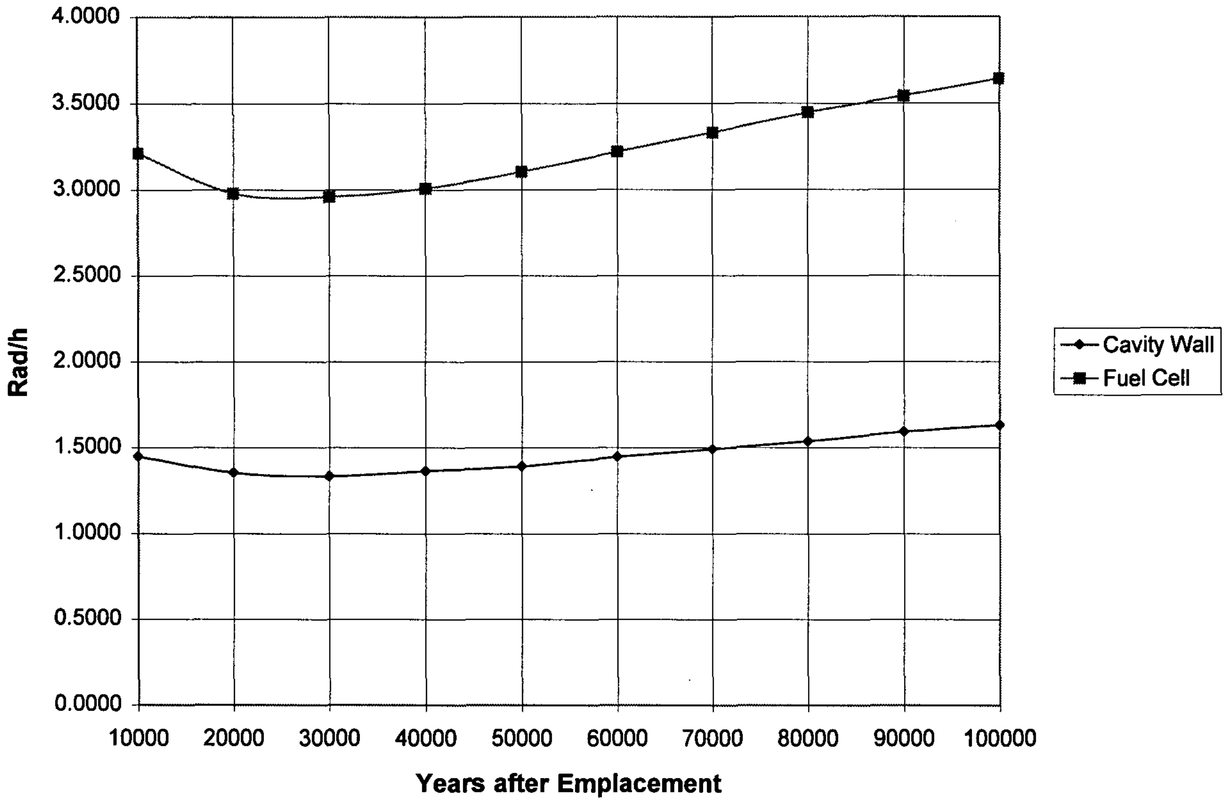

Figure 6. Gamma Dose Rates in the 21-PWR WP Calculated by MCNP

6.3 NITRIC ACID PRODUCTION IN THE 21-PWR WP

The gamma dose rates in the fuel cell calculated by MCNP in the previous section is used to determine the radiolytic production rate of nitric acid in the failed 21-PWR WP for the time period between 10,000 and 100,000 years. The dose rates in the fuel cells given in Figure 6 are converted to number of nitric acid molecules produced per year using the conversion factor of 4.14E+19 derived in Section 5.5. The nitric acid production rate is then integrated over time to obtain the total yield of the entire time period. Table 16 presents the production rate and cumulative yield of the nitric acid as a function of time and Figure 7 depicts the cumulative amount of nitric acid produced as a function of time.

The results for nitric acid production can be extended to determine the production of other chemical species so long as G values are known. As a matter of fact, the yield of any particular chemical species is equal to its G value divided by 1.5 and multiplied by the yield in Table 16.

Table 16. Nitric Acid Production in the 21-PWR WP over Time

Years after Emplacement	Dose Rate (Rad/h)	Yield Rate (Molecules/y)	Cumulative Yield (Molecules)
10000	3.2124	1.330E+20	0
20000	2.9773	1.233E+20	1.281E+24
30000	2.9590	1.225E+20	2.510E+24
40000	3.0055	1.244E+20	3.745E+24
50000	3.1034	1.285E+20	5.009E+24
60000	3.2193	1.333E+20	6.318E+24
70000	3.3309	1.379E+20	7.674E+24
80000	3.4462	1.427E+20	9.077E+24
90000	3.5432	1.467E+20	1.052E+25
100000	3.6436	1.508E+20	1.201E+25

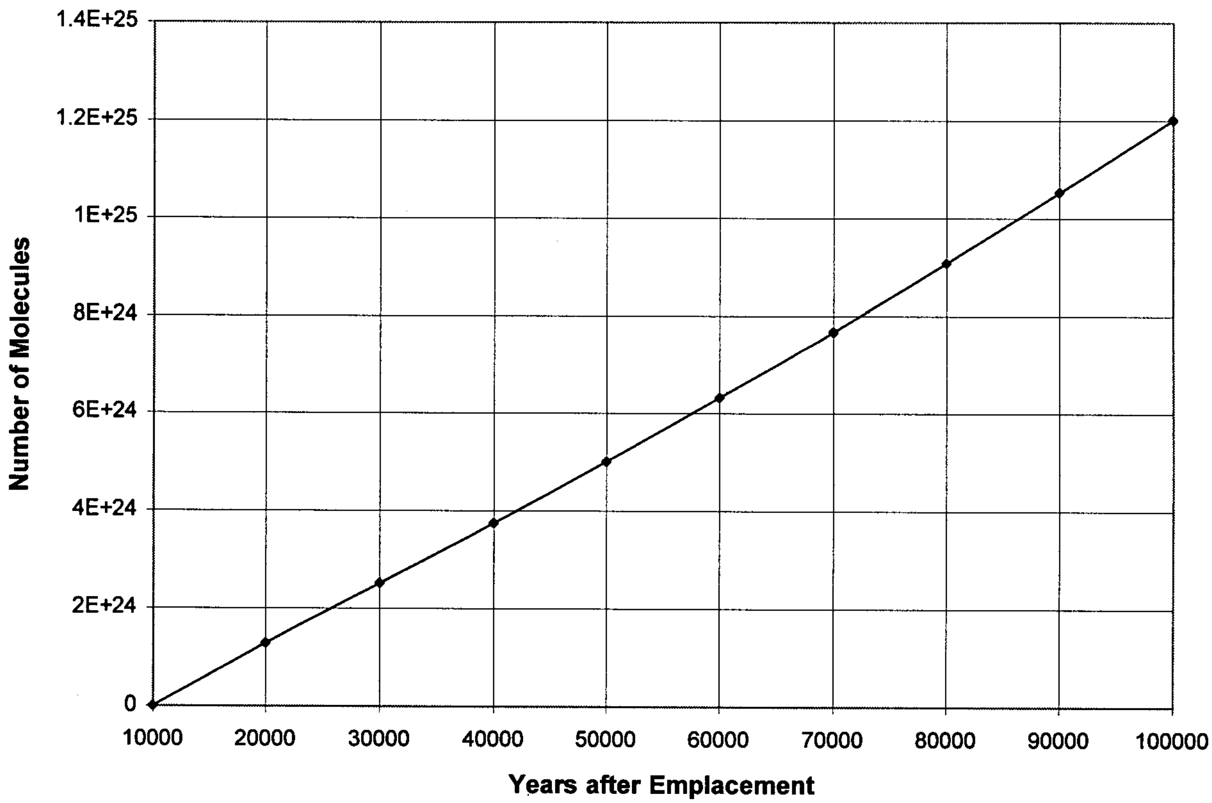

Figure 7. Cumulative Nitric Acid Production over Time

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8. ATTACHMENTS

The list of attachments is presented in Table 17. Electronic output files are provided on a compact disk that is Attachment III of this calculation. The files' attributes of the output files are listed in Table 18. Each file is identified by its name, size (in bytes), and the date and time. The files can be read using Word-Pad application in Microsoft Windows Explorer. It should be noted that the date and time reflect the time of transfer from the HP to the personal computer. The actual date and time of each run completion can be found in its corresponding file.

Table 17. List of Attachments

Description	Attachment Number	No. of Pages
SK – 0175 REV 02 21-PWR Waste Package Configurations for Site Recommendation	I	2
SK – 0191 REV 00 21-PWR Waste Package Weld Configuration	II	1
Compact Disk of SAS1 and MCNP Output Files	III	N/A

Table 18. SAS1 and MCNP Output Files

File Name	Description	Size (bytes)	Date	Time
A-rod-g-dr.out	SAS1 gamma dose rates	3,796,635	11/17/2000	3:36 p.m.
A-rod-n-dr.out	SAS1 neutron dose rates	3,789,897	11/17/2000	3:37 p.m.
g100k.io	Gamma dose rate at year 100,000	212,459	11/17/2000	11:27 a.m.
g10k.io	Gamma dose rate at year 10,000	205,707	11/17/2000	11:27 a.m.
g20k.io	Gamma dose rate at year 20,000	205,988	11/17/2000	11:28 a.m.
g30k.io	Gamma dose rate at year 30,000	213,256	11/17/2000	11:28 a.m.
g40k.io	Gamma dose rate at year 40,000	206,229	11/17/2000	11:28 a.m.
g50k.io	Gamma dose rate at year 50,000	206,144	11/17/2000	11:28 a.m.
g5k.io	Gamma dose rate at year 5,000	205,428	11/17/2000	11:28 a.m.
g60k.io	Gamma dose rate at year 60,000	212,180	11/17/2000	11:28 a.m.
g70k.io	Gamma dose rate at year 70,000	212,046	11/17/2000	11:28 a.m.
g7k.io	Gamma dose rate at year7,000	204,639	11/17/2000	11:28 a.m.
g80k.io	Gamma dose rate at year 80,000	212,192	11/17/2000	11:28 a.m.
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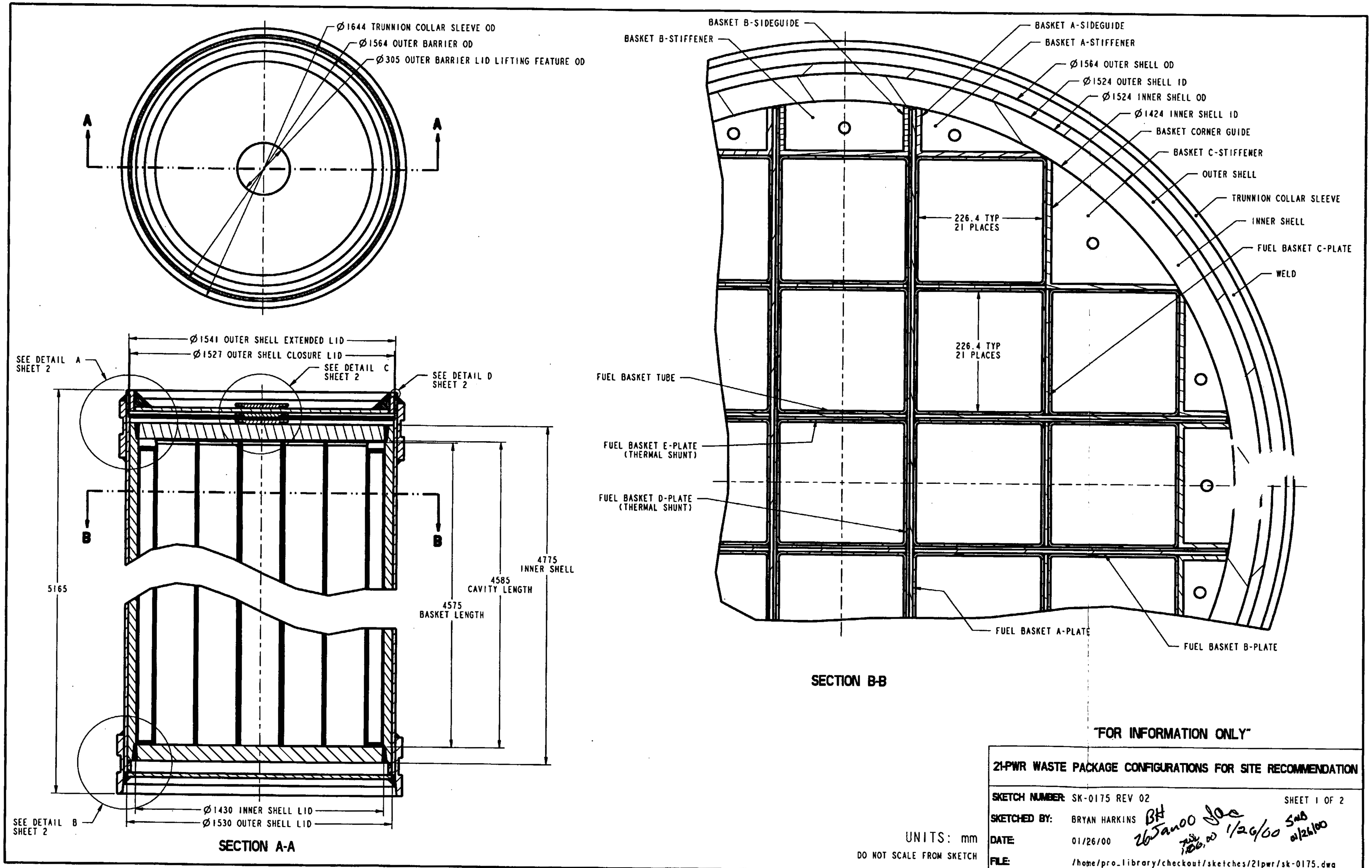

Ø1644 TRUNNION COLLAR SLEEVE OD
Ø1564 OUTER BARRIER OD
Ø305 OUTER BARRIER LID LIFTING FEATURE OD
A
A
Ø1541 OUTER SHELL EXTENDED LID
Ø1527 OUTER SHELL CLOSURE LID
SEE DETAIL A SHEET 2
SEE DETAIL C SHEET 2
SEE DETAIL D SHEET 2
B
B
5165
4775 INNER SHELL
4585 CAVITY LENGTH
4575 BASKET LENGTH
Ø1430 INNER SHELL LID
Ø1530 OUTER SHELL LID
SEE DETAIL B SHEET 2
SECTION A-A
BASKET B-SIDEGUIDE
BASKET B-STIFFENER
BASKET A-SIDEGUIDE
BASKET A-STIFFENER
Ø1564 OUTER SHELL OD
Ø1524 OUTER SHELL ID
Ø1524 INNER SHELL OD
Ø1424 INNER SHELL ID
BASKET CORNER GUIDE
BASKET C-STIFFENER
OUTER SHELL
TRUNNION COLLAR SLEEVE
INNER SHELL
FUEL BASKET C-PLATE
WELD
226.4 TYP 21 PLACES
226.4 TYP 21 PLACES
FUEL BASKET TUBE
FUEL BASKET E-PLATE (THERMAL SHUNT)
FUEL BASKET D-PLATE (THERMAL SHUNT)
FUEL BASKET A-PLATE
FUEL BASKET B-PLATE
SECTION B-B
"FOR INFORMATION ONLY"
21-PWR WASTE PACKAGE CONFIGURATIONS FOR SITE RECOMMENDATION
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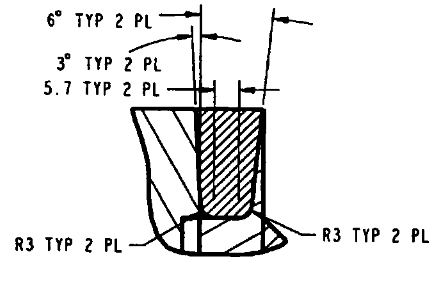
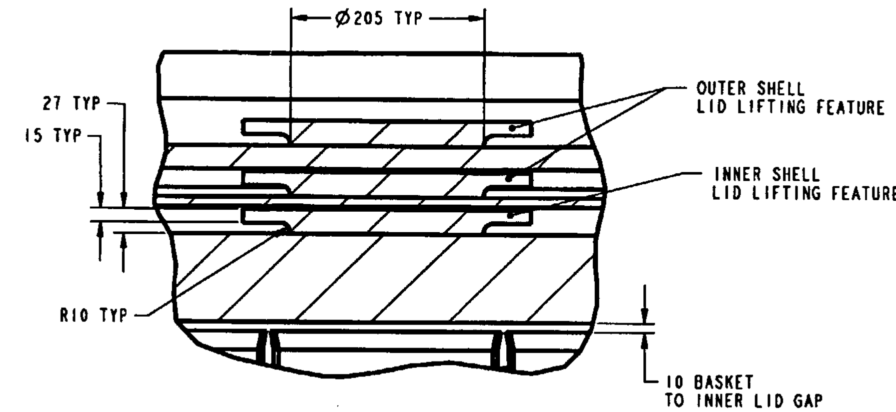
SHEET 1 OF 2
SKETCHED BY: BRYAN HARKINS
DATE: 01/26/00
FILE: /home/pro_library/checkout/sketches/21pwr/sk-0175.dwg
UNITS: mm
DO NOT SCALE FROM SKETCH



DETAIL D



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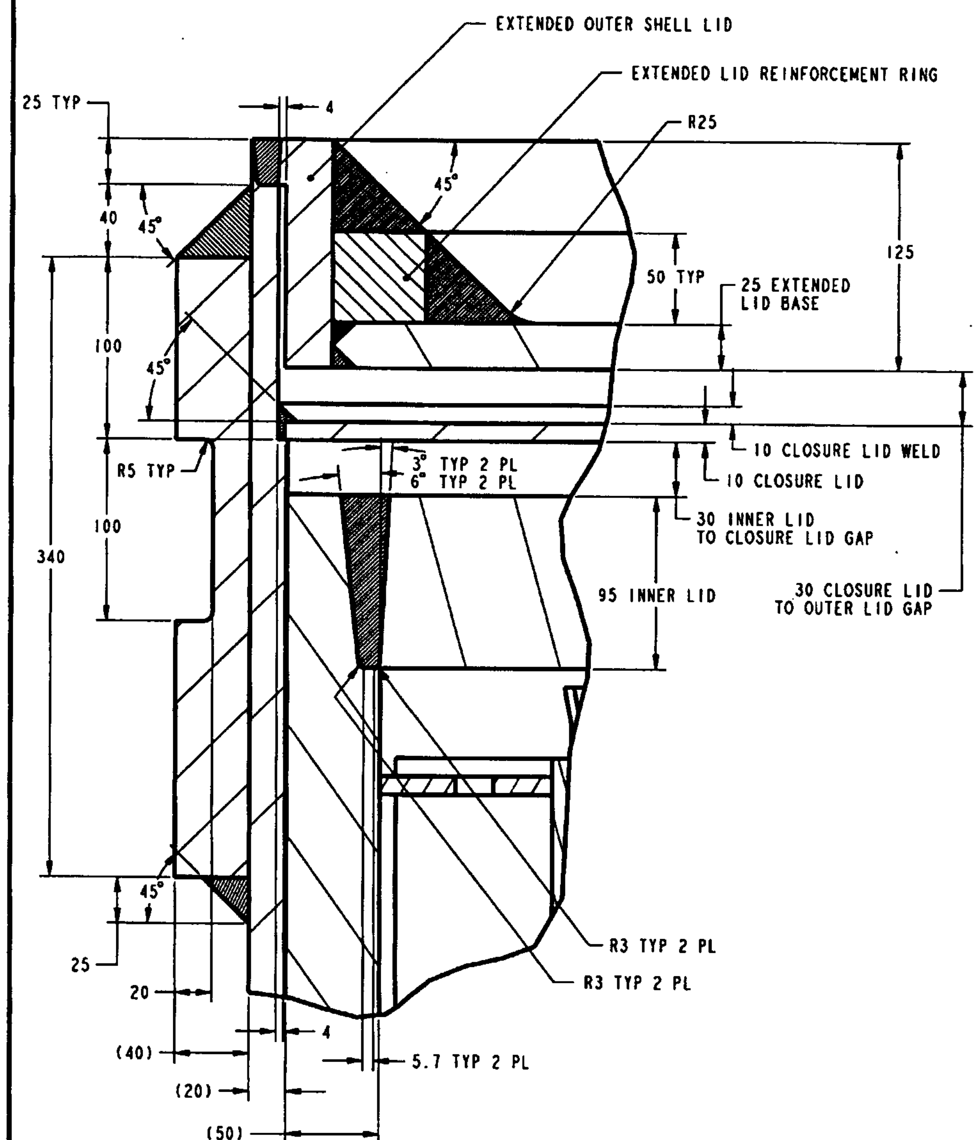
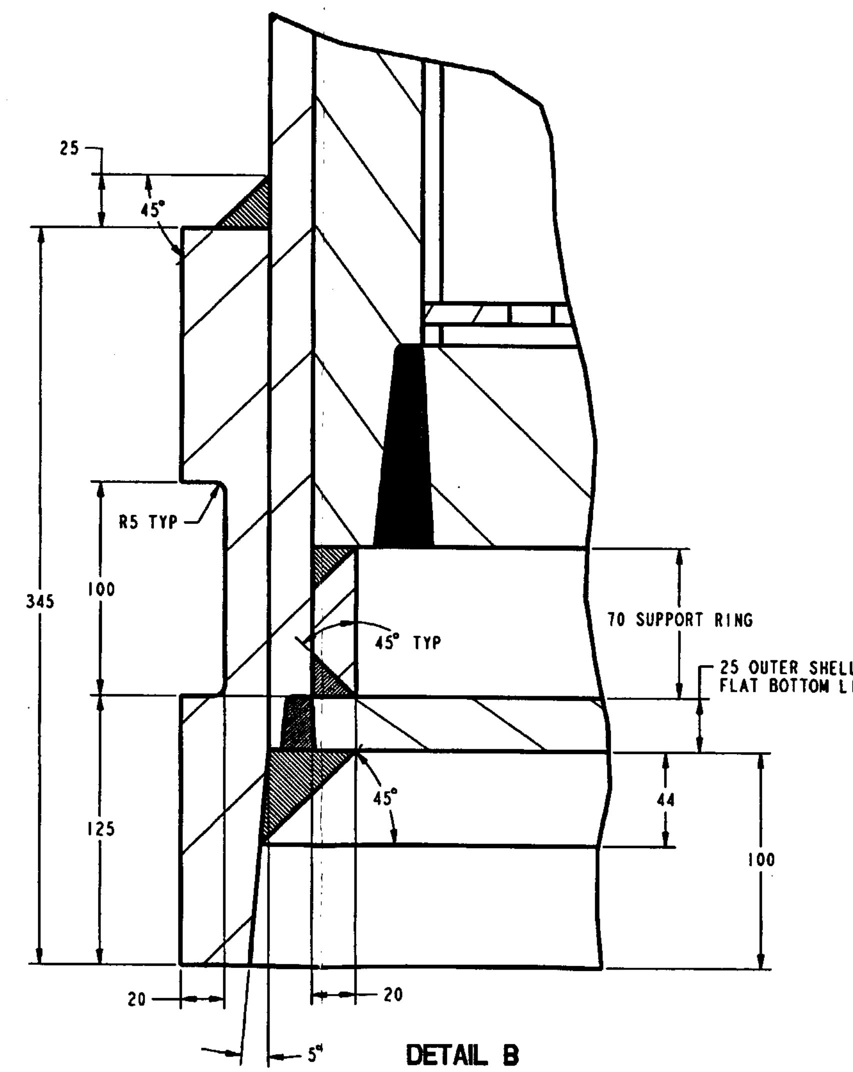


DETAIL A

21-PWR WASTE PACKAGE ASSEMBLY WITH STAINLESS STEEL/BORON PLATES

21-PWR CONTROL ROD WASTE PACKAGE ASSEMBLY WITH CARBON STEEL PLATES

COMPONENT NAME	MATERIAL	THICKNESS	MASS (KG)	QTY ROD
BASKET A-SIDEGUIDE	SA-516 K02700	10	27	32
BASKET A-STIFFENER	SA-516 K02700	10	0.72	64
BASKET B-SIDEGUIDE	SA-516 K02700	10	36	16
BASKET B-STIFFENER	SA-516 K02700	10	1.5	32
BASKET C-STIFFENER	SA-516 K02700	10	2.3	32
BASKET CORNERGUIDE	SA-516 K02700	10	42	16
FUEL BASKET A-PLATE	NEUTRONIT A 978	7	85	8
	#SA-516 K02700	#7	#86	#8
FUEL BASKET B-PLATE	NEUTRONIT A 978	7	85	8
	#SA-516 K02700	#7	#86	#8
FUEL BASKET C-PLATE	NEUTRONIT A 978	7	44	16
	#SA-516 K02700	#7	#45	#16
FUEL BASKET D-PLATE	SB-209 A96061 T4	5	21	8
FUEL BASKET E-PLATE	SB-209 A96061 T4	5	21	8
FUEL BASKET TUBE	SA-516 K02700	5	164	21
INNER SHELL	SA-240 S31600	50	8709	1
INNER SHELL LID	SA-240 S31600	95	1200	2
INNER LID LIFTING FEATURE	SA-240 S31600	27	12	1
OUTER SHELL	SB-575 N06022	20	4193	1
EXTENDED OUTER SHELL LID	SB-575 N06022	25	132	1
EXTENDED OUTER SHELL LID BASE	SB-575 N06022	25	366	1
OUTER LID LIFTING FEATURE	SB-575 N06022	27	13	2
EXTENDED LID REINFORCEMENT RING	SB-575 N06022	50	97	1
OUTER SHELL FLAT CLOSURE LID	SB-575 N06022	10	159	1
OUTER SHELL FLAT BOTTOM LID	SB-575 N0-6022	25	396	1
UPPER TRUNNION COLLAR SLEEVE	SB-575 N06022	40	507	1
LOWER TRUNNION COLLAR SLEEVE	SB-575 N06022	40	497	1
INNER SHELL SUPPORT RING	SB-575 N06022	20	41	1
TOTAL ALLOY 22 WELDS	SFA-5.14 N06022	-	249	**
TOTAL 316 WELDS	SFA-5.9 S31680	-	128	**
WASTE PACKAGE ASSEMBLY	-	-	26035	1
	-	-	#26059	#1
PWR FUEL ASSEMBLY	-	-	773.4*	21
WP ASSEMBLY WITH SNF	-	-	42277	1
	-	-	#42301	#1



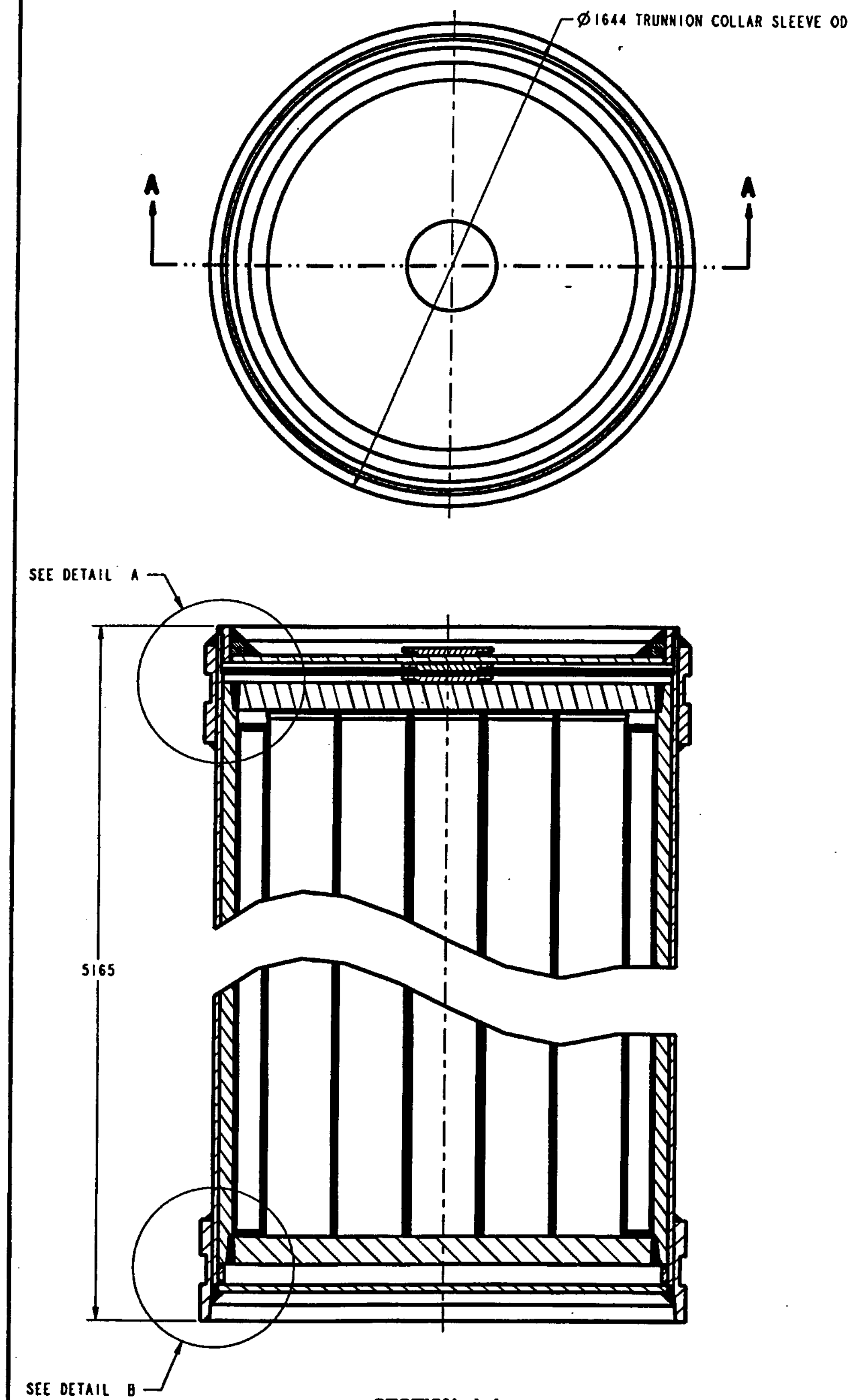
DETAIL B

* CRWMS M&O 1997. WASTE CONTAINER CAVITY SIZE DETERMINATION. BBAA00000-01717-0200-00026 REV 00. LAS VEGAS, NV: CRWMS M&O. ACC: MOL.19980106.0061

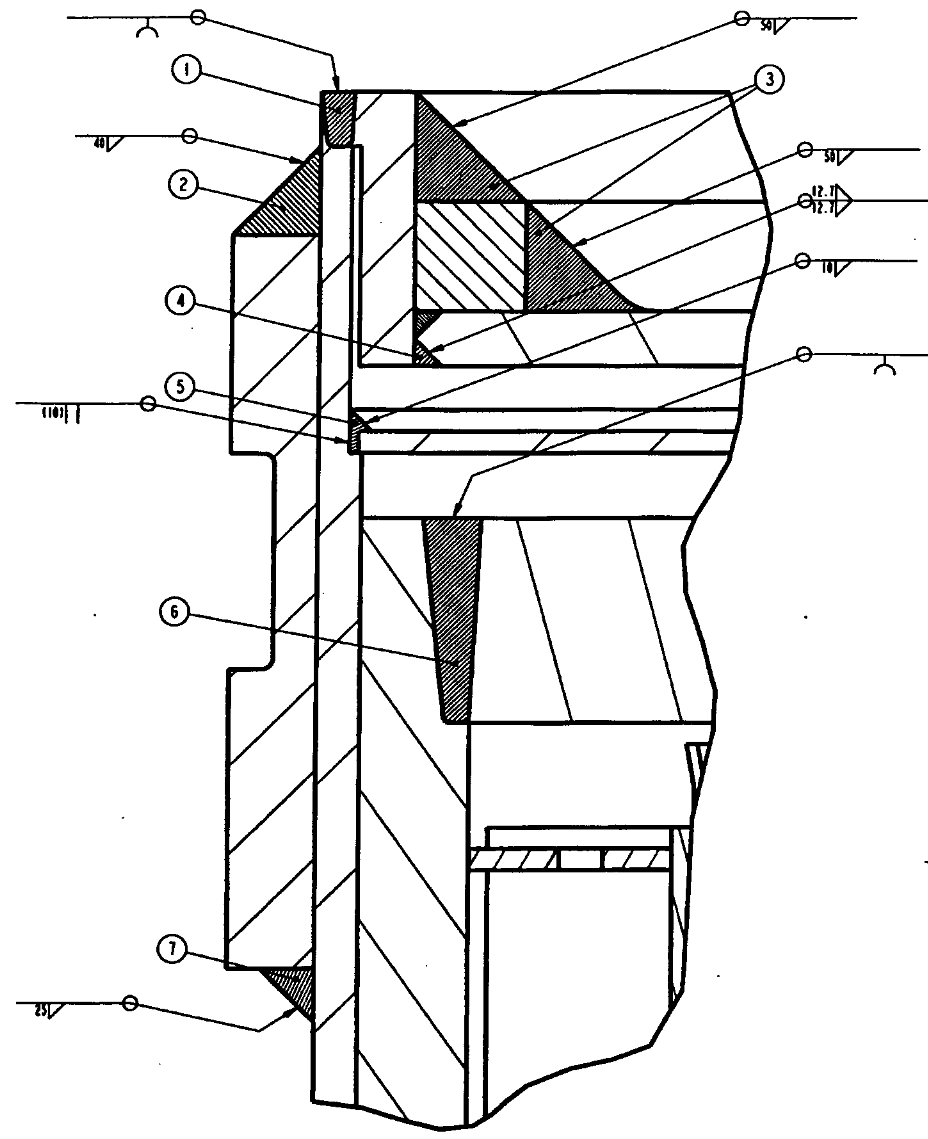
** REFER TO SK-0191 REV 00 "21-PWR WASTE PACKAGE WELD CONFIGURATION"

02 SMB 01/27/00

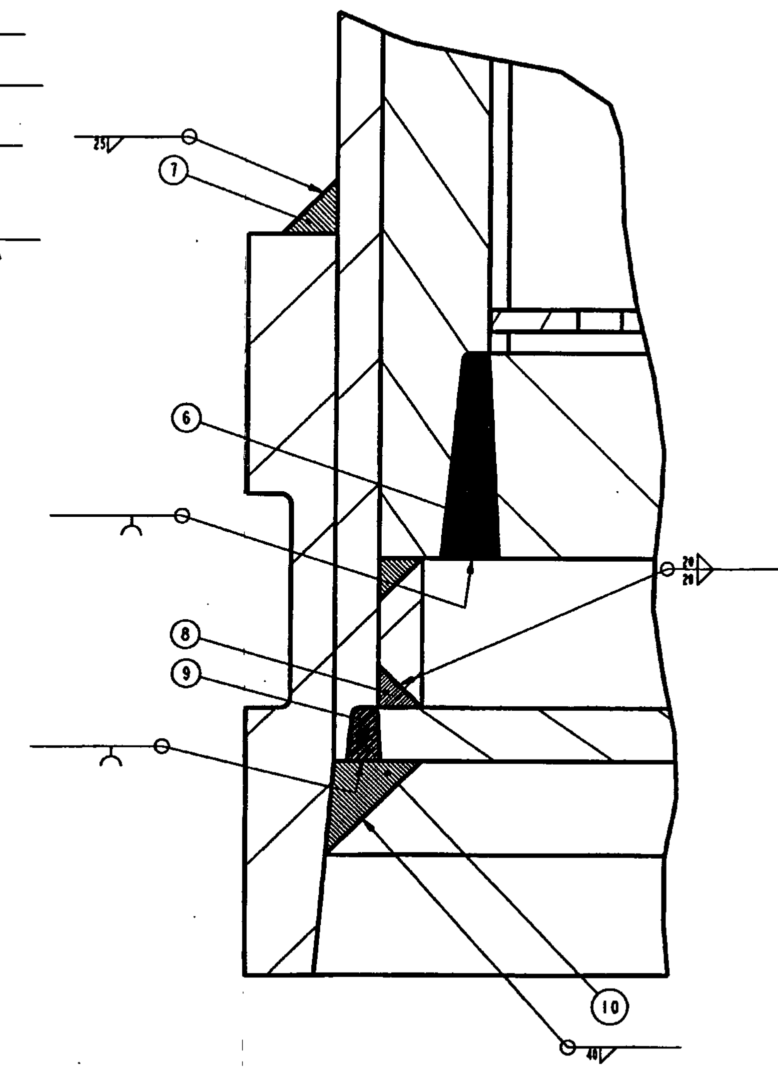
SK-0175 REV ~~01~~ 02 | SHEET 2 OF 2



SECTION A-A



DETAIL A



DETAIL B

WELD	MATERIAL	MASS (KG)	QTY ROD
1	SFA-5.14 N06022	14	1
2	SFA-5.14 N06022	35	1
3	SFA-5.14 N06022	96	1
4	SFA-5.14 N06022	3.1	2
5	SFA-5.14 N06022	3.8	1
6	SFA-5.9 S31680	64	2
7	SFA-5.14 N06022	13	2
8	SFA-5.14 N06022	8.2	2
9	SFA-5.14 N06022	14	1
10	SFA-5.14 N06022	37	1
TOTAL ALLOY 22 WELDS	SFA-5.14 N06022	249	-
TOTAL 316 WELDS	SFA-5.9 S31680	128	-

UNITS: mm

DO NOT SCALE FROM SKETCH

REVISIONS			
REV	DESCRIPTION	DRW BY	DATE
00	ISSUED APPROVED	BH	03/09/00

"FOR INFORMATION ONLY"

21-PWR WASTE PACKAGE WELD CONFIGURATION

SKETCH NUMBER: SK-0191 REV 00

SKETCHED BY: BRYAN HARKINS

DATE: 03/09/00

FILE: /home/pro_library/checkout/sketches/21pwr/sk-0191.dwg

BA 13March00 SMB 03/13/00 3/13/00

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
SPECIAL INSTRUCTION SHEET file dist 05-22-01 mk
Complete Only Applicable Items

1. QA: QA
Page: 1 of: 1

This is a placeholder page for records that cannot be scanned.

2. Record Date 05/22/2001	3. Accession Number ATT-TO MOL.20010522.0198
4. Author Name(s) JABO S. TANG	5. Author Organization N/A

6. Title/Description

GAMMA AND NEUTRON RADIOLYSIS IN THE 21-PWR WASTE PACKAGE

7. Document Number(s) CAL-MGR-NU-000006	8. Version Designator REV 0
9. Document Type DATA	10. Medium CD-ROM

11. Access Control Code
PUB

12. Traceability Designator
DC # 26929

13. Comments
THIS IS A SPECIAL PROCESS DUE TO THE CD-ROM ENCLOSED AS PART OF THE ATTACHMENT III, AND CAN BE LOCATED THROUGH THE RPC

NOTE: SEE ATTACHMENT OF ELECTRONIC SOURCE FILE VERIFICATION FORM PER AP-17.1Q/ICN 3, SECTION 5.1 (C), ELECTRONIC RECORDS

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DC # 26929

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

ELECTRONIC SOURCE FILE VERIFICATION

QA: N/A

1 of 2

1. DOCUMENT TITLE:	
GAMMA AND NEUTRON RADIOLYSIS IN THE 21-PWR WASTE PACKAGE	
2. DOCUMENT IDENTIFIER: CAL-MGR-NU-000006	3. REVISION DESIGNATOR: REV. 00

ELECTRONIC SOURCE FILE INFORMATION

4. ELECTRONIC SOURCE FILE NAME WITH FILE EXTENSION PROVIDED BY THE SOFTWARE: ATTACHMENT III (OUTPUT FILES)		
5. DATE LAST MODIFIED: 05/03/2001 / See ~~Pg~~ #16 (DDV 5-8-01)	6. ELECTRONIC SOURCE FILE APPLICATION: (I.E., EXCEL, WORD, CORELDRAW) Microsoft Word / Word-Pad	7. FILE SIZE IN KILOBYTES: 1,458kB / See ~~Pg~~. 16 (DDV 5-8-01)
8. FILE LINKAGE INSTRUCTIONS/INFORMATION: NONE/NONE		
9. FILE CUSTODIAN: (I.E., DC, OR DC APPROVED CUSTODIAN) DOCUMENT CONTROL	10. FILE LOCATION FOR DC APPROVED CUSTODIAN: (I.E., SERVER, DIRECTORY) N/A - N/A	
11. PRINTER SPECIFICATION (I.E., HP4SI) INCLUDING POSTSCRIPT INFORMATION (I.E., PRINTER DRIVER) AND PRINTING PAGE SETUP: (I.E., LANDSCAPE, 11 X 17 PAPER) Portrait, 8.5 x 11 paper, Hewlett Packard Laser Jet 5Si		
12. COMPUTING PLATFORM USED: (I.E., SUN) PC 116210	13. OPERATING EQUIPMENT USED: (I.E., UNIX, SOLARIS) MICROSOFT WINDOWS EXPLORER	
14. ADDITIONAL HARDWARE/SOFTWARE REQUIREMENT USED TO CREATE FILE(S): NONE	15. ACCESS RESTRICTIONS: (IF ANY) NONE	

COMMENTS/SPECIAL INSTRUCTIONS

16.

ATTACHMENT III FOR CAL-MGR-NU-000006 REV. 00 IS PROVIDED ON A CD.

SEE ATTACHED # 5, 7 for information on attachment

CERTIFICATION

17. NAME (Print and Sign) JABO S. TANG [signature]			18. DATE: 05/08/01
19. ORGANIZATION: WP PROJECT	20. DEPARTMENT: Nuclear Evaluations	21. LOCATION/MAILSTOP: 423/1026A	22. PHONE: 295-4575

DC USE ONLY

23. DATE RECEIVED: 05/09/01	24. DATE REVIEWED: 05/18/2001	25. DATE FILES TRANSFERRED: 05/18/2001
26. NAME (Print and Sign): Marina Blackwell [signature]		27. DATE: 05/18/2001

DI # CAL-MGR-NU-000006

InWPradiols (D:)

File Edit View Help

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A-rod-n-dr.out	3,702KB	OUT File	11/17/2000 3:37 PM
g100k.io	208KB	IO File	11/17/2000 11:27 AM
g10k.io	201KB	IO File	11/17/2000 11:27 AM
g20k.io	202KB	IO File	11/17/2000 11:28 AM
g30k.io	209KB	IO File	11/17/2000 11:28 AM
g40k.io	202KB	IO File	11/17/2000 11:28 AM
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