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Calculation Cover Sheet

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10. Remarks
Attachment IV in Section 8 provides the list of electronic files (Microsoft Excel spreadsheet files and MCNP output files) contained on a Compact Disk (CD), as indicated in Reference 7.17.

Revision History

11. Revision No.	12. Date Approved	13. Description of Revision
00		Initial Issue

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1. PURPOSE

The purpose of this calculation is to perform intact mode and partially degraded mode criticality evaluations of the Department of Energy's (DOE) Enrico Fermi (EF) Spent Nuclear Fuel (SNF) co-disposed in a 5 Defense High-Level Waste (5-DHLW) Waste Package (WP) and emplaced in a Monitored Geologic Repository (MGR). The criticality evaluations estimate the values of the effective neutron multiplication factor, k_{eff}, as a measure of nuclear criticality potential, for the 5-DHLW/DOE SNF WP with intact or partially degraded internal configurations. These evaluations contribute to the WP design.

This document has been prepared in accordance with Procedure NLP-3-27, REV 1, Engineering Calculations, and is subject to the Quality Assurance Requirements and Description (QARD) Document (Ref. 7.16).

2. METHOD

The following methodology is adopted to estimate the values of the effective neutron multiplication factor, k_{eff}, for intact and partially degraded internal configurations of the WP:

(a) computational cases, representing intact and partially-degraded DOE SNF configurations internal to the WP, are developed for the MCNP V4B2LV computer code (Ref. 7.1);

(b) spreadsheet calculations are conducted to determine the detailed input data, as required by the MCNP computer code, for the computational cases of interest developed in (a); and

(c) MCNP V4B2LV computer code (Ref. 7.1), a computer code appropriate for performing nuclear criticality analysis, is run for the computational cases developed above, to estimate the k_{eff} value and its corresponding standard deviation for each case.

3. ASSUMPTIONS

3.1 It is assumed that the fuel pin is a right cylinder. The basis for this assumption is that swaging the ends of a fuel pin does not change the mass of the fuel or its clad (Ref. 7.2, pp. 2, 4, 7, and 8). This assumption is used in Section 5.1.2.

3.2 It is assumed that the impurities in the fuel matrix (B, C, Cr, Fe, Ni, N, O, Zr, Cu, and other), Ref. 7.2, p. 9, are replaced with molybdenum (Mo). The basis for this assumption is that the replacement makes the calculations more conservative, as the majority of the elements present in the impurities have higher thermal neutron absorption cross sections than Mo. This assumption is used in Section 5.1.2.

3.3 It is assumed that the –01 aluminum canister is a right cylinder (ignoring the bail at the top and the short skirt at the bottom). The basis for this assumption is that the volume of the ignored parts is small, compared to the dimensions of the canister itself, and they are far from

the fuel section, which is inside the –04 aluminum canister (Ref. 7.2, p. 14). This assumption is used in Section 5.3.

3.4 It is assumed that the end cups of the –04 canister (made of aluminum 3003) are made of aluminum 6061, as is the main body of the –04 canister. The bases for this assumption are that the volume of end cups comprise a small fraction of the volume of the whole body of the –04 canister, they are at the ends of the canister, and the mass densities of the two kinds of aluminum are not considerably different. This assumption is used in Section 5.

3.5 It is assumed that the stainless steel (SS) 316 dividers and basket lifting rods may be ignored in the MCNP model and iron shot fills their place (Attachment III). The basis for this assumption is that the physical model will be easier to model for the MCNP computer code. The replacement results in more conservative estimates of k_{eff} value, as water fills the void space created by the replacement. This assumption was used in Section 5.3.

3.6 It is assumed that the iron shot bulk density is based on as-poured condition. The basis for this assumption is that the filler (iron shot) bulk density based on as-poured condition is lower than the bulk density based on vibrated condition, and this is conservative, as more void space would be filled with water when the waste package is flooded (Ref. 7.15, pp. 9-11). This assumption is used in Section 5.3 for the cases where the filler is considered.

3.7 It is assumed that waste package is surrounded by water reflector with a thickness of 30 cm. This is based on the established fact among the nuclear criticality safety community that 30 cm is an effectively infinite thickness for water reflectors (Ref. 7.18, p. 27)). This assumption is used in Section 5.3.

3.8 It is assumed that iron shot (Fe) and the aluminum present in the DOE SNF 18-inch canister degrade (oxidize) and produce FeOOH (goethite) and AlOOH (diaspore), respectively. The basis for this assumption is that the choice of FeOOH, as the oxidation product of Fe, over Fe_2O_3 (hematite) makes the calculations more conservative, as the hydrogen present in FeOOH acts as neutron moderator. This assumption is used in Section 5.3.4.

3.9 It is assumed that iron shot (in cases where it is present) and aluminum 6061 (in the case where it is corroded [oxidized]) contain no impurities. The basis for this assumption is that with no impurities the calculations are more conservative, as the impurities include elements, such as Mn, with thermal neutron absorption cross sections higher than that of Fe or Al. This assumption was used in Sections 5.3.1-5.3.4.

4. USE OF COMPUTER SOFTWARE

4.1 SOFTWARE APPROVED FOR QA WORK

The calculation of the WP k_{eff} for the intact and partially degraded modes of the DOE SNF 18-inch canister internal configurations was performed with the MCNP V4B2LV computer code, Computer Software Configuration Item (CSCI) number 30033 V4B2LV (Ref. 7.1). MCNP is

used as a general purpose Monte Carlo neutron, photon and electron transport code. The generalized geometry capability of the code allows the development of detailed, accurate representations of the systems of interest. MCNP calculates k_{eff} for a variety of geometric configurations with neutron cross sections for elements and isotopes described in the Evaluated Nuclear Data File Version B-V (ENDF-B/V). MCNP is appropriate for the fissile isotopes involved in the geometries, and materials required for these analyses. The calculations using the MCNP software were executed on a Hewlett-Packard workstation. The software qualification of the MCNP software is summarized in the Software Qualification Report for the Monte Carlo N-Particle Code (Ref. 7.1). The MCNP evaluations performed for this calculation, while not within the range of MCNP Software Qualification Report (Ref. 7.1), are appropriate for the MCNP physics representations. Access to and use of the MCNP software for this analysis was granted by Software Configuration Management (SCM) and performed in accordance with the QAP-SI series procedures.

The names and location of the electronic copies of the MCNP output files (containing their corresponding echoed input files) are provided in Section 8.

4.2 SOFTWARE ROUTINES

Microsoft Excel 97, loaded on a 266 MHz Pentium II PC. Arithmetic calculations involved in determining the input data for the MCNP computer code are performed electronically in this spreadsheet software package. Section 5.4 indicates the general equations used to calculate the number densities and the mass densities for homogenized mixtures. Other involved equations, if any, are documented within the spreadsheets. The names, locations, and other file attributes of the electronic copies of the well-documented spreadsheet files, along with a brief description of each file, as to what each spreadsheet does, are provided in Attachment IV. Hardcopies of the spreadsheet files are provided in Attachment V.

5. CALCULATION

The criticality evaluations are performed for the 5-DHLW/DOE SNF waste package assembly, considering the intact mode and partially degraded modes.

Existing data are used in this calculation. Therefore, the use of any data from this calculation for input into documents supporting procurement, fabrication, or construction is required to be identified and tracked as TBV (to be verified) in accordance with appropriate procedures.

Figure 5-1 shows the main components of a typical 5-DHLW/DOE SNF WP configuration. Attachment I provides a sketch of the 5-DHLW/DOE SNF disposal container utilized for the co-disposal of the EF SNF. For the criticality evaluations reported here the DOE SNF canister (the canister at the center of the WP [Figure 5-1]) contains Enrico Fermi SNF and the surrounding 5 canisters contain HLW glass.

Attachment II provides a sketch of the 18-inch outer diameter (OD) DOE standardized SNF canisters, referred to as the DOE 18-inch canisters, whose differences are in axial dimensions.

The short canister, with an internal length of 2575 mm and an external length of 2999 mm, is used for the co-disposal of EF SNF.

The DOE 18-inch canister accommodates a stack of two sets of 4-inch OD tubes, as indicated in Attachment III. Twelve tubes, welded to a base plate, comprise each set. A spacer at the top of the top tube set restrains the stacked set of tubes in place. A shipping canister made of aluminum and referred to as –01 canister (Ref. 7.2, p. 10) is contained in each tube. Each –01 canister contains an aluminum canister, referred to as the –04 canister (Ref. 7.2, p. 10). The –04 canister contains 140 SNF pins of the Enrico Fermi fast reactor. The fuel pins have zirconium clad and are derodded. The void space outside the tubes is filled with iron shot and gadolinium phosphate. 1%, by volume, of the Fe-$GdPO_4$ mixture is $GdPO_4$. The void space inside each tube, but outside the –01 canister, is filled with the same mixture of Fe-$GdPO_4$.

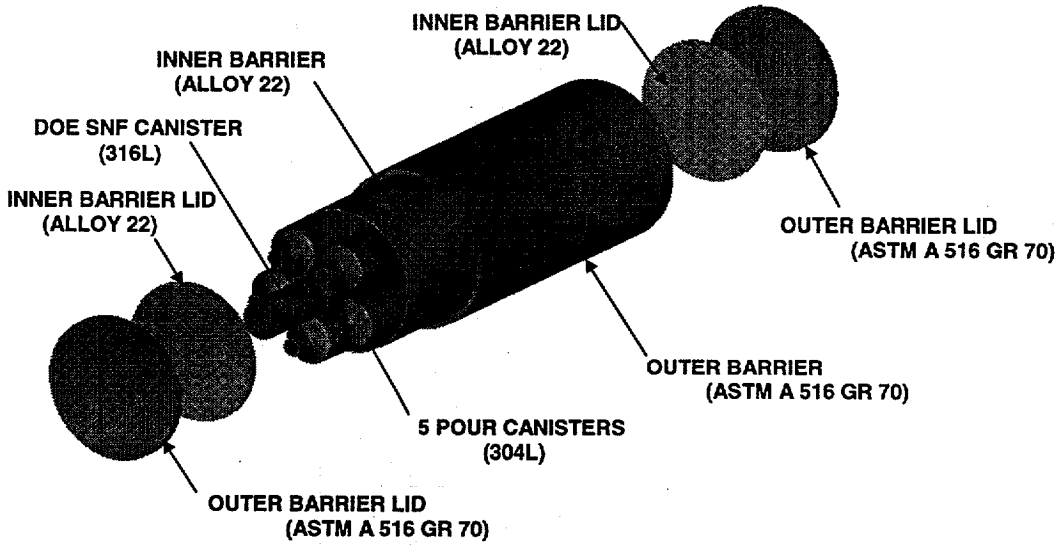

Figure 5-1. 5-DHLW/DOE SNF WP Design

5.1 ENRICO FERMI FAST REACTOR FUEL CHARACTERISTICS

The dimensions and composition of a typical fuel pin and its clad are provided in this section, as given in Ref. 7.2, pp. 7-8. The weight percent of each element or isotope in the fuel and the density of the fuel are calculated.

5.1.1 Fuel Pin Dimensions

The zirconium-clad fuel pins are 30.5 in. long (fuel matrix length). The diameter of the fuel matrix is 0.148 in. and the outer diameter of the clad is 0.158 in. There is no gap between the fuel and the clad.

5.1.2 Fuel Pin Composition and Density

Table 5-1 shows the composition of an Enrico Fermi fast reactor fuel pin. The composition of the fuel is that of fresh (non-irradiated) fuel, as no credit is taken for fuel burnup.

Table 5-1. Composition of an Enrico Fermi Fast Reactor Fuel Pin (Fresh Fuel)

Element/Isotope/Impurities[a]	Mass (g)	Weight Percent in Fuel Pin (No Clad)	Note
U (U-235 & U-238)	133.9		25.69% U-235 enriched[a]
U-235	34.4	22.96[b]	
U-238	99.5	66.41[b]	
Mo	15.31	10.63[b]	Impurities were added to Mo mass for conservatism
Impurities	0.609		
Total (U+Mo +Impurities)	149.819		
Zr Cladding	9.2		

(a) Reference 7.2, pp. 7-8.
(b) Calculated value.

The following calculations provide the density of a fuel pin (with no clad):

Fuel pin radius: $R = 0.148 \text{ in.} * (2.54 \text{ cm}/1 \text{ in.})/2 = 0.18796 \text{ cm}$
Fuel pin length: $H = 30.5 \text{ in.} * (2.54 \text{ cm}/1 \text{ in.}) = 77.47 \text{ cm}$
Fuel pin volume: $V = \pi R^2 H = \pi * (0.18796 \text{ cm})^2 * (77.47 \text{ cm}) = 8.598 \text{ cm}^3$
Fuel pin density: $\rho = (\text{fuel pin mass})/\text{fuel pin volume}$
$= (149.819 \text{ g})/8.598 \text{ cm}^3 = 17.424 \text{ g/cm}^3$

5.2 COMPOSITIONS AND DENSITIES OF NON-FUEL MATERIALS

Tables 5-2 through 5-7 show the composition of the non-fuel materials present in the 5-DHLW WP used for the co-disposal of Enrico Fermi SNF. A value of 6.5 g/cm^3 was used as the density of zirconium (the fuel clad material) (Ref. 7.2, p. 7). The density of anhydrous gadolinium phosphate was estimated to be 5 g/cm^3, which is the average density reported for monazite (anhydrous rare earth phosphate [Ref. 7.19, p. 413]).

Table 5-2. Chemical Composition of Aluminum 6061

Element	Weight Percent[a]	Value Used
Si	0.4 - 0.8	0.6
Fe	0.7 (max)	0.7
Cu	0.15 - 0.4	0.275
Mn	0.15 (max)	0.15
Mg	0.8 – 1.2	1.0
Cr	0.04 - 0.35	0.195
Zn[b]	0.25 (max)	0.25[b]
Ti	0.15 (max)	0.15
Others[c]	0.15 (Max)	0.15[c]
Al	Balance	96.93
Density = 2.71 g/cm^3 (Ref. 7.4, p. 619 and Ref. 7.6, p. 7; the range is 2.70-2.73)		

(a) Reference 7.3, p.338, Table 1.
(b) Replaced by Al in the input data for the MCNP computer code (MCNP cross section library does not contain Zn).
(c) Replaced by Al.

Table 5-3. Chemical Composition of Type 316L Stainless Steel

Element	Weight Percent[a]	Value Used
C	0.03 (max)	0.03
Mn	2.00 (max)	2.00
P	0.045 (max)	0.045
S	0.03 (max)	0.03
Si	1.00 (max)	1.00
Cr	16.00 - 18.00	17.00
Ni	10.00 - 14.00	12.00
Mo	2.00 - 3.00	2.50
N	0.10 (max)	0.10
Fe	Balance (assumed)	65.295
Density = 7.98 g/cm^3 (Ref. 7.6, p. 7)		

(a) Reference 7.5, P. 2, Table 1.

Table 5-4. Chemical Composition of Type 304L Stainless Steel

Element	Weight Percent[a]	Value Used
C	0.03 (max)	0.03
Mn	2.00 (max)	2.00
P	0.045 (max)	0.045
S	0.03 (max)	0.03
Si	0.75 (max)	0.75
Cr	18.00 - 20.00	19.00
Ni	8.00 - 12.00	10.00
N	0.10 (max)	0.10
Fe	Balance (assumed)	68.045
Density = 7.94 g/cm^3 (Ref. 7.6, p. 7)		

(a) References 7.7, p. 2, Table 1 and 7.8, p.315, Table 1.

Table 5-5. Chemical Composition of HLW Glass (TBV)

Element	Weight Percent[a]	Element	Weight Percent[a]
Li-6	9.5955E-02	Li-7	1.3804E+00
B-10	5.9176E-01	B-11	2.6189E+00
O	4.4770E+01	F	3.1852E-02
Na	8.6284E+00	Mg	8.2475E-01
Al	2.3318E+00	Si	2.1888E+01
S	1.2945E-01	K	2.9887E+00
Ca	6.6188E-01	Ti	5.9676E-01
Mn	1.5577E+00	Fe	7.3907E+00
Ni	7.3490E-01	P	1.4059E-02
Cr	8.2567E-02	Cu	1.5264E-01
Ag	5.0282E-02	Ba-137[b]	1.1267E-01[b]
Pb	6.0961E-02	Cl	1.1591E-01
Th-232	1.8559E-01	Cs-133	4.0948E-02
Cs-135	5.1615E-03	U-234	3.2794E-04
U-236	1.0415E-03	Zn[c]	6.4636E-02[c]
U-235	4.3514E-03	U-238	1.8666E+00
Pu-238	5.1819E-03	Pu-239	1.2412E-02
Pu-240	2.2773E-03	Pu-241	9.6857E-04
Pu-242	1.9168E-04		
Density at 25°C = 2.85 g/cm^3 (Ref. 7.10, p. 2.2.1.1-4)			

(a) Reference 7.9, p. 7.
(b) Ba-138 was used in the input data for the MCNP computer code (MCNP cross section library does not contain Ba-137).
(c) Replaced by Al in the input data for the MCNP computer code (MCNP cross section library does not contain Zn).

Table 5-6. Chemical Composition of Alloy 22

Element	Weight Percent[a]	Value Used
C	0.015 (max)	0.015
Mn	0.50 (max)	0.50
Si	0.08 (max)	0.08
Cr	20.0 - 22.5	21.25
Mo	12.5 - 14.5	13.50
Co	2.50 (max)	2.50
W	2.5 - 3.5	3.00
V	0.35 (max)	0.35
Fe	2.0 - 6.0	4.00
P	0.02	0.02
S	0.020	0.020
Ni	Balance	54.765
Density = 8.69 g/cm^3 (References 7.11, p. 3, and 7.12, p.2)		

(a) References 7.11, p. 678, Table 1 and 7.12, p.2, Table 1.

Table 5-7. Chemical Composition of ASTM A 516 Grade 70

Element	Weight Percent Range[a]	Value Used
C	0.30 (max)	0.30
Mn	0.85-1.20	1.025
P	0.035 (max)	0.035
S	0.035 (max)	0.035
Si	0.15-0.40	0.275
Fe	Balance (assumed)	98.33
Density = 7.85 g/cm^3 (Ref. 7.14, p. 21)		

(a) Reference 7.13, pp. 320-321.

5.3. NUCLEAR CRITICALITY CALCULATIONS

Nuclear criticality evaluations of the Enrico Fermi SNF, co-disposed in a 5-DHLW/DOE SNF WP, are performed for two different "modes" of the DOE 18-inch canister contained in the WP (Attachments II and III): intact mode and "partially degraded" mode. The EF fuel pins contained within and the WP contents outside of the DOE 18-inch canister are considered to be intact in all cases considered in this report. The cases considered for these two modes, and their associated MCNP computer code representations are discussed in Sections 5.3.1 through 5.3.3.

5.3.1 Intact Mode

For the intact mode, the contents of the DOE 18-inch canister are in "as-welded/loaded position and condition," as depicted in Figures 5-2 through 5-6 However, since the WP is to be emplaced horizontally in the MGR, the –01 and –04 canisters are considered to be settled inside the tubes and the –01 canisters, respectively, as depicted in Figure 5-7.

Moreover, to examine the impact of fuel pin arrangement on the MCNP code estimate of the k_{eff} value, different arrangements of the fuel pins inside the –04 canisters are considered. Figures 5-8 and 5-9 show different fuel pin arrangements.

As shown in Figures 5-5 and 5-6, the tubes are in their original (welded) positions and each tube is concentric with the –01 and –04 aluminum canisters contained therein. A case similar to the one shown in Figures 5-5 and 5-6, but with the –01 and –04 canisters contained in the three "central" tubes shifted toward the center of the DOE 18-inch canister was also studied. The void space outside and inside the tubes, but outside the –01 canisters, is filled with iron shot (Fe) and gadolinium phosphate ($GdPO_4$). The $GdPO_4$ is 1 percent, by volume, of the Fe-$GdPO_4$ mixture. The iron shot is used for moderator (water) exclusion and the gadolinium phosphate acts as neutron absorber.

It should be noted that the Fe and $GdPO_4$ used to fill the above-mentioned void space fill about 58.82% of the void space (Section 8, Attachment VI, based on Ref. 7.15, pp. 9-11). In other words, about 41.18% of the volume containing filler is void space and is filled with water when the WP is flooded. A case with no filler and no gadolinium phosphate was also studied to determine the impact of the absence of filler and neutron absorber on the k_{eff} of the WP in the intact mode. Water density was also varied to evaluate its impact on the k_{eff} value. This density variation simulates filling in the presence of an unspecified moderator displacer. The waste package is considered to be flooded in all cases. Water fills all void space inside the WP. Figure 5-10 shows that in the absence of filler (iron shot or gadolinium phosphate) water fills all void space available.

Spreadsheet calculations were performed for the cases where filler material is used to determine the required input data for the MCNP computer code. The names, locations, and other file attributes of the electronic copies of the well-documented spreadsheet files, along with a brief

description of each file, as to what each spreadsheet does, are provided in Attachment IV. Hardcopies of the spreadsheet files are provided in Attachment V. The spreadsheet files used, except for the one named "fuelcomp.xls," involve Fe, the filler material, in the calculations.

The calculations performed considered the WP to be surrounded by water (30 cm), as shown in Figures 5-2 and 5-3. This water acts as neutron reflector (Ref. 7.18, p. 27).

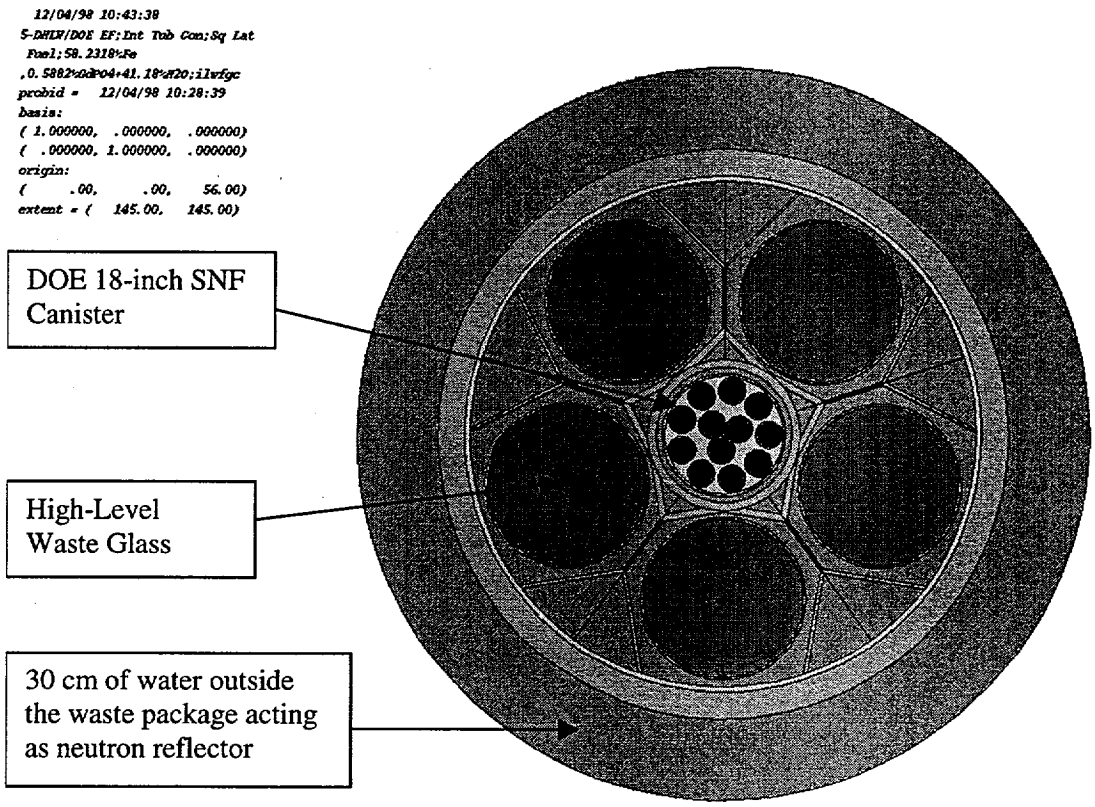

Figure 5-2. A Horizontal Cross-sectional View of the 5-DHLW/DOE SNF WP for the Intact Mode

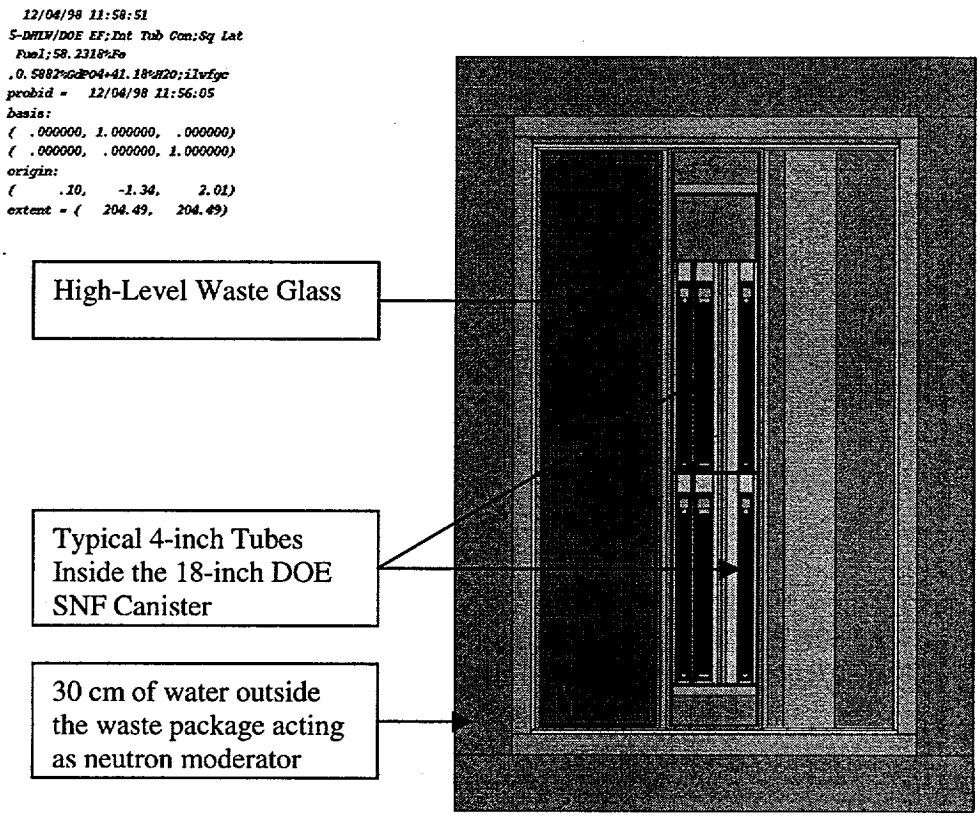

Figure 5-3. A Vertical Cross-sectional View of the 5-DHLW/DOE SNF WP for the Intact Mode

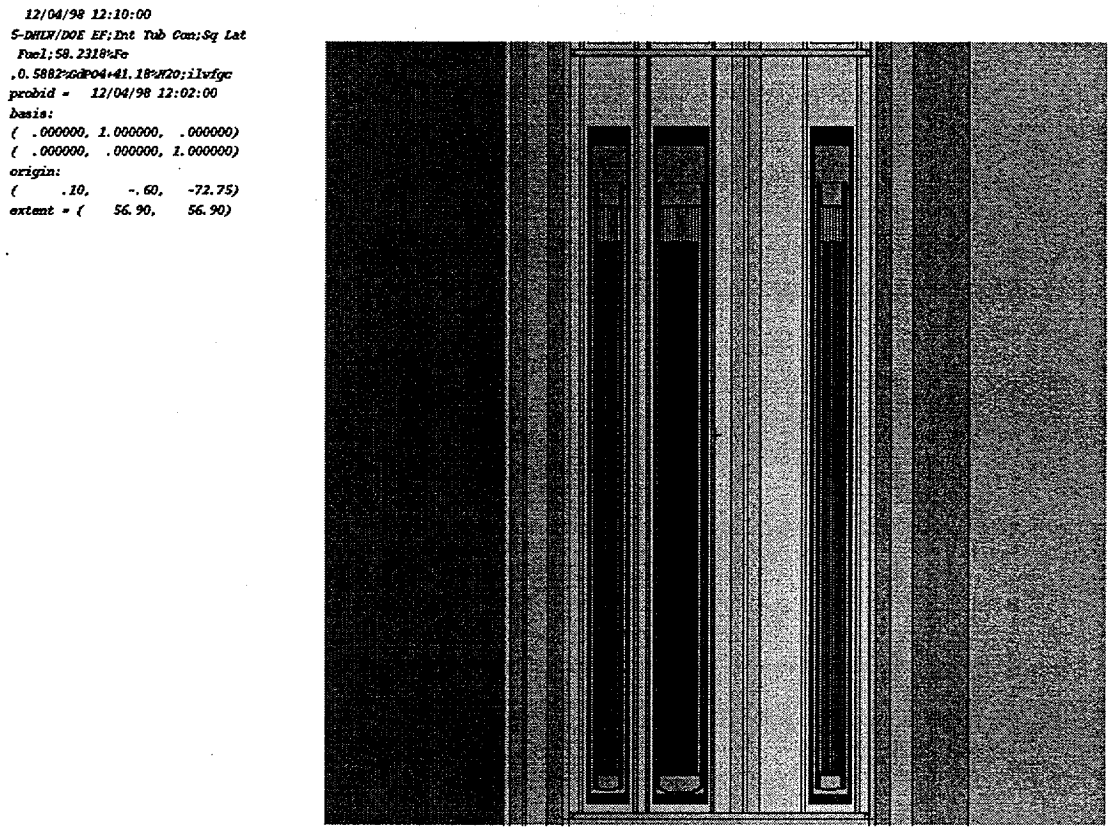

Figure 5-4. A Vertical Cross-sectional View of the 5-DHLW/DOE SNF WP Showing the Contents of Typical Tubes

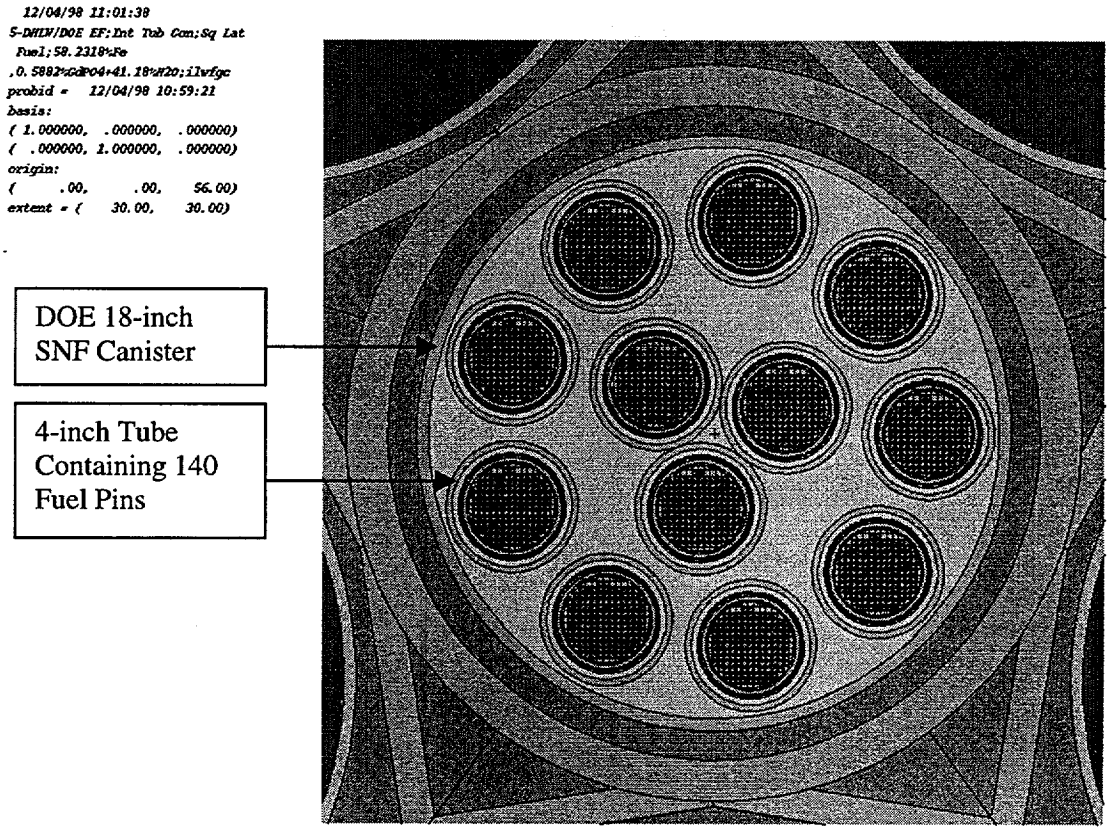

Figure 5-5. A Horizontal Cross-sectional View of the 5-DHLW/DOE SNF WP Showing the Contents of the DOE 18-inch SNF Canister for the Intact Mode

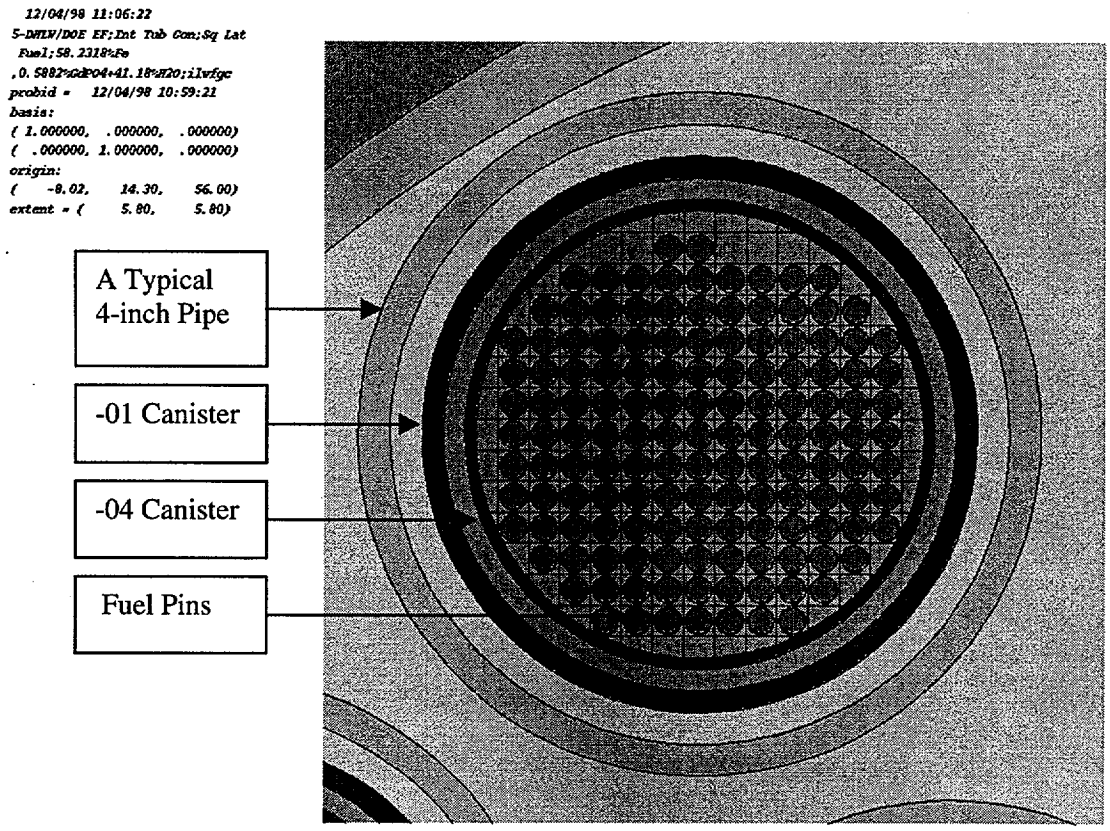

Figure 5-6. A Horizontal Cross-sectional View of the 5-DHLW/DOE SNF WP Showing the Contents of a Typical Tube for the Intact Mode

```
  12/04/98 11:25:28
5-DHLW/DOE EF:Int Tub Can;Sq Lat
 Fuel;58.2318%Fe
,0.5882%GdPO4+41.18%H2O; ilvfg
probid =  12/04/98 11:09:51
basis:
( 1.000000,  .000000,  .000000)
(  .000000, 1.000000,  .000000)
origin:
(    -8.06,    14.30,    56.00)
extent = (    6.00,    6.00)
```

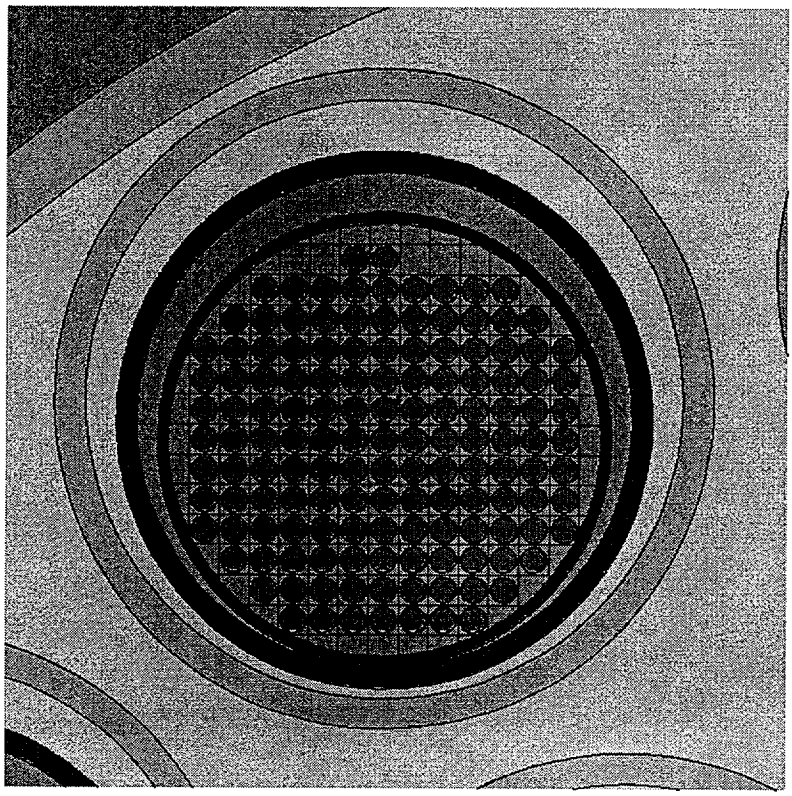

Figure 5-7. A Horizontal Cross-sectional View of the 5-DHLW/DOE SNF WP Showing the Contents of a Typical Tube, where the –01 and –04 Canisters are Settled

```
  12/04/98 11:33:39
S-DMIX/DOE EF;Int Tub Can;Dis
 Fuel;58.2318%Fe,0.
5882%Gd2O4+41.18%H2O; idxfg
probid =  12/04/98 11:29:50
basis:
( 1.000000,  .000000,  .000000)
(  .000000, 1.000000,  .000000)
origin:
(    -8.06,    14.26,    56.00)
extent = (    5.68,     5.68)
```

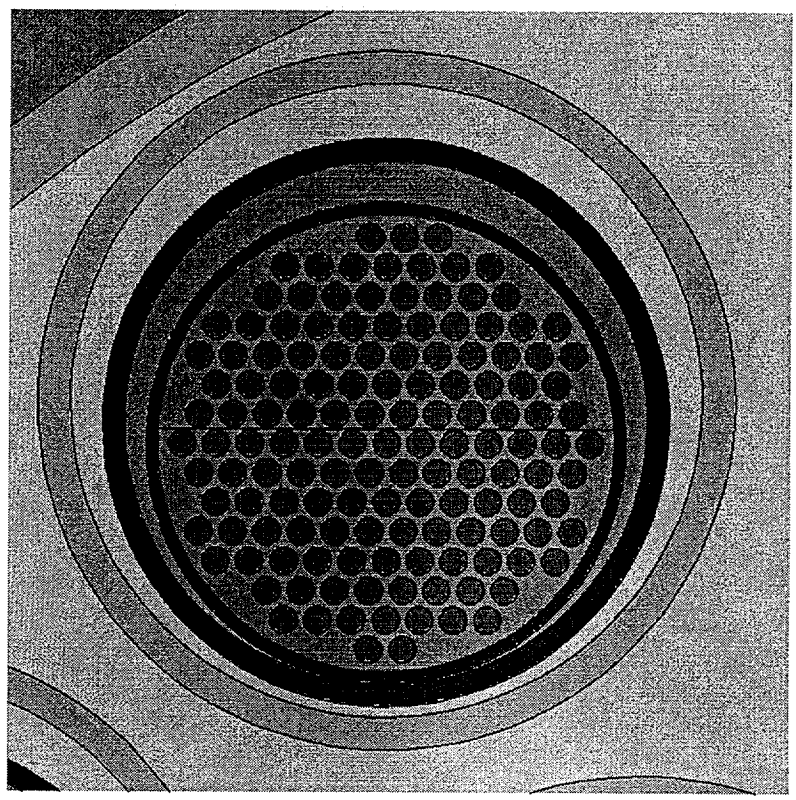

Figure 5-8. Hexagonal Arrangement of 140 Fuel Pins Contained in a Typical –04 Canister

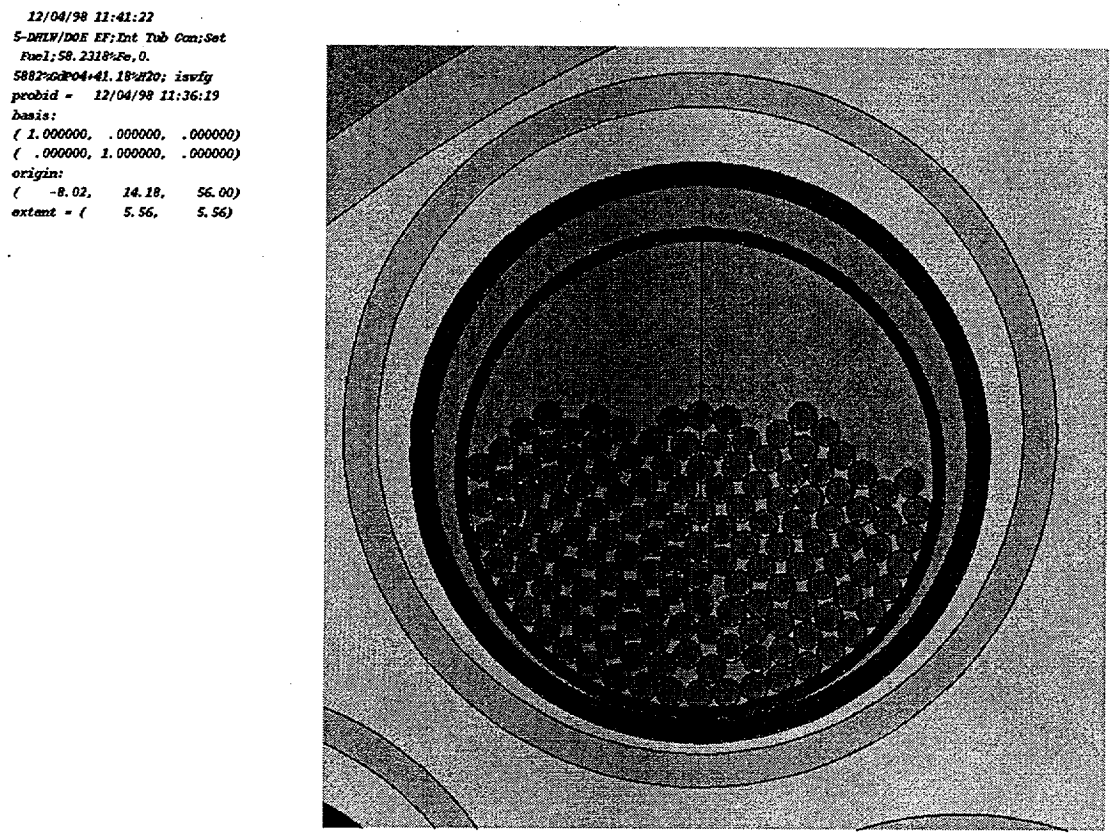

Figure 5-9. The Arrangement of 140 Fuel Pins when Randomly Settled Inside a Typical –04 Canister

```
  12/04/98 11:50:57
5-DHLW/DOE SNF VP;EF Fuel;Intact
 Tubes Con;Sq Lat Fuel;H2O
 everywhere; ilv
probid =  12/04/98 11:44:12
basis:
( 1.000000,  .000000,  .000000)
(  .000000, 1.000000,  .000000)
origin:
(    -8.22,    14.18,    56.00)
extent = (    5.68,     5.68)
```

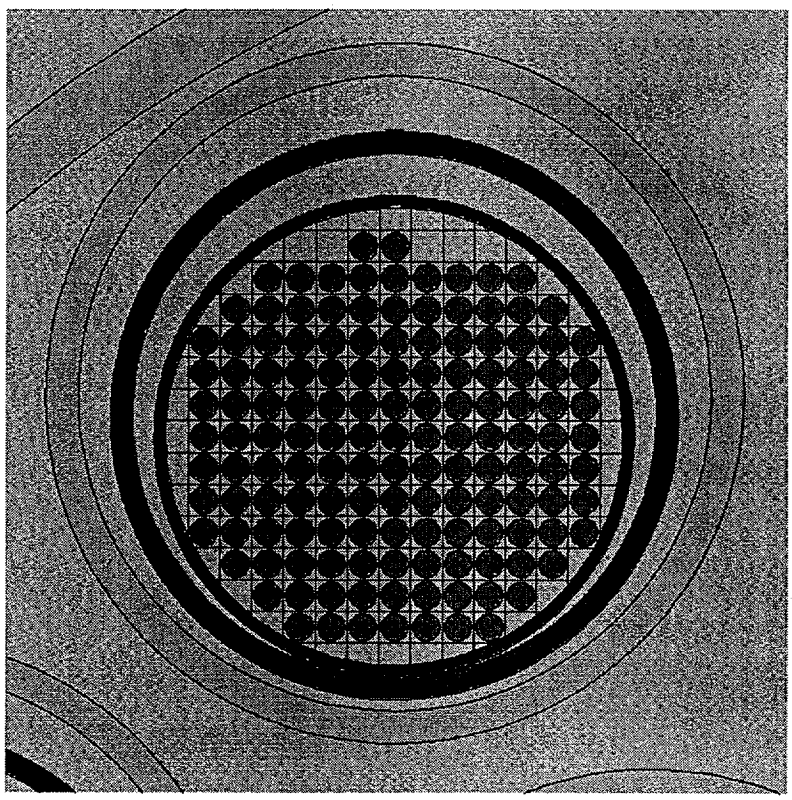

Figure 5-10. Water Fills All Void Space Available Inside the DOE 18-inch SNF Canister in the Absence of Fe-$GdPO_4$ Mixture

5.3.2 Partially Degraded Mode with no Oxidation of Fe or Al

The partially degraded mode refers to the cases where the 24 tubes contained in the DOE 18-inch SNF canister no longer remain in their original (welded) arrangement and settle into a possibly more reactive configuration. Alternative tube arrangements were evaluated to identify their impact on k_{eff} value. Figures 5-11 and 5-13 show the tube arrangements considered for this mode. In the calculations for this mode, the Fe (iron shot) and the –01 and –04 aluminum canisters are considered non-corroded.

Moreover, since the WP is to be emplaced horizontally in a MGR, the –01 and –04 canisters are considered to be settled inside the tubes and the –01 canisters, respectively, as depicted in Figure 5-7.

In addition to the configurations mentioned above the following conditions are also considered for the partially degraded mode criticality calculations:

(a) different arrangement of tubes
(b) presence of iron shot (Fe) and $GdPO_4$
(c) presence of Fe but absence of $GdPO_4$
(d) no Fe-$GdPO_4$ mixture (water fills all void space available [Figures 5-12 and 5-14])

Spreadsheet calculations were performed for this case to determine the required input data for the MCNP computer code. The names, locations, and other file attributes of the electronic copies of the well-documented spreadsheet files, along with a brief description of each file, as to what each spreadsheet does, are provided in Attachment IV. Hardcopies of the spreadsheet files are provided in Attachment V. The spreadsheets named fuelcomp.xls, Fe-W5882.xls, and degFeAl.xls do not involve $GdPO_4$ in their calculations.

5.3.3 Impact of Partial Flooding, Fuel Pin Spacing, and Absence of Manganese on k_{eff}

The partially degraded mode with gravitationally stable tube configuration and no oxidation of Fe or Al, Figure 5-11, was considered as the base case to study the impact on k_{eff} of partial flooding, fuel pin spacing, and absence of manganese (Mn) from the material compositions.

(a) Partial Flooding

To study the impact of partial flooding on the k_{eff} value, it was assumed that water fills the void space in –01 and –04 aluminum canisters, and that there is no water in the remaining void space.

(b) Fuel Pin Spacing

The fuel pin spacing was changed from 0.06 cm (surface to surface distance in the base case) to 0.48 cm in 7 steps to study the impact on the k_{eff} value when more spacing between adjacent fuel pins (less than 140 fuel pins in each –04 aluminum canister) is considered.

(c) No Mn in the Materials for which Maximum Amount of Mn was Used in their Compositions

Since Mn is a neutron absorber and the calculations performed considered the maximum amount of Mn for Al 6061, SS 316L, SS 304L, and Alloy 22 (Section 5.2), the base case (Fig. 5-11) with no Mn in the said materials (a conservative case) was run to determine the extent of increase in the k_{eff} value.

(d) Combined Effects of Partial Flooding, Optimum Fuel Pin Spacing, and Absence of Mn on the k_{eff} Value

The base case (Fig. 5-11) with partial flooding, as discussed in (a) above, with optimum fuel spacing, based on the study discussed in (b) above, and with no Mn in the materials listed in (c) above was run to determine the combined impact of all three conservative assumptions on the k_{eff} value.

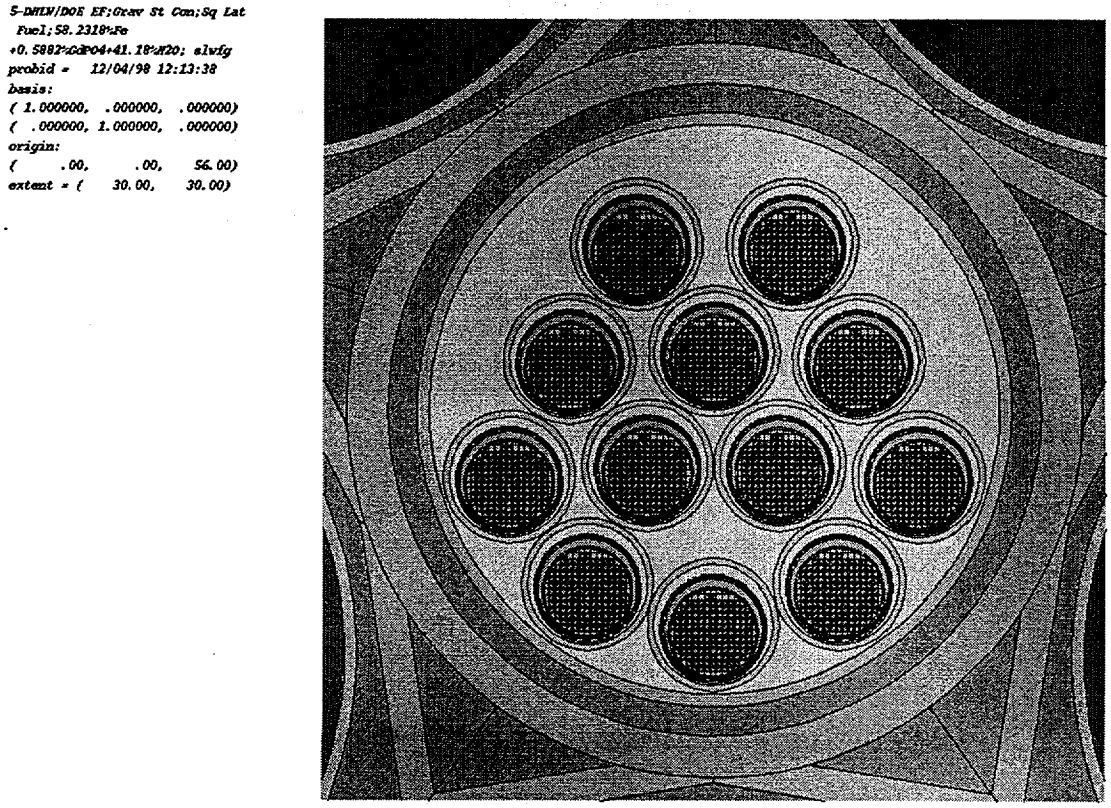

Figure 5-11. Gravitationally Stable Arrangement of Tubes Inside the DOE 18-inch SNF Canister

```
 12/04/98 12:23:16
5-DHLW/DOE EF; Gravitationally
 Stab Con; Sq Lat Fuel; H2O
 everywhere; slv
probid =  12/04/98 12:20:34
basis:
( 1.000000,  .000000,  .000000)
(  .000000, 1.000000,  .000000)
origin:
(     .00,     .00,    52.00)
extent = (   30.00,   30.00)
```

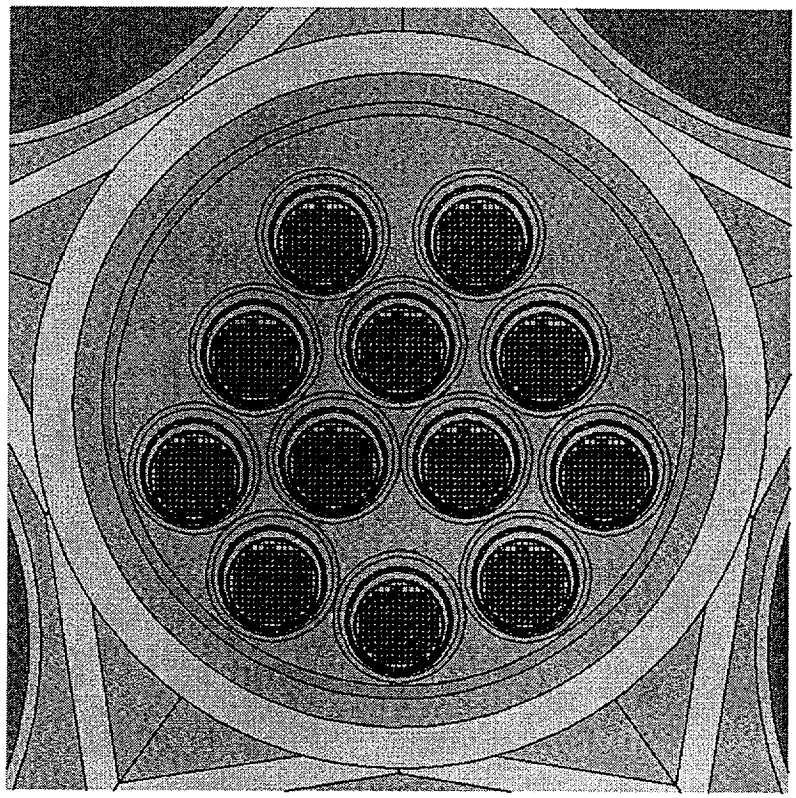

Figure 5-12. Water Fills All Void Space Available in the DOE 18-inch Canister in the Absence of any Filler Material – Gravitationally Stable Arrangement

```
  12/04/98 12:28:48
S-DHLW/DOE EF;HCP Conf;Sq Lat
 Fuel;59.2318%Fe,0.
5882%GdPO4+41.18%H2O; hlwfg
probid =  12/04/98 12:26:01
basis:
( 1.000000,  .000000,  .000000)
(  .000000, 1.000000,  .000000)
origin:
(      .00,      .00,    56.00)
extent = (    30.00,    30.00)
```

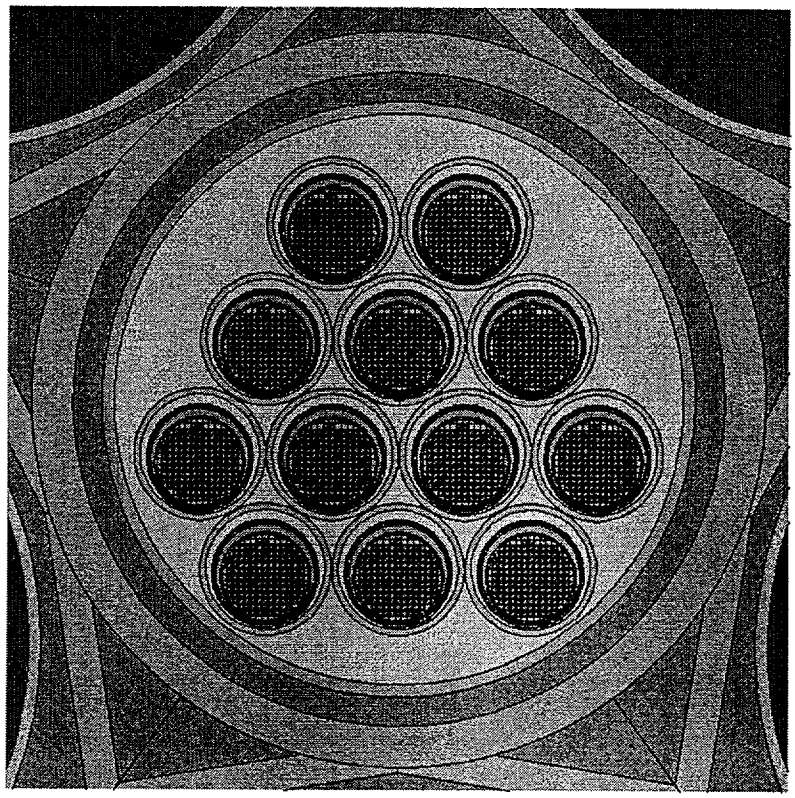

Figure 5-13. A Hexagonal Arrangement of the Tubes that is not Gravitationally Stable

```
  12/04/98 12:30:51
5-DHLW/DOE EF; Hex Close Packed
 Can; Sq Lat Fuel; H2O
 everywhere; hlw
probid =  12/04/98 12:27:49
basis:
( 1.000000,  .000000,  .000000)
(  .000000, 1.000000,  .000000)
origin:
(     .00,     .00,    56.00)
extent = (   30.00,   30.00)
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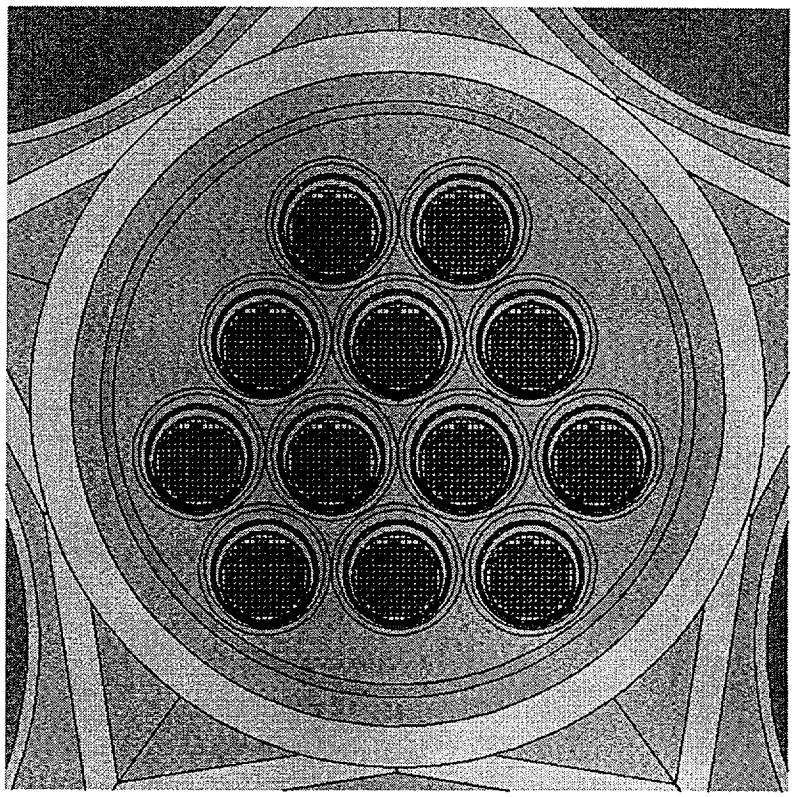


Figure 5-14. Water Fills All Void Space Available in the DOE 18-inch SNF Canister in the Absence of any Filler Material – Gravitationally Unstable Arrangement

5.3.4 Partially Degraded Mode with Corroded (Oxidized) Fe and Al

A case with a partial degradation more advanced than that involved in Section 5.3.2 was also studied. This case considered the oxidation of Fe (iron shot) and Al (aluminum body of the –01 and –04 canisters) into FeOOH (goethite) with a density of 4.2 g/cm^3 (Ref. 7.19, p. 240) and AlOOH (diaspore) with a density of 3.4 g/cm^3 (Ref. 7.19, p. 172), respectively. The neutron absorber, $GdPO_4$, remains insoluble.

The expansion ratio of FeOOH (volume of corrosion product divided by volume of corroded element) is 2.97 and that of AlOOH is 1.77. The name (degFeAl.xls), location, and other file attributes of the electronic copy of the spreadsheet file determining the expansion ratios, along with a brief description, as to what the spreadsheet does, are provided in Attachment IV. The hardcopy of the spreadsheet file is provided in Attachment V, p. 9.

The geometry of the material inside the tubes is depicted in Figures 5-15 and 5-16. FeOOH, and any non-oxidized portion of the original Fe fill the void space outside the tubes. Inside each tube, all Al is oxidized and AlOOH surrounds the fuel bundles like a cylindrical shell (radially bounded by the inner surface of the originally existing –04 canister and the outer shell of the originally existing –01 canister). The length of the shell was considered to be equal to that of the fuel bundle. A homogenized mixture of remaining AlOOH and H_2O fills the void space among the fuel pins. The void space outside the said shell (but inside the tube) is filled with FeOOH and any non-oxidized portion of the Fe originally filling the void space between the tube and the originally existing –01 canister.

Spreadsheet calculations were performed for this case to determine the required input data for the MCNP computer code. The name (FeOOH-AlOOH.xls), location, and other file attributes of the electronic copy of the corresponding well-documented spreadsheet file, along with a brief description, as to what the spreadsheet does, are provided in Attachment IV. The hardcopy of the spreadsheet file is provided in Attachment V, pp. 10-14.

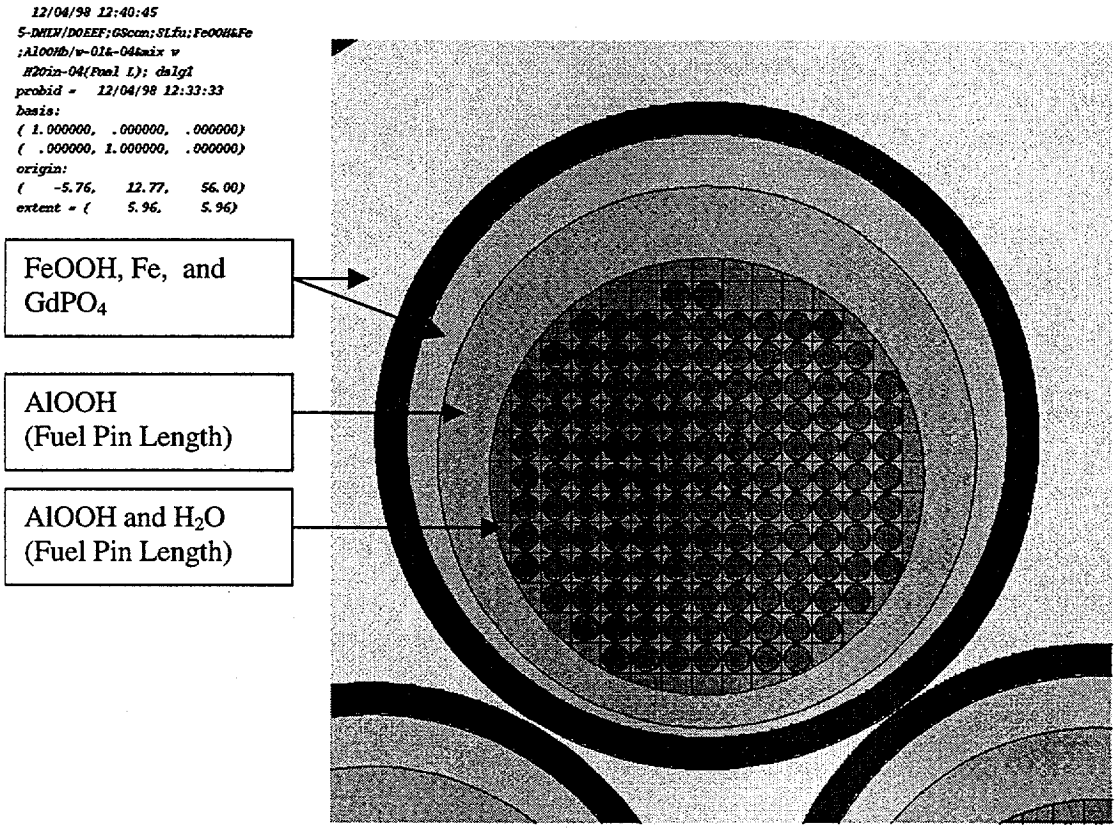


Figure 5-15. A Radial Cross-sectional View of the Contents of a Typical Tube for the Partially Degraded Mode with Fe and Al Oxidation

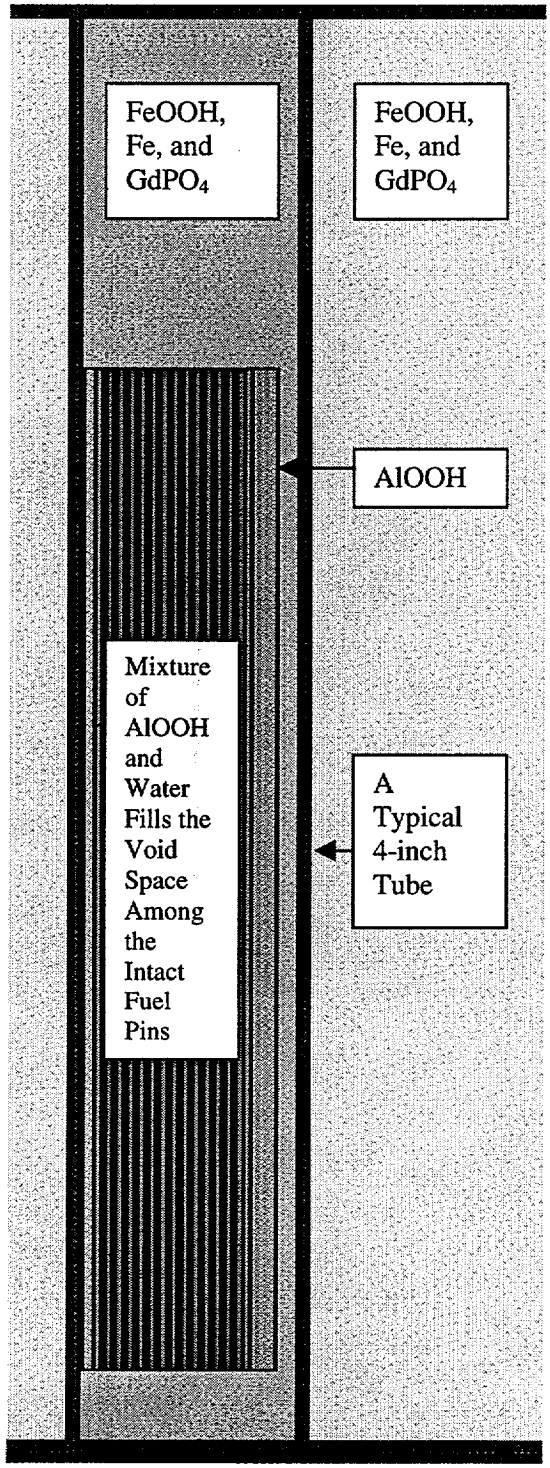


Figure 5-16. An Axial Cross-sectional View of the Contents of a Typical 4-inch Tube for the Partially Degraded Mode with Fe and Al Oxidation

5.4 CALCULATION OF NUMBER DENSITIES

Attachment V (Section 8) contains the hardcopies of the Microsoft Excel 97 spreadsheet files used to calculate the weight fractions, number densities, and mass densities required by the MCNP computer code, as well as to perform calculations involved in determining the said densities. Attachment IV (Section 8) provides the location of the electronic files of the spreadsheets; the table in this attachment provides a brief statement as to what each spreadsheet does.

The general equations used to calculate the number densities of materials involved in homogenized mixtures are shown below:

$$N_i = (d_i * v_i * N_a) / A_i$$

where,

N_i = atom density of i^{th} material (atoms/b-cm, 1 b (barn) = 10^{-24} cm^2).
d_i = mass density of i^{th} material (g/cm^3).
v_i = volume fraction of i^{th} material.
N_a = Avogadro's Number (0.6022 atoms-cm^2/mole-b).
A_i = atomic weight of i^{th} material (g).

The density of a homogenized mixture of n materials (d_{mix}), given the volume fraction and the mass density of each component, is calculated as follows:

$$d_{mix} = d_1 * v_1 + d_2 * v_2 + \ldots + d_n * v_n.$$

In the cases where filler (iron shot) is used, the number density calculations involve the volume occupied by Fe and the volume remained as void (or filled with water). These volumes are based on the calculations included in Attachment VI (Section 8).

Calculation of number densities involved in the partially degraded mode with corroded (oxidized) Fe and Al (see Section 5.3.4) required that the volumes of FeOOH, AlOOH, and the intact (non-corroded) Fe, be determined. A system of two linear equations in two unknowns was used to determine the volume of FeOOH and the intact Fe. A single equation was used to determine the volume of AlOOH. The hardcopy of the spreadsheet file FeOOH-AlOOH.xls in Attachment V (pages 11 and 14) provides the equations used to determine the said volumes (see Section 8 for the electronic file).

The expansion ratio of FeOOH (volume of FeOOH devided by the volume of Fe oxidized) and that of AlOOH (volume of AlOOH devided by the volume of Al oxidized) were involved in the equations mentioned above. The spreadsheet file degFeAl.xls calculates the expansion ratios. The hardcopy of this file is provided on page 9 of Attachment V (see Section 8 for the electronic file).

6. RESULTS

Existing data were used in the development of the results presented in this section. Therefore, the use of any data from this calculation for input into documents supporting procurement, fabrication, or construction is required to be identified and tracked as TBV in accordance with appropriate procedures.

The results of the intact mode and partially degraded mode criticality evaluations performed are summarized in this section. Section 6.1 summarizes the results of the calculations conducted for the intact mode; Section 6.2 summarizes the results obtained for the partially degraded mode; and Section 6.3 summarizes the results of the cases run to study the impact of partial flooding, fuel pin spacing, and absence of Mn on the k_{eff} value. In all cases the WP is considered to have been flooded unless stated otherwise.

6.1 INTACT MODE

Table 6-1 given below provides the results of the intact mode criticality calculations. In this table, each letter or digit in the case names has been chosen to serve as a pneumonic.

Table 6-1. Results of the Intact Mode

Case No.	Case Name	Description	Figure No.	Filler (Iron Shot)	Absorber (1% of the Fe-$GdPO_4$ mix by vol.)	Water Density (g/cm^3) [H/U-235][(b)]	k_{eff} [Std. Dev.]	AENCF[(a)] (MeV)
1	ilwfgc	Each tube is concentric with its -01 and –04 canisters. The fuel pins are in a square lattice arrangement.	5-2 5-3 5-4 5-5 5-6	Yes	Yes	1 [5.1]	0.7271 [0.0012]	0.3686
1-a	ilwfgo	Similar to Case 1, but the Al canisters inside the three "central" tubes are shifted toward the center of the WP.	See the discrip-tion for this case.	Yes	Yes	1 [5.1]	0.7310 [0.0011]	0.3711
2	ilwfg	Similar to Case 1, but –01 and –04 are settled in each tube.	5-7	Yes	Yes	1 [5.1]	0.7251 [0.0011]	0.3675
3	ilwfg9	Like Case 2, but water density is lowered.	5-7	Yes	Yes	0.9 [4.6]	0.7193 [0.0012]	0.3834
4	ilwfg8	Like Case 3, but water density is lowered.	5-7	Yes	Yes	0.8 [4.1]	0.7131 [0.0012]	0.3968
5	ilwfg5	Like Case 4, but water density is lowered.	5-7	Yes	Yes	0.5 [2.5]	0.6809 [0.0011]	0.4577
6	ilwfg0	Like Case 5, but no water in the waste package.	5-7	Yes	Yes	0 [0]	0.4107 [0.0006]	1.0332

7	idwfg	Similar to Case 2, but the fuel pins are hexagonal even spaced.	5-8	Yes	Yes	1	0.7273 [0.0011]	0.3705
8	iswfg	Similar to Case 2, but the fuel pins are randomly settled.	5-9	Yes	Yes	1	0.6484 [0.0011]	0.4701
9	ilwf	Similar to Case 2, but no neutron absorber is mixed with the iron shot.	5-7	Yes	No	1 [5.1]	0.8054 [0.0012]	0.3291
10	ilw	Similar to Case 2, but with no filler.	5-10	No	No	1 [5.1]	0.8327 [0.0013]	0.2995

(a) Average Energy of Neutrons Causing Fission (energy loss to fission divided by weight loss to fission, see "problem summary" table in the corresponding MCNP output file [Reference 7.17]).
(b) Moderator-to-fuel ratio for cases with fuel pins in square lattice arrangement (see Attachment VII).

Note: The alphanumeric characters in the case names have the following meanings:

i: intact mode;
l: (square) lattice arrangement of fuel pins;
d: fuel pins distributed in hexagonal array;
s: randomly settled fuel pins;
w: water filling all remaining voids in the WP;
f: Fe (iron shot) has been used as filler material;
g: $GdPO_4$ (gadolinium phosphate) has been mixed with the filler;
c: concentric tube and its –01 and –04 canisters; and
9, 8, 5, 0: **water density times 10** (e.g., 8 means that the water density is 0.8 g/cm^3).

6.2 EFFECT OF TUBE RE-ARRANGEMENT

Table 6-2 given below provides the results of the intact mode criticality calculations. In this table, each letter in the case names has been chosen to serve as a pneumonic.

Table 6-2. Results of the Partially Degraded Mode with no Oxidation of Fe or Al

Case No.	Case Name	Description	Figure No.	Filler (Iron Shot)	Absorber (1% of the Fe-$GdPO_4$ mix by vol.)	Water Density (g/cm^3) [H/U-235][(b)]	K_{eff} [Std. Dev.]	AENCF[(a)] (MeV)
11	slwfg	Tubes settle to form a gravitationally stable configuration.	5-11	Yes	Yes	1 [5.1]	0.8014 [0.0010]	0.3538
12	slwf	Similar to Case 11, but with no $GdPO_4$.	5-11	Yes	No	1 [5.1]	0.8756 [0.0039]	0.3195
13	slw	Similar to Case 11, but with no iron shot or no $GdPO_4$.	5-12	No	No	1 [5.1]	0.9039 [0.0033]	0.2893
14	hlwfg	Hex close-packed arrangement of tubes.	5-13	Yes	Yes	1 [5.1]	0.8299 [0.0037]	0.3524
15	hlwf	Similar to Case 14, but with no $GdPO_4$.	5-13	Yes	No	1 [5.1]	0.8993 [0.0034]	0.3170
16	hlw	Similar to Case 14, but with no iron shot or no $GdPO_4$.	5-14	No	No	1 [5.1]	0.9277 [0.0037]	0.2913

(a) Average Energy of Neutrons Causing Fission (energy loss to fission divided by weight loss to fission, see the "problem summary" table in the corresponding MCNP output file [Reference 7.17]).
(b) Moderator-to-fuel ratio for cases with fuel pins in square lattice arrangement (see Attachment VII).

Note: The alphanumeric characters in the case names have the following meanings:

- **h:** hex close-packed arrangement of tubes;
- **s:** gravitationally stable configuration for the tubes;
- **d:** partially degraded mode, where Fe and Al oxidation;
- **l:** (square) lattice arrangement of fuel pins;
- **w:** water filling all remaining voids in the WP;
- **f:** Fe (iron shot) has been used as filler material; and
- **g:** $GdPO_4$ (gadolinium phosphate) has been mixed with the filler.

6.3 IMPACT OF PARTIAL FLOODING, FUEL PIN SPACING, AND NO MN

Table 6.3 summarizes the results of the cases run to study the impact of partial flooding, fuel pin spacing, and absence of Mn on the k_{eff} value. The impact of each of the three factors on the k_{eff} value was studied individually as well as all combined.

Table 6-3. Impact of Partial Flooding, Fuel Pin Spacing, and the Amount of Mn Present in Materials on the k_{eff} of the 5-DHLW/DOE Enrico Fermi SNF Waste Package

Case No.	Case Name	Description	Distance Between Adjacent Pin Surfaces (cm) [H/U-235][b]	k_{eff} [Std. Dev.]	AENCF[a] (MeV)
17	slwfg	Base case; gravitationally stable tube configuration; full flooding.	0.06 [5.1]	0.8014 [0.0010]	0.3538
18	slwfgd	Like the base case, but partial flooding; water in –01 and –04 canisters only.	0.06 [5.1]	0.8632 [0.0037]	0.3405
19	slwfg1	Like the base case, but with fewer pins.	0.09 [6.8]	0.8240 [0.0032]	0.3175
20	slwfg2	Like the base case, but with fewer pins.	0.12 [8.5]	0.8372 [0.0037]	0.2936
21	swfg2a	Like the base case, but with fewer pins.	0.15 [10.4]	0.8309 [0.0043]	0.2592
22	slwfg3	Like the base case, but with fewer pins.	0.18 [12.4]	0.8263 [0.0035]	0.2456
23	swfg3a	Like the base case, but with fewer pins.	0.21 [14.5]	0.8308 [0.0035]	0.2217
24	slwfg4	Like the base case, but with fewer pins.	0.24 [16.7]	0.8284 [0.0041]	0.1974
25	slwfg8	Like the base case, but with fewer pins.	0.48 [38.2]	0.7723 [0.0035]	0.1295
26	s00mn3	Like the base case, but no Mn was considered in Al 6061, SS 316L, SS 304L, or Alloy 22.	0.06 [5.1]	0.8009 [0.0010]	0.3528
27	sl3d	Like the base case, but partial flooding; water in –01 and –04 canisters only; fewer fuel pins (optimum pin spacing).	0.18 [12.4]	0.8991 [0.0030]	0.2309
28	s3d0mn	Like the base case, but partial flooding; water in –01 and –04 canisters only; fewer fuel pins (optimum pin spacing); no Mn in Al 6061, SS 316L, SS 304L, or Alloy 22.	0.18 [12.4]	0.9033 [0.0038]	0.2319

(a) Average Energy of Neutrons Causing Fission (energy loss to fission divided by weight loss to fission, see the "problem summary" table in the corresponding MCNP output file [Reference 7.17]).
(b) Moderator-to-fuel ratio for cases with fuel pins in square lattice arrangement (see Attachment VII).

Comparison of the base case (Case 17) with the partially flooded base case (water in -01 and -04 canisters only, Case 18 [slwfgd]) increased the k_{eff} value by approximately 7.7% (an increase from 0.8014 to 0.8632).

The base case (fully flooded) with reduced number of fuel pins in each -04 canister (0.18 cm distance between the outer surfaces of adjacent fuel pins in a square lattice), Case 22 (slwfg3), resulted in a maximum k_{eff} increase of approximately 3.1% (an increase from 0.8014 to 0.8263).

Ignoring the presence of Mn in material compositions for Al 6061, SS 316L, SS 304L, and Alloy 22 resulted in changes in k_{eff} which are within statistical uncertainties. This is evident when Case17 (the base case) is compared with Case 26 (with no Mn), or when Case 27 (with Mn) is compared with Case 28 (with no Mn).

The combined effects of partial flooding, reduction in pin numbers (optimum pin separation), and ignoring the amount of Mn in the materials mentioned above (Case 28 [s3d0mn]) resulted in an increase in k_{eff} of approximately 12.7% (an increase from 0.8014 to 0.9033).

6.4 EFFECT OF FE AND AL OXIDATION

Table 6-3 provides the results of the partially degraded mode, where a fraction of the iron shot (Fe) in the DOE 18-inch SNF canister, and the entire aluminum bodies of the –01 and –04 canisters are oxidized.

Table 6-4. Results of the Partially Degraded Mode with Fe and Al Oxidation

Case No.	Case Name	Description	Figure No.	Filler (Iron Shot)	Absorber (1% of the Fe-$GdPO_4$ mix by vol.)	Water Density (g/cm^3) [H/U-235][(b)]	k_{eff} [Std. Dev.]	AENCF[(a)]
29	dslfg1	Partially degraded case; a fraction of the iron shot is oxidized and produces FeOOH; the Al in the –01 and –04 bodies is oxidized completely and produces AlOOH.	5-15 5-16	Yes	Yes	1 [3.6]	0.8205 [0.0038]	0.3550

(a) Average Energy of Neutrons Causing Fission (energy loss to fission divided by weight loss to fission, see the "problem summary" table in the corresponding MCNP output file [Reference 7.17]).
(b) Moderator-to-fuel ratio; the intact fuel pins are in square lattice arrangement (see Attachment VII).

6.5 COMPARISONS AND OBSERVATIONS

The following tables show the behavior of k_{eff} with variations in the key waste package parameters.

Table 6-5. Variations Having Small Effects upon k_{eff}

Cases Compared	Variations
1-1.a	Shifting of the Al canisters contained in the "central" tubes toward the center of WP
1-2	Settling of inner concentric tubes
1-3, 1-4, 1-5, 1-6	Decrease density of water to simulate the effect of a generic moderator displacement, and to test whether the nominal system is over-moderated
2-7	Square vs. hexagonal lattice of fuel pins uniformly spaced within a tube
11-29	Displacing water with oxides of Fe and Al

Table 6-6. Decrease in k_{eff} from Addition of Gadolinium

Cases Compared	k_{eff} Decrease	Common Conditions for Cases Compared
2-9	0.0803	Intact tube arrangement
11-12	0.0742	Gravitationally collapsed tube arrangement
14-15	0.0694	Hexagonal close packed tube arrangement

Table 6-7. Decrease in k_{eff} from Addition of Filler (Iron Shot)

Cases Compared	k_{eff} Decrease	Common Conditions for Cases Compared
9-10	0.0273	Intact tube arrangement, no Gd
12-13	0.0283	Gravitationally collapsed tube arrangement, no Gd
15-16	0.0284	Hexagonal close packed tube arrangement, no Gd

Table 6-8. Variations in k_{eff} from Variations in Geometry

Cases Compared	k_{eff} Change	Variation Causing Change
2-8	-0.0767	Moderator displacement from settling/collapsing of pins
2-11	+0.0763	Gravitational settling of tubes into closer proximity
2-14	+0.1048	Hexagonal closest packing of tubes

7. REFERENCES

7.1 Civilian Radioactive Waste Management System (CRWMS) Management and Operating Contractor (M&O) 1998. *Software Qualification Report for MCNP Version 4B2, A General Monte Carlo N-Particle Transport Code.* CSCI: 30033 V4B2LV, DI: 30033-2003 REV 01. Las Vegas, Nevada: M&O. MOL.19980622.0637.

7.2 DOE, Office of Environmental Management 1999. *Fermi (U-Mo) Fuel Characteristics for Disposal Criticality Analysis.* DOE/SNF/REP-035, Revision 0. Idaho Falls, Idaho: Idaho National Engineering and Environmental Laboratory. 242461.

7.3 American Society of Mechanical Engineers (ASME) 1995. *ASME Boiler and Pressure Vessel Code, Sec II B SB-308/SB-308M. Specification for Aluminum-Alloy 6061-T6 Standard Structural Shapes.* New York, New York: ASME. 239716.

7.4 ASME 1995. *ASME Boiler and Pressure Vessel Codes, ASME Sec II-D 95, Table NF-2, Typical Physical Properties of Materials.* New York, New York: ASME. 239587.

7.5 American Society for Testing and Materials (ASTM) 1991. *Standard Specification for Stainless and Heat-Resisting Steel Bars and Shapes.* ASTM A 276-91a. Philadelphia, Pennsylvania: ASTM. 240022.

7.6 ASTM 1994. *Standard Practice for Preparing, Cleaning, and Evaluating Corrosion Test Specimens.* ASTM G 1–90. Philadelphia, Pennsylvania: ASTM. 238771.

7.7 ASTM 1995. *Standard Specification for Heat-Resisting Chromium and Chromium-Nickel Stainless Steel Plate, Sheet, and Strip for Pressure Vessels.* ASTM A 240/A 240M-94b. Philadelphia, Pennsylvania: ASTM. 240020.

7.8 ASME 1995. *ASME Boiler and Pressure Vessel Code, Sec II A SA-240 Specification for Heat-Resisting Chromium and Chromium-Nickel Stainless Steel.* New York, New York: ASME. 239714.

7.9 CRWMS M&O 1999. *DOE SRS HLW Glass Chemical Composition.* BBA000000-01717-0210-00038 REV 00. Las Vegas, Nevada: M&O. MOL.19990215.0397.

7.10 Stout, Ray B. and Leider, Herman R., ed.'s 1991. *Preliminary Waste Form Characteristics Report.* Version 1.0. Livermore, California: Lawrence Livermore National Laboratory. MOL.19940726.0118.

7.11 ASME 1995. *ASME Boiler and Pressure Vessel Code, Sec II B SB-575 Specification for Low-Carbon Nickel-Molybdenum-Chromium, Low-Carbon Nickel-Chromium-Molybdenum, and Low carbon Nickel-Chromium-Molybdenum-Tungsten Alloy Plate, Sheet, and Strip.* New York, New York: ASME. 239753.

7.12 ASTM 1994. *Standard Specification for Low-Carbon Nickel-Molybdenum-Chromium, Low Carbon Nickel-Chromium-Molybdenum, and Low-Carbon Nickel-Chromium-Molybdenum-Tungsten Alloy Plate, Sheet, and Strip.* ASTM B 575-94. Philadelphia, Pennsylvania: ASTM. 239768.

7.13 ASTM 1991. *Standard Specification for Pressure Vessel Plates, Carbon Steel, for Moderate- and Lower-Temperature Service.* ASTM A 516/A 516M-90. Philadelphia, Pennsylvania: ASTM. 240032.

7.14 ASME 1995. 1995 *Boiler and Pressure Vessel Code - Section II Materials – Part A Material Specifications-Ferrous - SA-20/SA-20M, Specification for General Requirements for Steel Plates for Pressure Vessels.* New York, New York: ASME. 242374.

7.15 CRWMS M&O 1996. *Waste Package Filler Material Testing Report.* BBA000000-01717-2500-00008 REV 02. Las Vegas, Nevada: M&O. MOL.19970121.0004.

7.16 DOE 1998. *Quality Assurance Requirements and Description for the Civilian Radioactive Waste Management Program.* DOE/RW-0333P, Rev. 8. Washington, DC: DOE Office of Civilian Radioactive Waste Management. 226560.

7.17 CRWMS M&O 1999. *Electronic Media (CD): The Calculation Files for Enrico Fermi Fast Reactor Spent Nuclear Fuel Criticality Calculations: Intact Mode.* BBA000000-01717-0210-00037 REV 00. Compact Disk. Las Vegas, Nevada: M&O. MOL.19990125.0079.

7.18 Thomas, J. T., ed. 1978. *Nuclear Safety Guide TID-7016*, NUREG/CR-0095, ORNL/NUREG/CSD-6. Washington, DC: Nuclear Regulatory Commission. 242291.

7.19 Roberts, W. L., Rapp, Jr., G. B., and Weber, J. 1974. *Encyclopedia of Minerals.* New York, New York: Van Nostrand Reinhold Company. 238571.

7.20 CRWMS M&O 1996. Material Compositions and Number Densities for Neutronics Calculations. BBA000000-01717-0200-00002 REV 00. Las Vegas, Nevada: M&O. MOL.19960624.0023

8. ATTACHMENTS

Seven attachments are referenced in this calculation. Attachments I through III provide sketches. Attachment IV is a listing of the contents of a compact disk (CD) (Ref. 7.17), containing calculation files (spreadsheet files and MCNP output files). Attachment V provides a hardcopy of each spreadsheet file involved in the calculations reported in this document. Attachment VI provides the calculation of the fraction of an original void space that is left as void after "filling" the original void with small iron shot, Size S230. Attachment VII provides the calculation of the moderator-to-fuel ratios.

Attachment I (Sketch SK-0069 REV 01) shows a sketch of the 5-DHLW/DOE SNF disposal container.

Attachment II (DWG-507692) shows a sketch of the 18-inch OD DOE standardized SNF canister, referred to as the DOE 18-inch canister. The short canister, with an internal length of 2575 mm and an external length of 2999 mm, is considered for the co-disposal of the Enrico Fermi SNF.

Attachment III (Sketch SK-0117 REV 02) shows a sketch of the DOE Enrico Fermi fuel basket assembly.

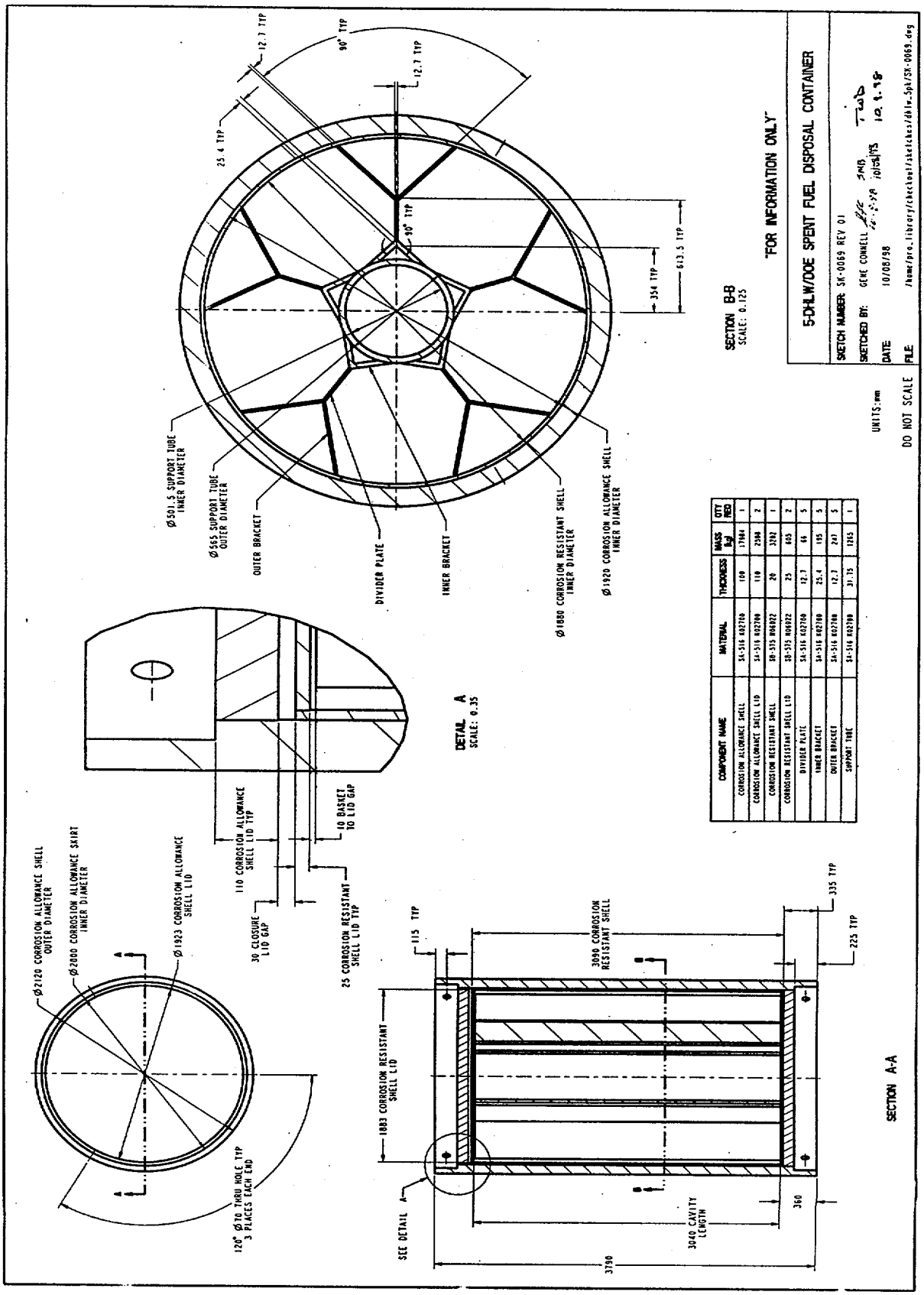
The files whose names appear in Attachment IV and are contained on the CD (Ref. 7.17) fall into two categories: Excel spreadsheet files and MCNP output files. The spreadsheet files are used to perform the required calculations to determine the number densities and mass densities of homogenized mixtures, as well as performing some pertinent calculations, as a part of the MCNP input data, for the cases of interest. The MCNP output files are the result of running the MCNP

code for the cases of interest. The contents of the input data file for each case are echoed in the output file for that case.

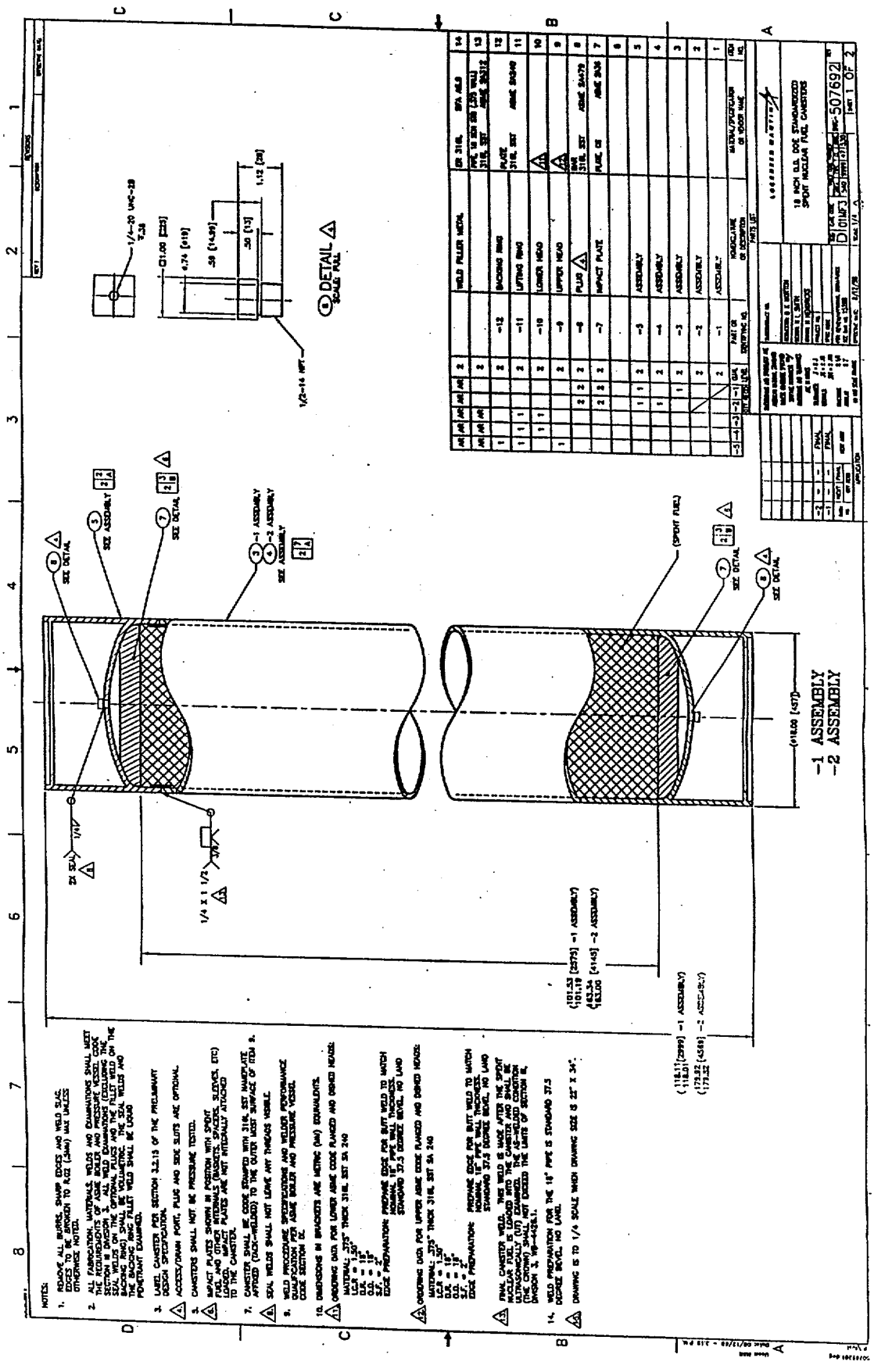
Brief descriptions of the spreadsheet files whose hardcopies are included in Attachment V are provided in the table in Attachment IV.

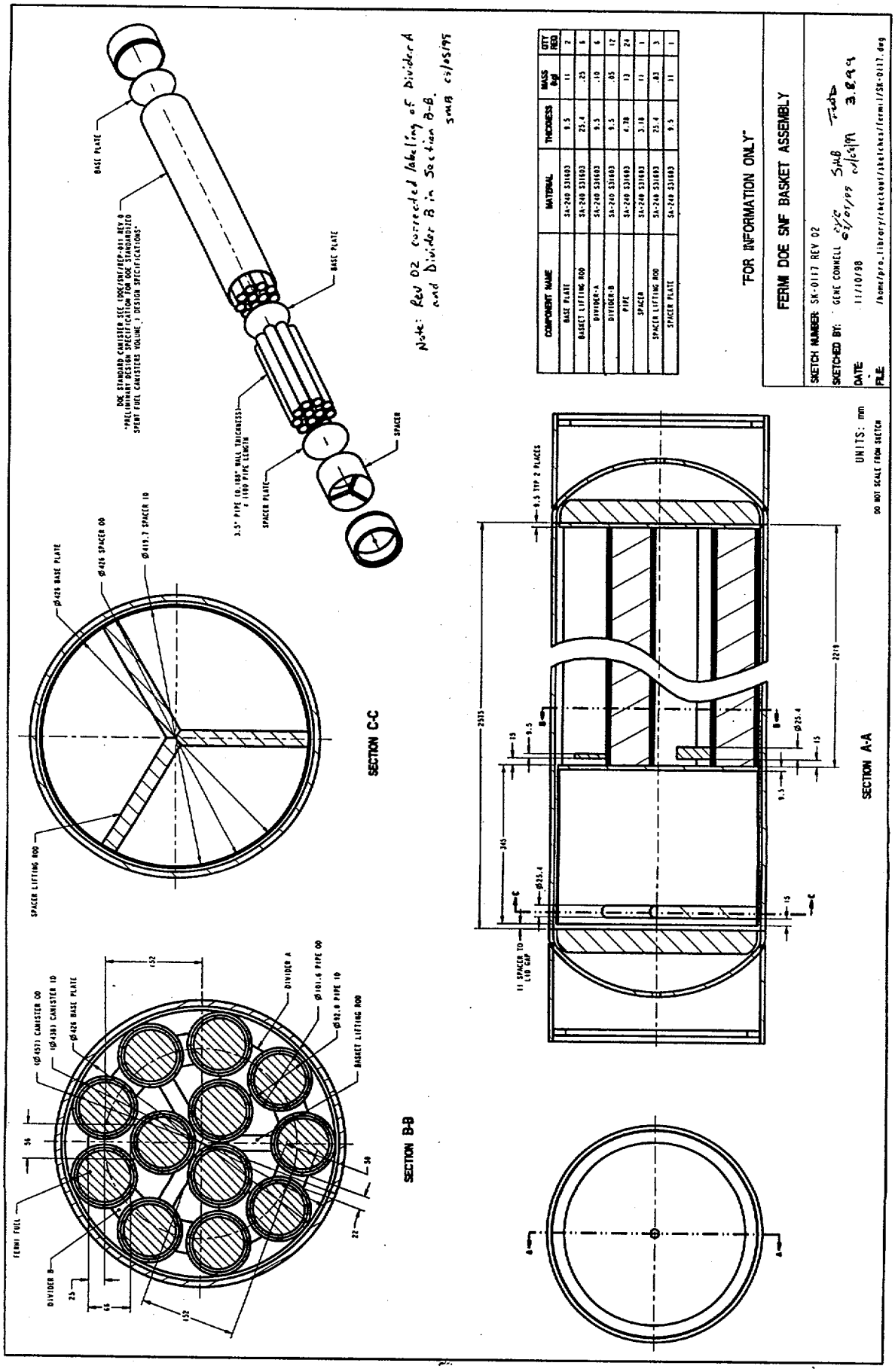
Attachment VI provides the volume fractions of Fe and remaining void space for the cases where filler (iron shot) is used. The number density calculations for these cases involve the volume occupied by Fe and the volume remained as void (or filled with water).

Attachment VII provides the moderator-to-fuel ratios for the cases with fuel pins in square lattice arrangement.



COMPONENT NAME	MATERIAL	THICKNESS	MASS kg	QTY REQ
CORROSION ALLOWANCE SHELL	SA-516 GR70N	100	17984	1
CORROSION ALLOWANCE SHELL LID	SA-516 GR70N	110	2548	2
CORROSION RESISTANT SHELL	SB-575 UNS N06022	20	3292	1
CORROSION RESISTANT SHELL LID	SB-575 UNS N06022	25	803	2
DIVIDER PLATE	SA-516 GR70N	12.7	66	5
INNER BRACKET	SA-516 GR70N	25.4	135	5
OUTER BRACKET	SA-516 GR70N	12.7	237	5
SUPPORT TUBE	SA-516 GR70N	31.75	1265	1


-1 ASSEMBLY
-2 ASSEMBLY
DETAIL
SCALE: FULL
SEE DETAIL
SEE ASSEMBLY
(SPENT FUEL)
18 INCH U.S. DOE STANDARDIZED
SPENT NUCLEAR FUEL CANISTER
DWG 507692
SHT 1 OF 2


Note: Rev 02 corrected labeling of Divider A and Divider B in Section B-B. SMB 05/05/99
FOR INFORMATION ONLY
FERMI DOE SNF BASKET ASSEMBLY
SKETCH NUMBER: SK-0117 REV 02
SKETCHED BY: GENE CONNELL
DATE: 11/10/98
FILE: /home/pro./library/checkout/sketches/fermi/SK-0117.dsg
UNITS: mm
DO NOT SCALE FROM SKETCH
SECTION A-A
SECTION B-B
SECTION C-C
BASE PLATE
SPACER
SPACER PLATE
SPACER LIFTING ROD
FERMI FUEL
DIVIDER A
DIVIDER B
BASKET LIFTING ROD

Attachment IV

This attachment provides a hardcopy listing of the contents of a CD (Ref. 7.17). As indicated in the table provided below, the CD contains 9 spreadsheet files, used to prepare the input data for the MCNP computer code, and 29 MCNP output files. The input files are echoed in their corresponding output files. The output files were transferred from a Hewlett Packard (HP) Series 9000 workstation to a Pentium II Personal Computer using a file transfer protocol. The HP file sizes differ from the file sizes on the CD due to the difference in the block sizes between the HP and the personal computer.

Contents of CD in Folder "Attach-IV"

File Name	Sub-folder	File Type	File Date (File Time)	Size (bytes)	Remarks
fuelcomp.xls	EF-Excel	Microsoft Excel	1/18/99 (5:53p)	15,872	This spreadsheet calculates the density and the number densities for the Enrico Fermi fuel.
Fe-GdPO4-Intact.xls	EF-Excel	Microsoft Excel	1/18/99 (4:25p)	18,432	This spreadsheet calculates the density and number densities for the homogenized mixture of Fe, $GdPO_4$, and H_2O (involved in the MCNP files whose names contain the letters "f" and "g").
Fe-GdPO4-Intact-9.xls	EF-Excel	Microsoft Excel	1/18/99 (8:46p)	17,920	Like Fe-$GdPO_4$-Intact.xls, but density of water is decreased to 0.9 g/cm^3. The calculated number densities are used in the MCNP file ilwfg9.O.
Fe-GdPO4-Intact-8.xls	EF-Excel	Microsoft Excel	1/18/99 (4:26p)	17,920	Like Fe-$GdPO_4$-Intact.xls, but density of water is decreased to 0.8 g/cm^3. The calculated number densities are used in the MCNP file ilwfg8.O.
Fe-GdPO4-Intact-5.xls	EF-Excel	Microsoft Excel	1/18/99 (3:26p)	17,920	Like Fe-$GdPO_4$-Intact.xls, but density of water is decreased to 0.5 g/cm^3. The calculated number densities are used in the MCNP file ilwfg5.O.
Fe-GdPO4-Intact-0.xls	EF-Excel	Microsoft Excel	1/18/99 (8:46p)	22,528	Like Fe-$GdPO_4$-Intact.xls, but density of water is decreased to 0 g/cm^3. The calculated number densities are used in the MCNP file ilwfg5.O.
Fe-W5882.xls	EF-Excel	Microsoft Excel	1/18/99 (4:36p)	16,384	This spreadsheet calculates the number densities for a homogenized mixture of Fe and H_2O. The calculated number densities are used in the MCNP files whose names contain "f", but not "g".

degFeAl.xls	EF-Excel	Microsoft Excel	1/18/99 (8:46p)	29,184	This spreadsheet calculates the volume expansion ratios involved in the oxidation of Fe and Al.
FeOOH-AlOOH.xls	EF-Excel	Microsoft Excel	1/19/99 (12:46p)	34,304	This spreadsheet calculates the number densities involved in the case where Fe and Al oxidize (MCNP case dslfg1).
ilwfgc.O	EF-mcnp	ASCII	2/22/99 (8:37p)	356,815	MCNP output file
ilwfgo.O	EF-mcnp	ASCII	2/22/99 (8:37p)	386,135	MCNP output file
ilwfg.O	EF-mcnp	ASCII	2/22/99 (8:38p)	356,294	MCNP output file
ilwfg9.O	EF-mcnp	ASCII	2/22/99 (8:38p)	356,292	MCNP output file
ilwfg8.O	EF-mcnp	ASCII	2/22/99 (8:38p)	357,372	MCNP output file
ilwfg5.O	EF-mcnp	ASCII	2/22/99 (8:39p)	356,041	MCNP output file
ilwfg0.O	EF-mcnp	ASCII	2/22/99 (8:39p)	355,267	MCNP output file
idwfg.O	EF-mcnp	ASCII	2/22/99 (8:40p)	479,864	MCNP output file
iswfg.O	EF-mcnp	ASCII	2/22/99 (8:40p)	479,215	MCNP output file
ilwf.O	EF-mcnp	ASCII	2/22/99 (8:40p)	355,045	MCNP output file
ilw.O	EF-mcnp	ASCII	2/22/99 (8:40p)	354,530	MCNP output file
slwfg.O	EF-mcnp	ASCII	2/22/99 (8:41p)	357,482	MCNP output file
slwf.O	EF-mcnp	ASCII	2/22/99 (8:41p)	287,236	MCNP output file
slw.O	EF-mcnp	ASCII	2/22/99 (8:41p)	286,389	MCNP output file
hlwfg.O	EF-mcnp	ASCII	2/22/99 (8:42p)	288,826	MCNP output file
hlwf.O	EF-mcnp	ASCII	2/22/99 (8:42p)	287,764	MCNP output file
hlw.O	EF-mcnp	ASCII	2/22/99 (8:42p)	286,632	MCNP output file
slwfgd.O	EF-mcnp	ASCII	2/22/99 (8:44p)	285,396	MCNP output file
slwfg1.O	EF-mcnp	ASCII	2/22/99 (8:45p)	288,951	MCNP output file
slwfg2.O	EF-mcnp	ASCII	2/22/99 (8:45p)	288,951	MCNP output file
swfg2a.O	EF-mcnp	ASCII	2/22/99 (8:45p)	288,853	MCNP output file
slwfg3.O	EF-mcnp	ASCII	2/22/99 (8:46p)	288,951	MCNP output file
swfg3a.O	EF-mcnp	ASCII	2/22/99 (8:46p)	289,000	MCNP output file
slwfg4.O	EF-mcnp	ASCII	2/22/99 (8:46p)	289,000	MCNP output file
slwfg8.O	EF-mcnp	ASCII	2/22/99 (8:46p)	288,806	MCNP output file
s00mn3.O	EF-mcnp	ASCII	2/22/99 (8:47p)	370,910	MCNP output file
sl3d.O	EF-mcnp	ASCII	2/22/99 (8:47p)	286,035	MCNP output file
s3d0mn.O	EF-mcnp	ASCII	2/22/99 (8:48p)	284,325	MCNP output file
dslfg1.O	EF-mcnp	ASCII	2/23/99 (10:08a)	281,759	MCNP output file

Attachment V

This attachment provides a hardcopy of each Microsoft Excel spreadsheet file involved in the calculations reported in this document. The location of the electronic copies of the spreadsheet files, and a brief description of each file, as to what it does, is explained in Attachment IV.

	A	B	C	D	E	F	G	H
1								
2		fuelcomp.xls						
3		Enrico Fermi fresh fuel composition						
4								
5		Weight	Weight					
6		(g)	(g)	Wt%				
7	U	133.9						
8	U-235		34.4	22.961				
9	U-238		99.5	66.4135				
10	Mo	15.31		10.6255	(Note: Impurities were added to Mo)			
11	Impurities	0.609						
12	Total weight	149.819	Total	100				
13	Zr Cladding	9.2						
14								
15	Vol of a fuel pin	8.59833	cm^3					
16	Den of a fuel pin	17.4242	g/cm^3					
17								
18								
19								

	A	B	C	D
1				
2				
3		Fe-GdPO4-Intact.xls		
4		**Homogenized mixture of Fe, GdPO4, and H2O**		
5		**water density: 1 g/cc**		
6	**Calculating number densities for the intact cases whose MCNP file names**			
7	**contain f" and "g", and the density of water is 1 g/cc**			
8				
9	**H2O**			
10	Vol Frac		0.4118	
11	Density (g/cm^3)		1	
12	Molar weight (g)		18.0105654	
13	n-H2O (moles/b-cm)		0.01376892	
14	n-H (atoms/b-cm)		0.02753783	
15	n-O (atoms/b-cm)		0.01376892	
16				
17	**Fe**			
18	Vol Frac		0.582318	
19	Density (g/cm^3)		7.85	
20	Molar weight (g)		55.847	
21	n-Fe (atoms/b-cm)		0.04929136	
22				
23	**GdPO4**			
24	Vol Frac		0.005882	
25	Density (g/cm^3)		5	
26	Molar weight (g)		252.203425	
27	n-GdPO4 (moles/b-cm)		7.0224E-05	
28	n-Gd (atoms/b-cm)		7.0224E-05	
29	n-P (atoms/b-cm)		7.0224E-05	
30	n-O (atoms/b-cm)		0.0002809	0.014049811
31				(total)
32		Density of the homogenized mixture (g/cm^3):	5.0124063	
33				
34				

	A	B	C	D
1				
2				
3		Fe-GdPO4-Intac-9.xls		
4		**Homogenized mixture of Fe, GdPO4, and H2O**		
5		**(water density: 0.9 g/cm^3)**		
6	**Calculating number densities for the intact case named ilwfg9**			
7				
8	**H2O**			
9	Vol Frac		0.4118	
10	Density (g/cm^3)		0.9	
11	Molar weight (g)		18.010565	
12	n-H2O (moles/b-cm)		0.012392	
13	n-H (atoms/b-cm)		0.024784	
14	n-O (atoms/b-cm)		0.012392	
15				
16	**Fe**			
17	Vol Frac		0.582318	
18	Density (g/cm^3)		7.85	
19	Molar weight (g)		55.847	
20	n-Fe (atoms/b-cm)		0.0492914	
21				
22	**GdPO4**			
23	Vol Frac		0.005882	
24	Density (g/cm^3)		5	
25	Molar weight (g)		252.20342	
26	n-GdPO4 (moles/b-cm)		7.022E-05	
27	n-Gd (atoms/b-cm)		7.022E-05	
28	n-P (atoms/b-cm)		7.022E-05	
29	n-O (atoms/b-cm)		0.0002809	0.012673
30				(total)
31		Density of the homogenized mixture (g/cr	4.9712263	
32				
33				

	A	B	C	D
1				
2				
3		Fe-GdPO4-Intac-8.xls		
4		**Homogenized mixture of Fe, GdPO4, and H2O**		
5		**(water density: 0.8 g/cm^3)**		
6	**Calculating the number densities for the intact case ilwfg8**			
7				
8	**H2O**			
9	Vol Frac		0.4118	
10	Density (g/cm^3)		0.8	
11	Molar weight (g)		18.011	
12	n-H2O (moles/b-cm)		0.011	
13	n-H (atoms/b-cm)		0.022	
14	n-O (atoms/b-cm)		0.011	
15				
16	**Fe**			
17	Vol Frac		0.5823	
18	Density (g/cm^3)		7.85	
19	Molar weight (g)		55.847	
20	n-Fe (atoms/b-cm)		0.0493	
21				
22	**GdPO4**			
23	Vol Frac		0.0059	
24	Density (g/cm^3)		5	
25	Molar weight (g)		252.2	
26	n-GdPO4 (moles/b-cm)		7E-05	
27	n-Gd (atoms/b-cm)		7E-05	
28	n-P (atoms/b-cm)		7E-05	
29	n-O (atoms/b-cm)		0.0003	0.0113
30				(total)
31		Density of the homogenized mixt	4.93	
32				
33				

	A	B	C	D
1				
2				
3		Fe-GdPO4-Intac-5.xls		
4		**Homogenized mixture of Fe, GdPO4, and H2O**		
5		**(water density: 0.5 g/cm^3)**		
6	**Calculating number densities for the intact case ilwfg5**			
7				
8	**H2O**			
9	Vol Frac		0.4118	
10	Density (g/cm^3)		0.5	
11	Molar weight (g)		18.011	
12	n-H2O (moles/b-cm)		0.0069	
13	n-H (atoms/b-cm)		0.0138	
14	n-O (atoms/b-cm)		0.0069	
15				
16	**Fe**			
17	Vol Frac		0.5823	
18	Density (g/cm^3)		7.85	
19	Molar weight (g)		55.847	
20	n-Fe (atoms/b-cm)		0.0493	
21				
22	**GdPO4**			
23	Vol Frac		0.0059	
24	Density (g/cm^3)		5	
25	Molar weight (g)		252.2	
26	n-GdPO4 (moles/b-cm)		7E-05	
27	n-Gd (atoms/b-cm)		7E-05	
28	n-P (atoms/b-cm)		7E-05	
29	n-O (atoms/b-cm)		0.0003	0.0072
30				(total)
31		Density of the homogenized m	4.8065	
32				
33				

	A	B	C	D
1				
2				
3		Fe-GdPO4-Intac-0.xls		
4		**Homogenized mixture of Fe, GdPO4, and H2O**		
5		**(water density: 0 g/cm^3 [no water, dry case])**		
6	**Calculating the number densities for the intact case ilwfg0**			
7				
8	**H2O**			
9	Vol Frac		0.412	
10	Density (g/cm^3)		0	
11	Molar weight (g)		18.01	
12	n-H2O (moles/b-cm)		0	
13	n-H (atoms/b-cm)		0	
14	n-O (atoms/b-cm)		0	
15				
16	**Fe**			
17	Vol Frac		0.582	
18	Density (g/cm^3)		7.85	
19	Molar weight (g)		55.85	
20	n-Fe (atoms/b-cm)		0.049	
21				
22	**GdPO4**			
23	Vol Frac		0.006	
24	Density (g/cm^3)		5	
25	Molar weight (g)		252.2	
26	n-GdPO4 (moles/b-cm)		7E-05	
27	n-Gd (atoms/b-cm)		7E-05	
28	n-P (atoms/b-cm)		7E-05	
29	n-O (atoms/b-cm)		3E-04	0.0003
30				(total)
31		Density of the homogenized mixt	4.601	
32				
33				

Fe-W5882.xls

Calculating number densities for a homogenized mixture of Fe and H2O

(involved in the MCNP cases whose file name contain "f", but not "g")

H2O vol Frac	H2O Den (g/cm^3)	Fe vol Frac	Fe Den (g/cm^3	Mix Den (g/cm^3)
0.4118	1	0.5882	7.85	5.02917

Avogadro's No (atoms-cm2/mole-barn)	AH2O	AFe	nH2O	nFe
0.602252	18.01056538	55.847	0.013770105	0.049793549

nH	nO	nFe
0.02754021	0.013770105	0.049793549

	A	B	C	D	E	F
1						
2						
3		degFeAl.XLS				
4						
5	Volume expansion due to oxidation					
6	**Calculation of volume expansion coefficient for FeOOH and AlOOH**					
7	**(Fe and Al expand when oxidized)**					
8						
9						
10	**Elements to be degraded**					
11	Element	Fe	Al			
12	Vol, cm3	1	1			
13	Den, g/cm3	7.85	2.702			
14	Wt, g	7.85	2.702			
15	At. Wt, g	55.847	26.9815389			
16	No. of moles	0.140563	0.100142546			
17						
18	**Degradation Products**					
19	Mineral	Goethite	Diaspore			
20	Mineral Chem Formula	FeOOH	AlOOH			
21	Mineral Den, g/cm3	4.2	3.4			
22	Moles of Mineral	0.140563	0.100142546			
23	Molar Wt of Mineral, g	88.84466	59.97919409			
24	Mineral Wt, g	12.48824	6.006469202			
25	Mineral Vol, cm3	2.97339	1.766608589			
26	Vol Expansion. Coeff.	2.97339	1.766608589			
27						
28						
29						

FeOOH-AlOOH.xls

	A	B	C
1	**Degradation of Fe into FeOOH and AL into AlOOH**		
2	The Al involved in -01 (including the bail) and -04 degrade and remain		
3	inside the outer boundary of the -01 canister along with non-degraded Al.		
4	The Fe inside each 4" pipe degrades and remain outside the outer		
5	boundary of the -01 (without its bail) along with the non-degraded portion		
6	of the original Iron shot.		
7	Outside the pipes, the degraded Fe and non-degraded Fe fill the avaiable vol.		
8	When no neutron absorber is used, Fe shot occupies 58.82% of available vol.		
9	**NOT CONSIDERING THE -01 BAIL**		
10	DOE Canister:		
11	Inner bottom of the DOE 18-inch canister	-128.75	cm
12	Bottom of the "central" ss plate	-17.7975	cm
13	Height of the active section (AS) (bottom part)	110.9525	cm
14	Heigt of AS - bottom ss plate thicknesses (pipe length)	110	cm
15	IR of the DOE canister	21.9075	cm
16	Tot vol of active section (bottom part)	165854.9	cm^3
17	4" Pipes:		
18	OR of a 4" pipe	5.08	cm
19	Number of 4" pipes (bottom section)	12	
20	Tot displacing Vol of 4" pipes	107016.6	cm^3
21	**Void space outside the 4" pipes (bot sec) for Fe, FeOOH, and GdPO4**	**58838.24**	**cm^3**
22	**Vol of the original intact Fe shot outside the bottom 12 4" pipes (Vi)**	**34262.57**	**cm^3**
23	**Vol of GdPO4 outside the bottom 12 4" pipes; 1% of Fe-GdPO4 vol**	**346.0865**	**cm^3**
24	**Void space avaiable for Fe and FeOOH outside the bottom 12 4" pipes (V)**	**58492.15**	**cm^3**
25			
26	IR of a 4" pipe	4.60248	cm
27	Height of a 4" pipe	110	cm
28	Inner vol of a 4" pipe	7320.258	cm^3
29	-01 Al Shipping Canister:		
30	OR of a -01 shipping canister	4.1275	cm
31	Outer Height of -01 (no bail)	98.425	cm
32	Displaced vol of cylindrical section of one -01	5267.802	cm^3
33	Vol of one bail IGN	34.75453	cm^3
34	Tot displacing vol of one -01	5267.802	cm^3
35	Vol inside the 4" pipe containing no Fe / FeOOH / GdPO4	4146.27	cm^3
36			
37	**Void space b/w a 4" pipe and a -01 (NOT CONSIDERING THE BAIL)**	**2052.456**	**cm^3**
38	**Vol of the original intact Fe shot b/w a 4" pipe and a -01 (NO BAIL)**	**1195.182**	**cm^3**
39	**Vol of GdPO4 b/w a 4" pipe and a -01 (No BAIL); 1% of Fe-GdPO4 vol**	**12.07254**	**cm^3**
40	**Void space avaiable for Fe and FeOOH b/w a 4" pipe and a -01 (NO BAIL)**	**3161.915**	**cm^3**
41	**Total volume occupied by Fe, FeOOH, and GdPO4 in a 4" pipe**	**3173.988**	**cm^3**

FeOOH-AlOOH.xls (Continued)

	D	E	F	G	H	I	J	K
1	(11/30/98)							
2	(d:\FERMIcalc\voids-113098.xls)							
3								
4								
5								
6								
7								
8								
9								
10								
11								
12	Calculation of Fe & FeOOH volumes:							
13	V = void space for Fe & FeOOH		58492.2	cm^3				
14	Vf = vol of original Fe		34262.6	cm^3				
15	Vi = vol of intact Fe							
16	Vo = vol of oxidized Fe							
17	E = expansion ratio		2.97	cm^3	(from degFeAl.XLS)			
18	Vi + Vo = Vf	(1)						
19	V - Vi = E Vo	(2)						
20	(1) +(2):							
21	Vo + V = Vf + E Vo							
22	(E -1) Vo = V - Vf							
23	**Vo = (V - Vf) / (E-1)**		12299.3	cm^3				
24	**Vi = Vf - Vo**		21963.3	cm^3				
25								
26	**FeOOH Volume (E Vo)**		**36528.9**	**cm^3**				
27	**Fe Volume (Vi)**		**21963.3**	**cm^3**				
28		Tot Vol	58492.2					
29	**Number density calculations:**			**Avogadro's No.**		**Atomic den**		
30	**Element/Minera**	**Den (g/cm^3)**	**Vol Frac**	**(atom - cm^2) / (mole - b)**	**Mol. Wt. (g)**	**(atoms / b - cm)**		
31								
32	**Fe**	7.85	0.37328	0.6022	55.847	**0.031597167**		
33	**FeOOH**	4.2	0.62084	0.6022	88.84465519	**0.017674018**		
34	**Fe**					0.017674018	**0.0492712**	**(Tot)**
35	O					0.035348037		
36	**H**					**0.017674018**		
37	**GdPO4**	5	0.00588	0.6022	192.2550655	**9.21209E-05**		
38		Tot Vol Check	1					
39	**Gd**					**9.21209E-05**		
40	**P**					**9.21209E-05**		
41	**O**					0.000368483	**0.0357165**	**(Tot)**
42				**Mixture Den:**	5.567186605	g/cm^3		

FeOOH-AlOOH.xls (Continued)

	A	B	C
42	Calculations needed for Al Degradation:		
43	Vol enclosed by the outer surface of		
44	the cylindrical section of one -01	5267.802	cm^3
45	OR of fuel pin (cladded fuel rod)	0.20066	cm
46	Length of a fuel pin	77.47	cm
47	Vol of one fuel pin	9.799525	cm^3
48	Vol of 140 fuel pins	1371.934	cm^3
49	IR of -01 (shell)	3.81	cm
50	Height of -01 shell	99.695	cm
51	Vol of Al in -01 shell	789.3157	cm^3
52	Tot Thickness of bot & top plates of -01	2.54	cm
53	Vol of Al in bot & top plates of -01	115.8333	cm^3
54	Vol of Al "spacer" in -01	18.45018	cm3
55	Tot vol of Al in -01 body and Al spacer (NOT CONSIDERING THE BAIL)	923.5992	cm^3
56	-04 Al Shipping Canister		
57	OR of -04	3.4925	cm
58	IR of -04	3.3274	cm
59	Inner height of -04	82.55	cm
60	Volume of -04 bounded by the inner surface	2871.289	cm^3
61	Length of the main single-layer shell of -04	82.55	cm
62	Length of the bent part of the single-layer shell	0.733235	cm
63	Total length of single-layer shell of -04	83.28323	cm
64	Vol of single-layer shell of -04	294.5999	cm^3
65	Length of double-layer shell of -04	6.985	cm
66	Thickness of the shell or end plates of -04	0.1651	cm
67	IR of -04 for the double-layer parts of the shell	3.1623	cm
68	Vol of the double-layer shell of -04	48.22013	cm^3
69	Vol of two plates at the ends of -04	10.37369	cm^3
70	Tot vol of Al in the -04 body and end plugs	353.1937	cm^3
71	**Tot vol of Al in each 4" pipe (NOT CONSIDERING THE -01 BAIL)**	**1276.793**	**cm^3**
72	**Void space enclosed by the outer surface of -01 for Al and ALOOH**	**1499.356**	**cm^3**

FeOOH-AlOOH.xls (Continued)

	D	E	F	G	H	I	J	K
43								
44	V = void space for Fe & FeOOH		3161.92					
45	Vf = vol of original Fe		1195.18					
46	Vi = vol of intact Fe							
47	Vo = vol of oxidized Fe							
48	E = expansion ratio		2.97	cm^3	(from degFeAl.XLS)			
49								
50	**Vo = (V - Vf) / (E-1)**		998.342					
51	**Vi = Vf - Vo**		196.84					
52								
53	**FeOOH Volume (E Vo)**		**2965.08**	**cm^3**				
54	**Fe Volume (Vi)**		**196.84**	**cm^3**				
55		Tot vol	3161.92					
56								
57	**Number density calculations:**			**Avogadro No.**		**Atomic den**		
58	**Element/Minera**	**Den (g/cm^3)**	**Vol Frac**	**(atom - cm^2) /**	**Mol. Wt. (g)**	**(atoms / b - cm)**		
59				**(mole - b)**				
60	**Fe**	**7.85**	0.06202	0.6022	55.847	**0.005249511**		
61	**FeOOH**	**4.2**	0.93418	0.6022	88.84465519	**0.026594338**		
62	**Fe**					0.026594338	**0.0318438**	**(Tot)**
63	**O**					0.053188677		
64	**H**					**0.026594338**		
65	**GdPO4**	**5**	0.0038	0.6022	192.2550655	**5.95699E-05**		
66		Tot Vol Check	1					
67	**Gd**					**5.95699E-05**		
68	**P**					**5.95699E-05**		
69	**O**					0.000238279	**0.053427**	**(Tot)**
70				**Mixture Den:**	**4.429403629**	**g/cm^3**		

FeOOH-AlOOH.xls (Continued)

	D	E	F	G	H	I	J	K
71								
72	Vol of Al to be oxidized		1276.793	cm^3				
73	E = expansion ratio		1.77	cm^3	(from degFeAl.XLS)			
74	Tot vol of AlOOH		2259.923	cm^3	Vol of AlOOH = Vol of Al * Expansion Ratio			
75	Vol of AlOOH between outer surf of -01							
76	and inner surface of -04 (fuel length):		1451.675	cm^3				
77	**Vol of AlOOH inside -04:**		**808.2479**	**cm^3**				
78	**Vol of H2O among fuel rods:**		**514.4132**	**cm^3**				
79	Check:	Tot	1322.661	cm^3				
80		Vol 0f -04 - fuel vol	1322.661	cm^3				
81								
82	**Number density calculations:**			**Avogadro's No.**		**Atomic den**		
83	**Element/Mi**	**Den (g/cm^3)**	**Vol Frac**	**(atom - cm^2) /**	**Mol. Wt. (g)**	**(atoms / b - cm)**		
84				**(mole - b)**				
85	**AlOOH**	3.4	1	0.6022	59.97919409	**0.034136504**		
86	**Al-27**					**0.034136504**		
87	**O**					**0.068273008**		
88	**H**					**0.034136504**		
89				**Density:**	3.4	g/cm^3		
90								
91	**AlOOH**	3.4	0.611077	0.6022	59.97919409	**0.020860036**		
92	**Al-27**					**0.020860036**		
93	O					0.041720071		
94	H					0.020860036		
95	**H2O**	1	0.388923	0.6022	18.01056538	**0.013003999**		
96		Tot vol check:	1					
97	**H**					0.026007998	**0.046868**	**(Tot)**
98	**O**					0.013003999	**0.0547241**	**(Tot)**
99				**Mixture Den:**	**2.466585015**	g/cm^3		

Attachment VI

This attachment provides the calculation of the fraction of an original void space that remains as void after "filling" the original void with small iron shot, Size S230.

Reference: CRWMS M&O 1996. *Waste Package Filler Material Testing Report.* BBA000000-01717-2500-00008 REV 02, pp. 9-11. Las Vegas, Nevada: M&O. MOL.19970121.0004

The steel shot bulk density (as poured condition) is 4.617 g/cm^3.

Considering 1 cm^3 of "void-Fe mixture," we can write:

$$v_{Fe} + v_{void} = 1 \text{ cm}^3$$

where, v_{Fe} is the fraction of 1 cm^3 occupied by the filler, and v_{void} is the remaining void fraction.

The mass of filler is determined as:

$$m_{Fe}/1 \text{ cm}^3 = 4.617 \text{ g/cm}^3, \text{ or}$$

$$m_{Fe} = 4.617 \text{ g} \qquad (1)$$

Considering the mass density of the filler as 7.85 g/cm^3, m_{Fe} can also be found as:

$$m_{Fe} = 7.85 \text{ g/cm}^3 * v_{Fe} \qquad (2)$$

Equating (1) and (2) results in:

$$4.617 = 7.85\, v_{Fe}$$

Then, the fraction of the 1 cm^3 original void space occupied by iron shot is:

$$v_{Fe} = 4.617/7.85$$
$$= 0.5882 \text{ cm}^3$$

In other words, 58.82% of the original void space is occupied by the filler (Fe).

The void volume out of 1 cm^3 is:

$$v_{void} = 1 - 0.5882 = 0.4118 \text{ cm}^3$$

In other words, 41.18% of the original void space is not occupied by Fe.

Attachment VII

This attachment provides the calculation of moderator-to-fuel ratios (H/X) for the cases where the fuel pins inside each –04 aluminum canister are in square lattice arrangement.

The H/X ratio is obtained by dividing the total number of hydrogen atoms (H population) present in a fuel cell by the total number of U-235 atoms (U-235 population) present in that cell.

The spreadsheet on pages 2 and 3 of this attachment shows the results of the calculations of the H/X ratios for three categories of cases:

(a) the water density changes,
(b) the pitch (the center-to-center distance between adjacent fuel cells ["squares"]) changes, and
(c) the fuel pins are surrounded by a mixture of water and AlOOH (Table 6-4 of this document, case No. 29 [dslfg1]).

The formulas corresponding to the calculations performed in the said spreadsheet are provided on pages 4 and 5 of this attachment.

H/X Calculations

(The corresponding formulas are provided on page 4 of this attachment.)

	A	B	C	D	E	F
1	**Calculation of H/X ratio;**					
2	**H is the atom population &**					
3	**X is the U-235 population in**					
4	**a square lattice cell**					
5	**Dimensions and volumes**					
6	Fuel pin height (cm)		77.47			
7	Fuel radius (cm)		0.18796			
8	Clad outer radius (cm)		0.20066			
9	Fuel volume (cm^3)		8.598333806			
10	Distance between adjacent pin surfaces (cm)		0.06			
11	Pitch (the same as fuel-cell side length) (cm)		0.46132			
12	"Moderator" volume, base case (cm^3)		6.687341117			
13	**Fuel pin composition (wt%)**					
14	U-235		22.96104			
15	U-238		66.41347			
16	Mo and impurities		10.62549			
17	**Calculation of number density for U-235**					
18	Density (g/cm^3)		17.42419			
19	Atomic weight of U-235 (g) (Ref. 7.20, p. 30)		235.043915			
20	Avogadro's number ([atom-cm^2]/mole-b])		0.602252			
21	(Ref. 7.20, p. 37)					
22	Number density of U-235 ([atom]/[b-cm])		0.010251169			
23	**Data for H2O**					
24	Atomoc weight of H (g) Ref. 7.20, p. 29)		1.00782519			
25	Atomic weight of O (g) (Ref. 7.20, p. 29)		15.994915			
26	Molecular weight of H2O (g/mole)		18.01056538			
27	**Partially degraded mode with**					
28	**Fe and Al oxidation**					
29	The 140 pins are in square lattice					
30	arrangement, case dslfg1.					
31	The fuel pins are surrounded by the following					
32	elements (based on 61.11% AlOOH and					
33	38.89% H2O; density=2.46658 g/cm^3					
34	(See p. 14 of Attachment V):					
35	**Element**		**No. Density**			
36			**(atom/b-cm)**			
37	H		0.046868			
38	O		0.0547241			
39	Al		0.02086			
40						

H/X Calculations (continued)

(The corresponding formulas are provided on page 5 of this attachment.)

	A	B	C	D	E	F
41	**H/X ratios for different H2O densities**					
42			**H2O Density**	**H2O Number**	**H Num. Den.**	**H/X**
43			**(g/cm^3)**	**Density**	**(atom/b-cm)**	
44				**(mole/b-cm)**		
45			1	0.033438817	0.06687763	5.073956
46			0.9	0.030094935	0.06018987	4.56656
47			0.8	0.026751054	0.05350211	4.059165
48			0.5	0.016719409	0.03343882	2.536978
49			0	0	0	0
50						
51	**H/X ratios for different pitch values**					
52			**Distance**	**Pitch (cm)**	**H2O Volume**	**H/X**
53			**Between**		**(cm^3)**	
54			**Adjacent Pin**			
55			**Surfaces (cm)**			
56			0.06	0.46132	6.68734112	5.073956
57			0.09	0.49132	8.90137174	6.75383
58			0.12	0.52132	11.2548484	8.539508
59			0.15	0.55132	13.747771	10.43099
60			0.18	0.58132	16.3801396	12.42827
61			0.21	0.61132	19.1519542	14.53136
62			0.24	0.64132	22.0632149	16.74025
63			0.48	0.88132	50.3733559	38.2203
64						
65	**H/X ratio for partially degraded mode**		3.555839949			
66						
67						

Note: The reference provided in the above spreadsheet corresponds to Ref 7.20 in Section 7 of the main text.

Formulas Involved in the H/X Calculations

(The formulas correspond to the results provided on p. 2 of this attachment.)

	C	D	E	F
1				
2				
3				
4				
5				
6	=30.5*2.54			
7	0.18796			
8	0.20066			
9	=PI()*(C7^2)*C6			
10	0.06			
11	=2*C8+C10			
12	=((C11^2)-PI()*(C8^2))*C6			
13				
14	22.96104			
15	66.41347			
16	10.62549			
17				
18	17.42419			
19	235.043915			
20	0.602252			
21				
22	=C18*(C14/100)*C20/C19			
23				
24	1.00782519			
25	15.994915			
26	=(2*C24+C25)			
27				
28				
29				
30				
31				
32				
33				
34				
35	**No. Density**			
36	**(atom/b-cm)**			
37	0.046868			
38	0.0547241			
39	0.02086			
40				

Formulas Involved in the H/X Calculations (continued)

(The formulas correspond to the results provided on p. 3 of this attachment.)

	C	D	E	F
41				
42	H2O Density	H2O Number	H Num. Den.	H/X
43	(g/cm^3)	Density	(atom/b-cm)	
44		(mole/b-cm)		
45	1	=C45*$C$20/$C$26	=D45*2	=($C$12*E45)/($C$9*$C$22)
46	0.9	=C46*$C$20/$C$26	=D46*2	=($C$12*E46)/($C$9*$C$22)
47	0.8	=C47*$C$20/$C$26	=D47*2	=($C$12*E47)/($C$9*$C$22)
48	0.5	=C48*$C$20/$C$26	=D48*2	=($C$12*E48)/($C$9*$C$22)
49	0	=C49*$C$20/$C$26	=D49*2	=($C$12*E49)/($C$9*$C$22)
50				
51				
52	Distance	Pitch (cm)	H2O Volume	H/X
53	Between		(cm^3)	
54	Adjacent Pin			
55	Surfaces (cm)			
56	0.06	=2*$C$8+C56	=(D56^2-(PI()*$C$8^2))*$C$6	=(E56*$E$45)/($C$9*$C$22)
57	0.09	=2*$C$8+C57	=(D57^2-(PI()*$C$8^2))*$C$6	=(E57*$E$45)/($C$9*$C$22)
58	0.12	=2*$C$8+C58	=(D58^2-(PI()*$C$8^2))*$C$6	=(E58*$E$45)/($C$9*$C$22)
59	0.15	=2*$C$8+C59	=(D59^2-(PI()*$C$8^2))*$C$6	=(E59*$E$45)/($C$9*$C$22)
60	0.18	=2*$C$8+C60	=(D60^2-(PI()*$C$8^2))*$C$6	=(E60*$E$45)/($C$9*$C$22)
61	0.21	=2*$C$8+C61	=(D61^2-(PI()*$C$8^2))*$C$6	=(E61*$E$45)/($C$9*$C$22)
62	0.24	=2*$C$8+C62	=(D62^2-(PI()*$C$8^2))*$C$6	=(E62*$E$45)/($C$9*$C$22)
63	0.48	=2*$C$8+C63	=(D63^2-(PI()*$C$8^2))*$C$6	=(E63*$E$45)/($C$9*$C$22)
64				
65	=($C$12*$C$37)/($C$9*$C$22)			
66				
67				

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