Hydrogen Generation from Sludge Sample Bottles Caused by Radiolysis and Chemistry with Concentration Determination in a SWB or Drum for Transport

Prepared for the U.S. Department of Energy
Assistant Secretary for Environmental Management

Contractor for the U.S. Department of Energy
under Contract DE-AC06-08RL14788

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EDC #: PRC-EDC-10-45750

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Document Type: TR

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Ascendent Engineering & Safety Solutions

Date Published
March 2010

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Total Pages: 50

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HNF-43821 Rev.3 CHPRC Calculation Cover Sheet and Revision Summary

Section 1: Identification						
1. Project Identifier		2. Modification Description Title/Subject Hydrogen Generation from Sludge Sample Bottles Caused by Radiolysis and Chemistry with Concentration Determination in a SWB or Drum for Transport			3. Page 1 of 46	
4. Use of Form ☒ Calculation ☐ Engineering Analysis ☐ Software Installation ☐ Technical Basis ☐ Other						
5. Job Title Hydrogen Generation from Sludge Sample Bottles Caused by Radiolysis and Chemistry with Concentration Determination in a SWB or Drum for Transport		6. WBS Number NA		7. Department/Organization Transportation Safety / Nuclear Safety		
8. Calculation Number HNF-43821		9. Affected Building Numbers NA		10. Room NA		11. Floor NA
12. Independent Verification Required? ☒ Yes ☐ No		13. Performance Category (PC) ☐ 0 ☐ 1 ☐ 2 ☐ 3 ☒ N/A				
Section 2: Preparation, Review, and Approval						
14. Rev. No.	15.	16. Originator	17. Checker	18. Approver: Design Authority or System Engineer	19. Supersedes Calc. No. or Rev. No.	20. Field Confirmation Required?
3	Print Name Sign Date	D. L. Riley 3/24/2010	A. E. Bridges 3/24/2010	W. S. Edwards 3/25/10	NA	☐ Yes ☒ No
	Print Name Sign Date					☐ Yes ☐ No
Section 3: Revision Summary						
21. Rev. No.	22. Description/Reason for Revision					23. Affected Pages
0	This calculation determines the hydrogen concentration in a SWB or drum with sludge sample bottles. The hydrogen results from radiolysis and chemistry from the sludge sample bottles inside a Superpig or Piglet. Two Super pigs are placed within a SWB while two Piglets are placed within a drum.					ALL
1	Complete revision to incorporate comments from DOE reviewer(s). Added section on thermal load from radiolysis and chemical reaction.					ALL
2	Complete revision to incorporate comments from DOE reviewer(s). Added information regarding plutonium water reactions and from PNNL Letter Report 46497-RPT14, "Enthalpies and Free Energies of Reaction for Uranium Phases and Metals of Interest to Transportation of K Basin Sludge."					ALL
3	Complete revision to incorporate comments from DOE reviewer(s).					ALL
Registration Stamp (as applicable): Signature/Date: _____				Classification Review: Signature/Date: 3-29-10		

**Hydrogen Generation from Sludge Sample Bottles
Caused by Radiolysis and Chemistry with Concentration
Determination in a SWB or Drum for Transport**

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1.0 OBJECTIVE

A volume of 600 mL of sludge, in 4.1 L sample bottles (Appendix 7.6), will be placed in either a Super Pig (Ref. 1) or Piglet (Ref. 2, 3) based on shielding requirements (Ref. 4). Two Super Pigs will be placed in a Standard Waste Box (SWB, Ref. 5), as their weight exceeds the capacity of a drum; two Piglets will be placed in a 55-gallon drum (shown in Appendix 7.2). The generation of hydrogen gas through oxidation/corrosion of uranium metal by its reaction with water will be determined and combined with the hydrogen produced by radiolysis. The hydrogen concentration in the 55-gallon drum and SWB will be calculated to show that the lower flammability limit of 5% hydrogen is not reached. The inner layers (i.e., sample bottle, bag and shielded pig) in the SWB and drum will be evaluated to assure no pressurization occurs as the hydrogen vents from the inner containers (e.g., shielded pigs, etc.).

The reaction of uranium metal with anoxic liquid water is highly exothermic; the heat of reaction will be combined with the source term decay heat, calculated from Radcalc, to show that the drum and SWB package heat load limits are satisfied.

This analysis does five things:

1. Estimates the H_2 generation from the reaction of uranium metal with water
2. Estimates the H_2 generation from radiolysis (using Radcalc 4.1)
3. Combines both H_2 generation amounts, from Items 1 and 2, and determines the percent concentration of H_2 in:
 - a. the interior of an SWB with two Super Pigs, and
 - b. the interior of a 55-gallon drum with two Piglets
4. From the combined gas generation rate, shows that the pressure at internal layers is minimal
5. Calculates the maximum thermal load of the package, both from radioactive decay of the source and daughter products as calculated/reported by Radcalc 4.1, and from the exothermic reaction of uranium metal with water

Current analysis restrictions and assumptions:

- Steady state, no functions of time
- H_2 generation calculated based on:
 - one temperature, but the temperature is selectable
 - one volume, 600 mL
- The Design Basis inventory is used to calculate:
 - the H_2 production from the chemical reaction of water with uranium metal
 - the H_2 production from radiolysis

Definitions used:

Define a cc:

$$\text{cc} := \text{cm}^3$$

Density of uranium metal:
(Ref. 6, pg B44)

$$\rho_U := 19.0 \frac{\text{gm}}{\text{cc}}$$

Gas constant:
(Ref. 6, pg F-245)

$$R_g := 8.3145 \frac{\text{J}}{\text{K} \cdot \text{mole}}$$

Ambient pressure:

$$P := 1 \text{ atm}$$

As both packages and inner layers are vented, the ambient pressure will always be assumed 1 atm.

1.1 Calculation Methodology

This report was prepared using the MathCAD™ program to perform most calculations. This report includes many instances where output from that program is inserted into the text to provide numbers that support the conclusion of this report. That MathCAD™ source file is available upon request.

1.2 Inputs Used in this Worksheet

The default sludge volume will be 600 mL, which is the per-sample-bottle maximum sludge amount. The default temperature will be three different values that will allow the equations to be simultaneously solved to show the results from these three temperatures. The three temperatures correspond to:

- 115 °F The assumed ambient temperature of the sludge
- 145 °F From Section 3.2.2.1, the assumed temperature of the sludge, based on the maximum temperature for a 55-gallon drum, with solar insolation, assuming a 115 °F ambient air temperature (from Ref. 7)
- 157 °F From Section 3.2.1.1, the assumed temperature of the sludge, based on the maximum temperature of the SWB, with solar insolation, assuming a 115 °F ambient air temperature (from Ref. 8)

Assumed sludge volume:
(per sample bottle)

$$V_{\text{sludge}} := 600 \cdot \text{mL}$$

$$V_{\text{sludge}} = 600 \cdot \text{cc}$$

Assumed temperatures:

$$T_{\text{init}} := \begin{pmatrix} 115 \\ 145 \\ 157 \end{pmatrix} \cdot ^\circ\text{F}$$

$$T_{\text{init}} = \begin{pmatrix} 46.1 \\ 62.8 \\ 69.4 \end{pmatrix} \cdot ^\circ\text{C}$$

2.0 H₂ GENERATION

The hydrogen generation will be calculated from two sources, the chemistry of the uranium metal – water interaction and from radiolysis.

In Pacific Northwest National Laboratory's (PNNL) report "Enthalpies and Free Energies of Reaction for Uranium Phases and Metals of Interest to Transportation of K Basin Sludge" (Ref. 9) an evaluation of the hydrogen generation from chemical reactions within the sludge other than the uranium metal-water (the aluminum-water and zirconium-water reactions) showed that "the gas generation testing results with sludge provide no evidence that appreciable Al or Zr metal reacted with water to generate H₂ over the temperature range of 40 to 95 °C." (Ref. 9, section 5).

Since "no evidence" was observed for the generation of H₂ gas from Al or Zr, the PNNL laboratory tests accounted for all H₂ gas generated. Thus the use of the rate equation in section 2.1.2 will be used to account for all H₂ gas produced, other than that by radiolysis.

2.1 H₂ Generation from the Chemistry of Uranium Metal and Water

2.1.1 Sludge Parameters Used

The sludge parameters were obtained from Ref. 10, Table 2-3 "Properties for Container and Settler Sludge" the "Uranium Metal Fraction in Settled Sludge - Non-Segregated." Ref. 10 establishes the basis for all settler sludge design activities and is appropriate to use for this evaluation.

Design Basis values for uranium metal fraction in sludge:

$$UM_{con} := 0.052 \cdot \frac{gm}{cc}$$

The resulting mass of metallic uranium in the sludge is:

$$M_{MU} := UM_{con} \cdot V_{sludge} = 31.2 \cdot gm$$

From Ref. 11, Table 4-5b "Reactive Sludge Particle Size for Uranium Metal - Segregated," given the largest particle diameter in the sludge is less than 500 μm (as is the case for Integrated Water Treatment System (IWTS) Settler sludge) then the average effective particle diameter is 375 μm . That value is then used to calculate the total number of uranium metal particles in the container and the total uranium surface area in the sample bottle, which is used to determine the overall uranium metal-water reaction rate.

Uranium metal particle diameter:

$$d := 375 \cdot \mu m = 1.23 \times 10^{-3} ft$$

Volume of a single particle:

$$Vol_{part} := \frac{\pi}{6} \cdot d^3 = 2.761 \times 10^{-5} \cdot cc$$

Mass of a single particle:

$$M_{part} := Vol_{part} \cdot \rho_U = 5.246 \times 10^{-4} \cdot gm$$

Surface area of a single particle:

$$A_{single} := \pi \cdot d^2 = 4.418 \times 10^{-3} \cdot cm^2$$

Number of particles:

$$N_{part} := \text{ceil} \left(\frac{M_{MU}}{M_{part}} \right) = 59472$$

Note: "ceil" is the MathCAD™ abbreviation for the mathematical function "ceiling" which rounds toward positive infinity generating the nearest integer greater than or equal to the number of particles in question.

Surface area of all particles:

$$A_{all} := N_{part} \cdot A_{single} = 262.7 \cdot cm^2$$

The hydrogen gas produced from chemical reaction is determined by the Sludge Treatment Project (STP) rate law (Ref. 11). The rate law represents the culmination of reviewing 60 years of technical literature and is based on a survey of 32 studies resulting in 128 data points. The data points are between the temperatures of 24 °C and 350 °C. The entire 128-point dataset is plotted in Figure 2.2 of Ref. 12 and closely follows an Arrhenius dependence on temperature (the logarithm of the rate is proportional to the inverse absolute temperature) over the range of temperature. As there is some data spread over the range of temperature relative to the Arrhenius fit, an upper and lower bound is provided to allow a 95% confidence limit for the rate equation. The upper and lower bound for 95% confidence is approximately a factor of 3 and is very nearly a constant over the temperature range and is known as the Enhancement Factor.

As discussed in Appendix A of Reference 13, the overall technical basis for using the literature rate for the uranium metal in sludge is supported by the central limit tendency for averages. A sludge sample bottle holds the equivalent of many sludge samples used in the gas generation experiments (note: sample sizes ranged from ~10 to 400 g of sludge). As demonstrated in Figure 2.2 of Ref. 12, there is wide, nonsystematic scatter in the literature data, with some points above and some points below the average. It is expected that a collection of independent sludge samples (equivalent to what may be contained in 600 mL of sludge in a sample bottle) will behave like the literature average.

Over the past 12 years gas generation and uranium corrosion testing has been conducted in support of the STP with genuine sludge, irradiated N-Reactor uranium metal fuel, and un-irradiated uranium metal beads (Ref. 12). In all cases, with sludge and N-Reactor fuel, the measured rate from the testing has been within or below the 95% confidence bounds established from the STP rate law. In one case, with natural uranium beads in a grout waste form, the observed rate was slightly greater than the upper 95% confidence bound.

Consistent with the above from Ref. 11, Table 4-10 "Reaction Rate Enhancement Factor for Reaction of U Metal with Oxygen-Free Water," for the design basis Enhancement Factor (the high value for 95% confidence) is:

Enhancement Factor: $EF := 3$

[Note: from Ref. 11, Table 4-10, the rate enhancement factors for design basis are the same as used for safety basis]

2.1.2 Sludge Equations Used and H₂ Produced

From Ref. 11, Table 4-9 "KE & KW Sludge Reaction Rate for Uranium Metal Particulate" shows the equations for weight loss per unit of time and the surface area basis equation (R_c).

From section 1.1:

$$T_{\text{init}} = \begin{pmatrix} 115 \\ 145 \\ 157 \end{pmatrix} \cdot ^\circ\text{F} \quad T_{\text{init}} = \begin{pmatrix} 46.1 \\ 62.8 \\ 69.4 \end{pmatrix} \cdot ^\circ\text{C}$$

Rate constant:

$$R_c := \left(\frac{\text{mg}}{\text{cm}^2 \cdot \text{hr}} \right) \cdot 10^{\left(9.975 - \frac{3565\text{K}}{T_{\text{init}}} \right)} = \begin{pmatrix} 0.0644 \\ 0.2305 \\ 0.3708 \end{pmatrix} \cdot \frac{\text{mg}}{\text{cm}^2 \cdot \text{hr}}$$

Weight loss:

$$\text{Rate} := A_{\text{all}} \cdot EF \cdot R_c = \begin{pmatrix} 50.7 \\ 181.7 \\ 292.3 \end{pmatrix} \cdot \frac{\text{mg}}{\text{hr}} \quad \begin{matrix} 115^\circ\text{F} \\ \text{for } 145^\circ\text{F} \\ 157^\circ\text{F} \end{matrix}$$

Two moles of hydrogen are produced for every mole of uranium (i.e., $U + 2 H_2O = UO_2 + 2 H_2$), so the H_2 production is:

$$\text{Moles of } H_2 \text{ produced: } n_{H_2_chem} := \text{Rate} \cdot \frac{1 \text{ mol}}{238.05 \cdot \text{gm}} \cdot \frac{2 \text{ mol}}{1 \text{ mol}} = \begin{pmatrix} 4.26 \times 10^{-4} \\ 1.53 \times 10^{-3} \\ 2.46 \times 10^{-3} \end{pmatrix} \cdot \frac{\text{mol}}{\text{hr}}$$

$$n_{H_2_chem} = \begin{pmatrix} 1.18 \times 10^{-7} \\ 4.24 \times 10^{-7} \\ 6.82 \times 10^{-7} \end{pmatrix} \cdot \frac{\text{mol}}{\text{sec}} \quad \begin{matrix} 115^\circ\text{F} \\ \text{for } 145^\circ\text{F} \\ 157^\circ\text{F} \end{matrix}$$

2.2 H_2 Generation from Radiolysis

Ref. 10 provides the source term that is being used for all settler sludge design activities and is appropriate to use for this evaluation. Ref. 14 was used for the water transported in the sample bottles in addition to the sludge. The following summarizes the related applications of these for the analyses:

- 1) The sludge source data is taken from Ref. 10, Table 2-2a *Sludge Radionuclide Inventories (Decayed to 5-31-1998)*. The sludge inventory is shown in Table 7.7.1 in Appendix 7.7.
- 2) The volume in the 4.1 L bottle that is not sludge is conservatively assumed to be KE canister water, from Ref. 14, Table 4-1 *Nominal Inventory for K Basin Water Associated with Sludge*. The "nominal" water source term from this table is used for the design basis inventory.

KE canister water was selected because it has conservative radionuclide content (i.e., ^{137}Cs concentration is an order of magnitude greater than that in KW canister water) and some of the settler sludge originated in the KE Basin. It could be argued that it would be appropriate to use the lower water radionuclide values provided in TI-015 (Ref. 11) Table 4-22 when the settler sludge is in the IWTS settler tanks. However, it would not be appropriate when the settler sludge is retrieved into Engineered Container SCS-CON-230. The TI-015 (Ref. 11) Table 4-22, in the 'Note:' to the table, states its values are valid for flowing basin water or sludge staged in a large container such as the Weasel Pit. For small to moderate size vessels or containers, such as the Engineered Container and the sample bottles, Table 4-22 directs the use of HNF-SD-SNF-TI-009 Table 4-1, which is used here.

The water inventory is shown in Table 7.7.1 in Appendix 7.7.

The inventory shown in Table 7.7.1 in Appendix 7.7 was further decayed by a nominal 15 days to establish a minimal-time Radcalc run to estimate the initial heat and gas generated. The inventory was also decayed in Radcalc 4.1 to 1/1/2010. The largest H_2 generation and thermal heat load, from either the 15-day decayed inventory or the inventory decayed to 1/1/2010 (4,234 days) is conservatively used. Both Radcalc results are included in the Appendix.

An Excel spreadsheet was used to determine the specific inventory for an arbitrary volume of sludge, with the remaining volume consisting of water, as defined above. The results from the spreadsheet were used as inputs for Radcalc which resulted in the H_2 generation results from radiolysis used in this report. The spreadsheet produced the source inventory for 600 mL of sludge (with the remaining volume water) and is shown in Appendix 7.7, Table 7.7.1. The results of the 600 mL Radcalc 4.1 run are shown in Appendix

7.7, Sections 7.7.1 and 7.7.2 for the Design Basis for the two different decay times. In this report, only 600 mL of sludge is considered.

Radcalc performs gas calculations at standard pressure and temperature (1 atm and 0 °C). When volume calculations are used throughout this report, the volume flow rate will be temperature adjusted.

Appendix 7.7, Sections 7.7.1 and 7.7.2 contain the complete Radcalc 4.1 output files for 600 mL Design Basis sludge for the two different decay times. Of the two output files, the largest H₂ generation rate for the 600 mL Design Basis sludge is: 0.1002 cc/hr.

2.2.1 H₂ Molar Generation Rate from Radiolysis

The volumetric H₂ generation value from Appendix 7.7, Sections 7.7.1 and 7.7.2 is for 0 °C (Radcalc 4.1 default), and the volumetric generation rate needs to be converted to the molar generation rate at the Radcalc 4.1 default temperature. Note that pressure, at 1 atm, does not need to be adjusted (all layers are vented).

The default Radcalc temperature used in the generated values:

$$T_{\text{Radcalc}} = 0^{\circ} \text{ C} = 273.15 \text{ K}$$

The default Radcalc pressure:

$$P = 1 \text{ atm}$$

The volume of sludge is from the input section:

$$V_{\text{sludge}} = 0.6 \cdot \text{L}$$

The max. resulting H₂ generation rate is:
(Appendix 7.7, Section 7.7.2, from the nominal 15-day decay)

$$H2_{\text{rad_D}} = .1002 \cdot \frac{\text{cc}}{\text{hr}}$$

$$n_{H2_rad_D} = H2_{\text{rad_D}} \frac{P}{R_g \cdot T_{\text{Radcalc}}} = 1.242 \times 10^{-9} \cdot \frac{\text{mol}}{\text{s}}$$

Moles of H₂ generated from radiolysis:

$$n_{H2_rad} = n_{H2_rad_D} \quad \text{Design Basis}$$

The Radcalc temperature at 0 °C is used to determine the hydrogen generation from radiolysis in moles per second, and this rate will be used throughout this analysis and is temperature independent. When a volumetric rate is needed, it will be determined based on the temperature of interest in the particular analysis.

2.3 Combined Total H₂ Generation and Percent Contributions

The two sources of hydrogen will now be combined and the resulting percent contribution of each source will be shown.

Total moles of H_2 produced:
(from one bottle, at
three temperatures)

$$n_{\text{total}} := n_{H_2_rad} + n_{H_2_chem} = \begin{pmatrix} 1.20 \times 10^{-7} \\ 4.25 \times 10^{-7} \\ 6.83 \times 10^{-7} \end{pmatrix} \cdot \frac{\text{mol}}{\text{s}} \quad \begin{matrix} 115^\circ\text{F} \\ \text{for } 145^\circ\text{F} \\ 157^\circ\text{F} \end{matrix}$$

Percent contribution from radiolysis:

$$\text{cont}_{\text{rad}} := \frac{n_{H_2_rad}}{n_{\text{total}}} = \begin{pmatrix} 1.0 \\ 0.3 \\ 0.2 \end{pmatrix} \cdot \%$$

Percent contribution from chemistry:

$$\text{cont}_{\text{chem}} := \frac{n_{H_2_chem}}{n_{\text{total}}} = \begin{pmatrix} 99.0 \\ 99.7 \\ 99.8 \end{pmatrix} \cdot \%$$

Clearly, the chemical reaction is the predominant form of H_2 generation.

From section 1.1:

$$T_{\text{init}} = \begin{pmatrix} 115 \\ 145 \\ 157 \end{pmatrix} \cdot ^\circ\text{F} \quad T_{\text{init}} = \begin{pmatrix} 46.1 \\ 62.8 \\ 69.4 \end{pmatrix} \cdot ^\circ\text{C}$$

Total volumetric H_2 generation is:
(from one bottle)

$$\text{Vol}_{\text{total}} := \frac{n_{\text{total}} \cdot R_g \cdot T_{\text{init}}}{P} = \begin{pmatrix} 11.28 \\ 42.19 \\ 69.15 \end{pmatrix} \cdot \frac{\text{cc}}{\text{hr}} \quad \begin{matrix} 115^\circ\text{F} \\ \text{for } 145^\circ\text{F} \\ 157^\circ\text{F} \end{matrix}$$

3.0 DIFFUSION OF HYDROGEN

The hydrogen generation rates, from radiolysis and the metal/water reaction will now be used with the law of diffusion to calculate the percent H_2 concentrations inside the SWB (with Super Pigs) and inside the 55-gallon drum (with Piglets).

Only diffusion will be assumed, which is conservative, as this ignores pressure driven flow from the gas creation, temperature driven flow from temperature differences over time creating pressure differences, convection flow, or buoyant flow.

3.1 Fick's Law for Hydrogen Diffusion

The release of hydrogen gas (H_2) from a vented package by diffusion through air is modeled according to Fick's law of diffusion (Ref. 15), which is in the form:

$$j = Q \cdot \frac{dc}{dz}$$

where:

Q = Diffusion constant for hydrogen in air, cm^2/s
 dc = Concentration gradient across path, moles/cm^3
 dz = Diffusion path length, cm
 j = Molar flux, $\text{moles}/\text{cm}^2/\text{s}$

The diffusion flow rate is given by:

$$\dot{n} = A \cdot j$$

where:

A = Cross-sectional area of diffusion path, cm^2
 $\dot{n}$ = Diffusion flow rate, moles/s

Substituting Fick's law into the diffusion flow rate (for j) gives the following expression for the diffusion flow rate $\dot{n}$:

$$\dot{n} = \left(\frac{Q \cdot A}{dz} \right) \cdot dc$$

The quantity inside the parenthesis is defined as the diffusivity, D , with units of cm^2/s :

$$D = \left(\frac{Q \cdot A}{dz} \right)$$

The diffusion flow rate can now be simply expressed as:

$$\dot{n} = D \cdot dc$$

The driving force for hydrogen diffusion from a package is the concentration gradient between the package interior and the surrounding atmosphere, which is approximated as having a hydrogen concentration of zero. Ref. 6 lists the hydrogen concentration of atmospheric air at 0.5 ppm by volume, or 0.00005 vol%. In this context, dc represents the overall concentration difference between the package interior and exterior and can be relabeled Δc to distinguish it from the differential concentration gradient. Because the external hydrogen concentration can be assumed zero, Δc is simply the hydrogen concentration inside the package, expressed in volume percent (vol%).

The diffusion flow rate equation is solved for dc , the hydrogen concentration differential. It will be renamed Δc as discussed above to represent the overall concentration difference between the package interior and exterior. Also, the diffusivity will be renamed to represent the total package diffusivity D_{pkg}

and the flow rate is the molar hydrogen generation rate $\dot{n}_{H_2}$ from combining the Radcalc 4.1 radiolysis and the uranium water chemistry interaction.

$$\Delta c = \frac{\dot{n}_{H_2}}{D_{pkg}}$$

This equation will be used to determine the volume percent of H_2 in the containment boundary.

3.1.1 Diffusion Constant for Hydrogen in Air - Temperature Corrected

The Hydrogen diffusion constant will be corrected for the particular temperature given from the parameter input section above.

Ref. 16, the diffusion constant for hydrogen in air at 273K is: $Q_{273} := 0.611 \frac{\text{cm}^2}{\text{s}}$

Ref. 16, Perry's Chemical Engineers' Handbook Eq. (3-133) shows that the diffusion constant is proportional to $T^{1.75}$; the power to which T is raised depends on the actual temperature (Perry's Sixth Edition, Diffusion Coefficients, page 3-285).

The assumed temperature: $T_{\text{init}} = \begin{pmatrix} 319.3 \\ 335.9 \\ 342.6 \end{pmatrix} \text{ K} \quad T_{\text{init}} = \begin{pmatrix} 115 \\ 145 \\ 157 \end{pmatrix} \cdot ^\circ\text{F} \quad T_{\text{init}} = \begin{pmatrix} 46.1 \\ 62.8 \\ 69.4 \end{pmatrix} \cdot ^\circ\text{C}$

Temperature corrected Q value: $Q_{\text{H2}} := Q_{273} \cdot \left(\frac{T_{\text{init}}}{273\text{K}} \right)^{1.75} = \begin{pmatrix} 0.804 \\ 0.878 \\ 0.909 \end{pmatrix} \cdot \frac{\text{cm}^2}{\text{sec}} \quad \begin{matrix} 115^\circ\text{F} \\ \text{for } 145^\circ\text{F} \\ 157^\circ\text{F} \end{matrix}$

3.2 Diffusion in Transport System

The transport system consists of a Standard Waste Box (SWB, Ref. 5), which contains two Super Pigs (Ref. 1) or a 55-gallon drum (Ref. 17, typical) that contains two shielded container assemblies, Piglets, Ref. 2 and 3. One 4.1 L sample bottle is placed in a vented 12 mil polyurethane bag (Ref. 18) prior to placement in the Super Pig (Ref. 1) or Piglet (Ref. 2 and 3).

The two boundaries that are being credited as the containment boundaries are the SWB for the Super Pig and the 55-gallon drum for the Piglet. Both of these boundaries are vented and the percent H_2 concentration in these boundaries will be calculated.

3.2.1 Hydrogen Concentration in the SWB

Assume the SWB is vented with "n" NucFil-019 filters, with minimum $n = 2$ and maximum $n = 4$. The SWB has two Super Pigs, with each Super Pig containing one sample bottle.

From manufacturers specification sheet:
(for one model NucFil NFT-013 filter
Appendix 7.1) $D_{013} := 1.1 \times 10^{-5} \cdot \frac{\text{mol}}{\text{s}}$

From manufacturers specification sheet:
(for one model NucFil NFT-019 filter
Appendix 7.1) $D_{019} := 2.4 \times 10^{-5} \cdot \frac{\text{mol}}{\text{s}}$

The assumed temperature:
(ambient) $T_{\text{init}_0} = 319.3\text{K} \quad T_{\text{init}_0} = 115 \cdot ^\circ\text{F} \quad T_{\text{init}_0} = 46.1 \cdot ^\circ\text{C}$

The assumed pressure: $P = 1 \cdot \text{atm}$

Volumetric filter flow:

$$D_{\text{NFT019}} := D_{019} \cdot \frac{R_g \cdot T_{\text{init}_0}}{P} = 0.629 \cdot \frac{\text{cc}}{\text{s}}$$

Assume the SWB has "n" filters:

$$n_{\text{swb}} := 2$$

The SWB has two Super Pigs:

$$n_{\text{pigs}} := 2$$

"n" filters in parallel on SWB:

$$D_{\text{swb}} := n_{\text{swb}} \cdot D_{019} = 4.8 \times 10^{-5} \cdot \frac{\text{mol}}{\text{s}}$$

The volume percent of H_2 in the SWB is:
(For two Super Pigs in the SWB)

$$\% \text{SWB}_{\text{H}_2_2_ \text{PIG}} := \frac{n_{\text{pigs}} n_{\text{total}_0}}{D_{\text{swb}}} = 0.5 \cdot \%$$

This is for the input parameters:

$$V_{\text{sludge}} = 600 \cdot \text{mL} \quad T_{\text{init}_0} = 115 \cdot ^\circ\text{F}$$

The concentration of hydrogen in the SWB is less than 5%, for the design basis sludge at 115 °F. However, the volume percent will be checked at the solar insolation temperature of the SWB.

3.2.1.1 Hydrogen Concentration in the SWB at Solar Insolation Temperature

The SWB Safety Analysis Report for Packaging (SARP Ref. 8, page xxi-xxii) shows that the maximum SWB temperature does not exceed 69 °C, (157 °F) from solar insolation with an outside air temperature of 115 °F. Page B8-6 shows the maximum temperature is 154.9 °F, which is independent of the internal heat load, from 0 to 4 Watts, which bounds the sludge samples as two bottles produce 0.43 Watts (see section 3.3.3). The assumptions listed for the thermal analysis are on page B8-5 of Ref. 8. The H_2 concentration in the SWB (with up to four filters) will be calculated at 157 °F, to determine if controls are needed to avoid exposure of the SWB to solar insolation.

This worksheet allows the temperature to be adjusted to any value to produce the total H_2 generation. The hydrogen generation value calculated in section 2.3 for 157 °F will now be used.

The assumed temperature:
(SWB maximum Solar)

$$T_{\text{init}_2} = 342.6\text{K} \quad T_{\text{init}_2} = 157 \cdot ^\circ\text{F} \quad T_{\text{init}_2} = 69.4 \cdot ^\circ\text{C}$$

The total moles of H_2 produced is:
(from one bottle, at 157 °F)

$$n_{\text{total}_2} = 6.83 \times 10^{-7} \frac{\text{mol}}{\text{s}}$$

The volumetric total H_2 generation is:
(from one bottle, at 157 °F)

$$V_{\text{total}_2} = 69.15 \cdot \frac{\text{cc}}{\text{hr}}$$

Assume the SWB has "n" filters:

$$n_{\text{swb_max_13}} := 3 \quad n_{\text{swb_max_19}} := 2$$

"n" filters in parallel on SWB:
(for -013 and -019)

$$D_{\text{swb_max_19}} := n_{\text{swb_max_19}} \cdot D_{019} = 4.8 \times 10^{-5} \cdot \frac{\text{mol}}{\text{s}}$$

$$D_{\text{swb_max_13}} := n_{\text{swb_max_13}} \cdot D_{013} = 3.3 \times 10^{-5} \cdot \frac{\text{mol}}{\text{s}}$$

The volume percent of H_2 in the SWB is:
(For two Super Pigs in the SWB at 157 °F
with either the -013 or -019 filter).

$$\%SWB_{H2_2_PIG_157F_19} := \frac{2n_{total_2}}{D_{swb_max_19}} = 2.8 \cdot \%$$

$$\%SWB_{H2_2_PIG_157F_13} := \frac{2n_{total_2}}{D_{swb_max_13}} = 4.1 \cdot \%$$

Note that this is for the input parameters: $V_{sludge} = 600 \text{ mL}$, and $T_{init} = 157 \text{ °F}$

This shows that the SWB does not need controls for solar insolation and can be shipped at ambient temperatures as high as 115 °F when fitted with minimum two NucFil-019 filters or equivalent, or minimum three NucFil-013 filters or equivalent.

3.2.2 Hydrogen Concentration in 55-gallon Drum

Assume the 55-gallon drum is vented with a single NucFil-019 filter (or equivalent) and that the drum contains two Piglets, each with one sample bottle. Assume the temperature is at the ambient 115 °F.

The assumed temperature:
(Drum ambient)

$$T_{init_0} = 319.3K \quad T_{init_0} = 115 \cdot \text{°F} \quad T_{init_0} = 46.1 \cdot \text{°C}$$

The drum filter:
(Assume one drum filter)

$$D_{drum} := D_{019} = 2.4 \times 10^{-5} \cdot \frac{\text{mol}}{\text{sec}}$$

The volume percent of H_2 in the drum is:
(For two Piglets in the drum)

$$\%Drum_{H2_2_PIG} := \frac{2n_{total_0}}{D_{drum}} = 1.0 \cdot \%$$

This is for the input parameters:

$$V_{sludge} = 600 \cdot \text{mL} \quad T_{init_0} = 115 \cdot \text{°F}$$

3.2.2.1 Hydrogen Concentration in 55-gallon Drum at Solar Insolation Temperature

The previous section shows that the 55-gallon drum meets the less-than 5% H_2 concentration at 115 °F. Ref. 7 shows that 55-gallon drum surface temperatures with solar insolation can reach 145 °F with ambient air at 115 °F, so this analysis will be done using a sludge temperature of 145 °F. This temperature is independent of the internal heat load, from 0 to 12 Watts, which bounds the sludge samples as two pigs produce 0.43 Watts (see section 3.3.3).

The hydrogen generation value calculated in section 2.3 for 145 °F will now be used, which occurs at the maximum temperature for the drum.

For this case, a single 3/4-in filter (-019) will be used:

The assumed temperature:
(Drum maximum Solar)

$$T_{init_1} = 335.9K \quad T_{init_1} = 145 \cdot ^\circ F \quad T_{init_1} = 62.8 \cdot ^\circ C$$

The total moles of H_2 produced is:
(from one bottle, at 145 °F)

$$n_{total_1} = 4.25 \times 10^{-7} \cdot \frac{mol}{s}$$

The volumetric total H_2 generation is:
(from one bottle, at 145 °F)

$$Vol_{total_1} = 42.19 \cdot \frac{cc}{hr}$$

The volume percent of H_2 in the drum is:
(For two Piglets in the drum at 145 °F)

$$\%Drum_{H_2_2_PIG_145F} := \frac{2 n_{total_1}}{D_{drum}} = 3.5 \cdot \%$$

Note that this is for the input parameters: $V_{sludge} = 600$ mL, and $T_{init} = 145$ °F

This shows that the drum does not need controls for solar insolation and can be shipped at ambient temperatures as high as 115 °F when fitted with a single NucFil-019 filter or equivalent.

3.3 Heat Source

The total heat will be calculated for both exothermic chemical reaction and from the decay, as reported in the Radcalc 4.1 runs.

In Ref. 9, PNNL evaluated heat production from chemical reactions within the sludge other than the uranium metal-water reaction. PNNL specifically analyzed the aluminum-water and zirconium-water reactions, and concluded that "the gas generation testing results with sludge provide no evidence that appreciable Al or Zr metal reacted with water to generate H_2 over the temperature range of 40 to 95 °C." PNNL further stated that hydrogen production measured in their sampling activities would have been assumed to have been produced by uranium metal, but an over-prediction of uranium metal with a corresponding under-prediction of "reactable Zr and Al metal" would only result in a small underestimate of total reaction enthalpy (Section 5 of Ref. 9).

3.3.1 Decay Heat from Radcalc

The decay heat from radioactive decay of the source and daughter isotopes is shown in Appendix 7.7, Sections 7.7.1 and 7.7.2 for the two different decay times. The maximum decay heat is 0.032 W for the 600 mL sample of sludge at a decay time of 15 days. Since there will be two sample bottles in each drum or SWB, the maximum radiolytic decay heat is 0.064 W.

3.3.2 Heat from Exothermic Chemical Reaction

In the sections that follow it will be shown that there are small quantities of Al, Zr, and Pu, in comparison with the quantity of U in the sludge. Due to the small quantities and Ref. 9 indicating there is no evidence of appreciable reaction of these materials, the heat from exothermic chemical reaction will be ignored for Al, Zr, and Pu.

There is a large margin between the total heat load calculated in section 3.3.3 (0.43 W for the SWB and 0.29 W for the drum) and the heat load assumed in the referenced thermal analyses of the drum (12 W) and the SWB (4 W) that resulted in the maximum package temperatures with solar insolation used in this report. It was the solar insolation temperatures for the SWB and Drum, with internal heat loads of 4 W and 12 W, respectively, that were used to establish the temperatures assumed in this report. The total

sludge heat load would need to be on the order of ten times greater for the heat load to increase the assumed package temperature for the SWB, or thirty times greater for the heat load to increase the assumed package temperature for the Drum.

Due to these large margins, as shown in Section 3.3.2.2, the increases in the heat load that could be shown for Al, Zr, or Pu would have negligible effects on reducing the margin.

3.3.2.1 Uranium Water Reaction

The uranium metal in the sludge is transported with basin water in the sample container. It is assumed that the mass of water is sufficient to react all the uranium metal and is considered unlimited for the purposes of modeling the exothermic uranium metal and water reaction. The heat for the uranium-water reaction is 127.4 kcal/mole-U (Ref. 19, section 8.1.2.2).

The reaction of uranium in water is represented by
(Ref. 19)

The two solar insolation temperatures:

$$\text{SWB: } T_{\text{init}_2} = 157^\circ \text{F}$$

$$\text{Drum: } T_{\text{init}_1} = 145^\circ \text{F}$$

From section 3.2.1.1 and 3.2.2.1 (SWB and Drum):

The total moles of H_2 produced is:

(from one bottle, at 157 °F and 145 °F)

$$n_{\text{H}_2_total} := \left(\frac{n_{\text{total}_2}}{n_{\text{total}_1}} \right) = \left(\frac{6.833 \times 10^{-7}}{4.252 \times 10^{-7}} \right) \cdot \frac{\text{mol}}{\text{sec}}$$

SWB@157 °F

Drum@145 °F

Thus the moles of uranium reacted is one half the moles of hydration produced:

Moles uranium reacted:

$$n_{\text{U_reacted}} := \frac{n_{\text{H}_2_total}}{2} = \left(\frac{3.416 \times 10^{-7}}{2.126 \times 10^{-7}} \right) \cdot \frac{\text{mol}}{\text{sec}}$$

SWB@157 °F

Drum@145 °F

Exothermic reaction rate:

$$U_thermal_rate := 127.4 \cdot \frac{\text{kcal}}{\text{mol}} \quad (\text{per mol uranium})$$

The number of sample bottles in the package:

$$n_{\text{pigs}} = 2$$

The exothermic heat produced is then:
(For two sample bottles, the package)

$$\text{Heat}_{\text{exo_U}} := n_{\text{pigs}} \cdot n_{\text{U_reacted}} \cdot U_thermal_rate$$

$$\text{Heat}_{\text{exo_U}} = \left(\frac{0.364}{0.227} \right) \cdot W$$

SWB@157 °F

Drum@145 °F

3.3.2.2 Aluminum and Zirconium Reaction

Section 5.0 of Ref. 9 discusses the confirmation of the corrosion resistance and lack of significant reactivity of aluminum in the K basin water. It also discusses how zirconium has demonstrated outstanding corrosion resistance. The ratio of Al and Zr to that of uranium will be calculated and the low quantity of Al and Zr, along with its corrosion resistance, justifies ignoring the heat source from these materials.

Table 2-3 of Ref. 10 shows the total uranium in the sludge is 1.34 g U/cc. Table 2-5 (Ref. 10) shows the nominal chemical constituents for Al and Zr. Aluminum, in the form of aluminum hydroxide, is present in the sludge at 0.125 g/cc. Zirconium is identified as not being present in the sludge by the table. Comparing the Al in the sludge to the uranium:

Molecular weight of aluminum hydroxide: $MW_{Al_{OH_3}} := (26.982 + 3 \cdot 15.999 + 3 \cdot 1.008) \frac{g}{mol} = 78.003 \cdot \frac{g}{mol}$

Molecular weight of aluminum: $MW_{Al} := 26.982 \cdot \frac{g}{mol}$

The ratio of aluminum in aluminum hydroxide: $ratio_{Al} := \frac{MW_{Al}}{MW_{Al_{OH_3}}} = 34.6 \cdot \%$

Aluminum hydroxide in settler sludge:
(Ref. 10, Table 2-5) $Al_{hydro} := 0.125 \cdot \frac{g}{cc}$

The portion of aluminum in settler sludge: $Al_{sludge} := ratio_{Al} \cdot Al_{hydro} = 0.043 \cdot \frac{g}{cc}$

Total uranium in settler sludge:
(Ref. 10, Table 2-3, design basis) $U_{sludge} := 1.34 \cdot \frac{g}{cc}$

Ratio of aluminum to total uranium: $ratio_{al_to_u} := \frac{Al_{sludge}}{U_{sludge}} = 3.2 \cdot \%$

With such a small amount of aluminum relative to uranium in the sludge, the discussion in Ref. 9 on the corrosion resistance of aluminum in the K Basin water, and the large margin of safety discussed in Section 3.3.2, aluminum reactions can be ignored. Also, as Ref. 10, Table 2-5 does not identify any zirconium in the settler sludge and the discussion in Ref. 9 on the outstanding corrosion resistance of zirconium, zirconium reactions will also be ignored.

3.3.2.3 Plutonium Water Reaction

The reaction of plutonium metal with water is shown (Ref. 9) to have slightly less enthalpy and Gibbs free energy to that of uranium (discussed above in section 3.3.2.1). Appendix 7.7 shows the quantity of plutonium and uranium. The ratio of the two quantities will be calculated to show that the plutonium reaction may be ignored.

Using the design basis, decayed to 1/1/2010, Radcalc 4.1 results from Section 7.7.1 shows the quantity, in grams, of uranium as:

$$\begin{aligned} Qnt_{U233} &:= 8.633 \times 10^{-8} \cdot gm & Qnt_{U234} &:= 4.853 \times 10^{-2} \cdot gm & Qnt_{U235} &:= 4.767 \times 10^0 \cdot gm \\ Qnt_{U235m} &:= 2.728 \times 10^{-9} \cdot gm & Qnt_{U236} &:= 5.323 \times 10^{-1} \cdot gm & Qnt_{U237} &:= 4.531 \times 10^{-10} \cdot gm \\ Qnt_{U238} &:= 6.248 \times 10^2 \cdot gm \end{aligned}$$

Total uranium is:

$$Qnt_{total\ U} := Qnt_{U233} + Qnt_{U234} + Qnt_{U235} + Qnt_{U235m} + Qnt_{U236} + Qnt_{U237} + Qnt_{U238} = 630.1gm$$

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Using the design basis, decayed to 1/1/2010, Radcalc 4.1 results from Section 7.7.1 shows the quantity, in grams, of plutonium as:

$$Q_{ntPU238} := 1.252 \times 10^{-3} \cdot \text{gm} \quad Q_{ntPU239} := 1.354 \times 10^0 \cdot \text{gm} \quad Q_{ntPU240} := 2.020 \times 10^{-1} \cdot \text{gm}$$

$$Q_{ntPU241} := 1.451 \times 10^{-2} \cdot \text{gm} \quad Q_{ntPU242} := 5.235 \times 10^{-3} \cdot \text{gm}$$

Total plutonium is:

$$Q_{nt_totalPU} := Q_{ntPU238} + Q_{ntPU239} + Q_{ntPU240} + Q_{ntPU241} + Q_{ntPU242} = 1.6 \text{ gm}$$

The ratio of plutonium to uranium is: $\text{Ratio}_{Pu_to_U} := \frac{Q_{nt_totalPU}}{Q_{nt_totalU}} = 0.002503 \quad \frac{1}{\text{Ratio}_{Pu_to_U}} = 399.6$

Due to the fact that there is approximately 400 times the amount of uranium to that of plutonium, the plutonium's contribution to thermal heating and hydrogen generation will be ignored.

3.3.3 Total Thermal Load

The total thermal heat load is the sum of that from radiolysis and the exothermic heat of reaction of uranium with water for two sample bottles in either the drum or SWB. This is calculated as

The Radcalc 4.1 reported thermal load (one pig):
(Appendix 7.7.1 or 7.7.2)

$$\text{Heat}_{radcalc} := 0.032 \text{ W}$$

$$n_{pigs} = 2$$

The total package thermal load is: (two sample bottles)

$$\text{Heat}_{total_per_package} := \text{Heat}_{exo_U} + n_{pigs} \cdot \text{Heat}_{radcalc} = \begin{pmatrix} 0.43 \\ 0.29 \end{pmatrix} \cdot \text{W} \quad \begin{matrix} \text{SWB} \\ \text{Drum} \end{matrix}$$

3.3.4 Thermal Comparison to Referenced Analyses

As shown in sections 2.1.2, 2.3, and 3.3.2.1, the assumed temperature of the settler sludge determines the volumetric hydrogen gas produced and the exothermic heat load generated. As shown in section 1.2, three temperatures were assumed and used for calculations. The assumed settler sludge temperature used in this report, for the drum and SWB packages, was determined from the maximum reported temperature as shown in the Drum and SWB SARP. The Drum and SWB SARPs assumed a bounding internal heat load used in the calculations for maximum package temperature with solar insolation. For the drum, the thermal source assumed in Ref. 7 (Drum SARP, Part B, Section 8.2.2.1) is 12 W. For the SWB, the thermal source assumed in Ref. 8 (SWB SARP, Part B, Section 8.3) is 4 W.

There is a large margin between the total heat load calculated in section 3.3.3 (0.43 W for the SWB and 0.29 W for the drum) and the heat load assumed in the reference thermal analyses of the drum (12 W) and the SWB (4 W) that resulted in the maximum package temperature with solar insolation used in this report. Thus the maximum solar insolation temperature reported in Ref. 7 and Ref. 8 is bounding for this analysis, and the assumed reaction rate temperatures are conservative.

4.0 INTERIOR LAYER PRESSURE AVOIDANCE

The NucFil filters have a stated flow rate (air) at 1-in. water column (WC) pressure differential of 200 mL/min. The filters flow rate will be equated to the flow rate through an equivalent cylindrical hole of a known length and known diameter, to show that the filter is equivalent to a hole that gas must pass through. The equivalent hole will then be compared to the holes in the inner layers of the SWB or Drum, to show that inner-layer pressures will not occur.

Density of water:

(25 °C, or 77 °F, Ref. 20)

$$\rho_{h2o} := 997 \frac{\text{kg}}{\text{m}^3} = 62.24 \cdot \frac{\text{lb}}{\text{ft}^3}$$

Differential pressure at 1-in water column:

$$P_{1in} := \rho_{h2o} \cdot g \cdot 1in = 0.036 \cdot \text{psi}$$

Filter specification flow rate:

(for one filter on the drum, -019)

$$\text{Spec}_{019} := 200 \frac{\text{mL}}{\text{min}} = 3.333 \cdot \frac{\text{cc}}{\text{s}}$$

The highest flow rate that one filter will see is the single filter on a drum, which was calculated in section 2.3.

$$T_{\text{init}_1} = 145 \cdot ^\circ\text{F}$$

The H₂ flow rate in the drum at 145 °F:

(two pigs and one filter on the 55-gallon drum)

$$\text{Max}_{\text{flow}} := 2 \cdot \text{Vol}_{\text{total}_1} = 84.4 \cdot \frac{\text{cc}}{\text{hr}}$$

Note: The hydrogen generation could be greater in the SWB due to possible higher temperatures, but the SWB vent path requires multiple filters. The drum only has one filter, so this will be bounding.

The ratio of the gas volume vented at 1-in WC
to the gas volume produced:

$$\text{Ratio}_{\text{vent_prod}} := \frac{\text{Spec}_{019}}{\text{Max}_{\text{flow}}} = 142$$

This ratio shows that even at the highest rate of gas production from both pigs that the drum and SWB filters can easily pass this gas without building any pressure. Finding an equivalent "hole" equal to the filter's flow rate will show that the inner layers will not build pressure.

Poiseuille's law (Ref. 20) relates the volume flow rate for laminar flow through horizontal tubes of diameter D and length L as:

Poiseuille's law:

$$V_{\dot{}} = \frac{\Delta P \cdot \pi \cdot D_{eq}^4}{128 \cdot \mu \cdot L_{eq}}$$

Dynamic viscosity:
(air at 68 °F, Ref. 20))

$$\mu := 1.825 \times 10^{-5} \frac{\text{kg}}{\text{m} \cdot \text{s}}$$

The pressure is the 1-in. WC:

$$\Delta P := P_{1in} = 0.036 \cdot \text{psi}$$

The flow rate is:

$$V_{\dot{}} := \text{Spec}_{019} = 3.333 \cdot \frac{\text{cc}}{\text{s}}$$

Solving for the diameter:
(as a function of L)

$$D_{eq}(L_{eq}) := \sqrt[4]{V_{\dot{}} \cdot \frac{(128 \cdot \mu \cdot L_{eq})}{(\Delta P \cdot \pi)}}$$

Assume a 3-in. equivalent L:

$$D_{eq_3} := D_{eq}(3in) = 0.037 \cdot \text{in}$$

Note that the 3-in. length is just to demonstrate the methodology, actual lengths will be used below.

The area of the 3-in. equivalent hole:

$$A_{eq_3} := \frac{1}{4} \pi \cdot D_{eq_3}^2 = 1.062 \times 10^{-3} \cdot \text{in}^2$$

The methodology of this equivalent "hole" calculation will now be compared to the vent holes in the Super Pig, Piglet, and sample bottle.

4.1 Super Pig Vent Hole, Flow, and Pressure

The Super Pig has four vent holes, the holes are half-circles with an $r = 0.06$ inch. The half-hole area will be calculated, then the Super Pigs equivalent vent hole size will be determined, and then compared to the size of hole required to vent the Super Pig with a flow rate equal to the filters.

Length of horizontal vent path:

$$L_{s_pig_h} := \frac{(12.75 - 6.27)}{2} \text{in} = 3.24 \cdot \text{in}$$

Diameter of horizontal vent path:

$$Dia_{s_pig_h} := 2 \cdot 0.06 \text{in} \quad \text{Area will be half, as vent is half circle}$$

Area of horizontal lid vent path:
(one vent path)

$$Area_{s_pig_h} := \frac{\frac{1}{4} \pi \cdot Dia_{s_pig_h}^2}{2} = 5.655 \times 10^{-3} \cdot \text{in}^2$$

Diameter of a circular cross section vent
with the same area as the Super Pig
(one vent path)

$$Dia_{s_pig_h_eq} := \sqrt{\frac{Area_{s_pig_h}}{\frac{1}{4} \pi}} = 0.085 \cdot \text{in}$$

The equivalent diameter of the Super Pig's vent hole (one) to have the same air flow rate as a NucFil filter at 1-in. WC pressure (equation from Section 4.0):

$$D_{eq_Superpig} := D_{eq}(L_{s_pig_h}) = 0.037 \text{ in}$$

Ratio of actual vent hole (one)
to equivalent vent hole:

$$\text{ratio}_{superpig} := \frac{Dia_{s_pig_h_eq}}{D_{eq_Superpig}} = 2.3$$

This shows the Super Pig is adequately vented (assuming just one of the four holes) to avoid pressure in the Super Pig.

Check the Reynolds number to assure the use of Poiseuille's law was correct (properties at room temperature will be conservative).

Average velocity:
(for 200 mL/min)

$$Vel_{air} := \frac{V_{dot}}{Area_{s_pig_h}} = 35.97 \cdot \frac{\text{in}}{\text{sec}}$$

kinematic viscosity:
(at 68 °F)

$$\nu := 1.55 \cdot 10^{-05} \frac{\text{m}^2}{\text{sec}}$$

Reynolds number:

$$R_e := \frac{Vel_{air} \cdot Dia_{s_pig_h_eq}}{\nu} = 127$$

Clearly the flow is laminar (R_e less than 2300), the use of Poiseuille's law is valid, and the Super Pig will not build pressure.

4.2 Piglet Vent Hole, Flow, and Pressure

The Piglet has one vent hole, the hole has a diameter = 0.159-in. This hole will be compared to the size of hole required to vent the Piglet as well as a NucFil filter could vent air at 1-in. WC pressure.

Length of lid vent path:

$$L_{lid_vent} := 1.75 \text{ in} + 2.09 \text{ in} = 3.84 \cdot \text{in}$$

Diameter of lid vent path:

$$Dia_{lid_vent} := 0.159 \text{ in}$$

Area of lid vent path:

$$Area_{lid_vent} := \frac{1}{4} \pi \cdot Dia_{lid_vent}^2 = 0.020 \cdot \text{in}^2$$

The equivalent diameter of the Piglet's vent hole to have the same air flow rate as a NucFil filter at 1-in. WC differential pressure (equation from section 4.0):

$$D_{eq_Piglet} := D_{eq}(L_{lid_vent}) = 0.039 \cdot \text{in}$$

Ratio of actual vent hole
to equivalent vent hole:

$$\text{ratio}_{Piglet} := \frac{Dia_{lid_vent}}{D_{eq_Piglet}} = 4.1$$

This shows the Piglet is adequately vented to avoid pressure in the Piglet.

Check the Reynolds number to assure the use of Poiseuille's law was correct.

$$Re_{piglet} := \frac{Vel_{air} \cdot Dia_{lid_vent}}{v} = 238.1$$

Clearly the flow is laminar (Re less than 2300), the use of Poiseuille's law is valid, and the Piglet will not build pressure.

4.3 Vented Nalgene® Bottle, Flow, and Pressure

Drawing H-1-90493 (Ref. 21) shows the lid of the bottle has a 1/16-in. diameter hole. Per a telephone conversation with technical support at Nalgene®, the thickness of the lid of the bottle does not exceed 5 mm.

Length of 1/16-in dia. hole in bottle lid: $L_{bottle_lid_hole} := 5mm = 0.197 \cdot in$

Diameter of bottle lid hole: $Dia_{bottle_lid_hole} := \frac{1}{16} in = 0.063 \cdot in$

Area of hole in the bottle lid: $Area_{bottle_hole} := \frac{1}{4} \pi \cdot Dia_{bottle_lid_hole}^2 = 3.068 \times 10^{-3} \cdot in^2$

The equivalent diameter of the bottle's vent hole to have the same air flow rate as a NucFil filter at 1-in. WC differential pressure (equation from section 4.0):

$$D_{eq_Bottle} := D_{eq}(L_{bottle_lid_hole}) = 0.019in$$

Ratio of actual vent hole to equivalent vent hole: $ratio_{Bottle} := \frac{Dia_{bottle_lid_hole}}{D_{eq_Bottle}} = 3.4$

This shows the bottle is adequately vented to avoid pressure.

Check the Reynolds number to assure the use of Poiseuille's law was correct.

$$Re_{Bottle} := \frac{Vel_{air} \cdot Dia_{bottle_lid_hole}}{v} = 93.6$$

Clearly the flow is laminar (Re less than 2300), the use of Poiseuille's law is valid, and the bottle will not build pressure.

4.4 Vented Bag with a BOP Filter, Flow, and Pressure

The vented bag that surrounds the bottle has a BOP filter. The filter has a stated flow rate of 4.0 L/min of air at 1-in. water column differential pressure uncorrected to STP conditions, see Appendix 7.5. This flow is about 20 times that of the NucFil filter and will easily vent any pressure coming from the bottle to the pig. No analysis is necessary.

5.0 RESULTS AND CONCLUSIONS

The hydrogen generation rate has been determined for both radiolysis and chemical reaction of uranium metal and water. The hydrogen generation rate was calculated for a sludge volume of 600 mL in the sample bottle. For a volume of 600 mL sludge, the maximum reported package temperature with solar insolation was used to show that the percent of hydrogen in the SWB (for two Super Pigs) and in a 55-gallon drum (for two Piglets) will be less than 5%.

The thermal heat load (from radioactive decay of the source and daughter isotopes and the exothermic heat of reaction of uranium metal with water) for two sample bottles in either the drum or SWB (shown to be a maximum of 0.43 W) is less than the assumed heat load used in either the SWB or Drum SARP to establish the maximum solar package temperature. With the resulting bounding temperature, the reaction rates in this report are conservative.

The following constraints are required:

For the SWB:

1. A minimum of two NucFil-019 filters or equivalent (H_2 diffusivity of 2.4×10^{-5} Mol/sec/mol fraction or greater for each filter) are required, or a minimum of three NucFil-013 filters or equivalent (H_2 diffusivity of 1.1×10^{-5} Mol/sec/mol fraction or greater for each filter) are required.
2. Two Super Pigs, each containing 600 mL of sludge, are allowed in the SWB.
3. The SWB is known (Ref. 8) to reach container temperatures no greater than 157 °F due to solar insolation. The H_2 gas generated at 157 °F was calculated and the volume percent of H_2 is 2.8% with two -019 filters, and 4.1% for three -013 filters.
4. This configuration requires no protection from solar insolation and may be transported in ambient conditions up to 115 °F.

For the 55-gallon drum with a single ¾-in. filter (-019 or equivalent):

1. One NucFil-019 or equivalent (H_2 diffusivity of 2.4×10^{-5} Mol/sec/mol fraction or greater) filter is required.
2. Two Piglets, each containing 600 mL of sludge, are allowed in the drum.
3. 55-gallon drums have been shown (Ref. 7) to reach no greater than 145 °F due to solar insolation. The H_2 gas generated at 145 °F was calculated and the volume percent of H_2 is 3.5% with one -019 filter.
4. This configuration requires no protection from solar insolation and may be transported in ambient conditions up to 115 °F.

Using a method of equivalent "holes," e.g. a hole with the same flow rate as the SWB or drum filter, it has been shown that each layer (bottle, bag and pig) in the containment boundary is designed with a vent path that exceeds that of the SWB or drum filter. No internal pressurization will occur.

6.0 REFERENCES

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7.0 APPENDIX

7.1 NucFil Product Specification Data Sheets (-013, and -019)

9/02

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741 Corporate Circle, Suite R Golden, Colorado 80401

Product Specification Data Sheet

Model: NucFil®013
 Specification #: NFT-013
 Engineering
 Drawing #: 05130000

Date: 12/22/2003
 Revision: 5

Usage:

Control VOC release and ventilation of hydrogen gas generated in 55 gal drums, containers, and Standard Waste Boxes containing TRU, Low Level, Hazardous or Mixed Wastes. Installed into ¾" flange of newly generated drum lids with 10-foot pounds of torque. Torque to 15-foot pounds on drums weighing more than 900 lbs.

Performance Characteristics:

Particle Removal Efficiency:	Tested at greater than 99.97% of 0.3 μ to 0.5 μ poly-dispersed (DOP) aerosol.
Resistance to Flow:	Less than 1.0" W.C. DP @ 200 ml/min
Hydrogen Diffusivity:	1.1 E-05 Mol/Sec/mol Frac
Notes:	

Physical Characteristics:

Filter Media:	Carbon-bonded-Carbon
Size:	Overall Height: 1.10"
	Diameter: 1.64"
	Thread Type ¾" - 14 NPS
	Profile: .358"
Material of Construction:	Type 304 Stainless steel
Type of Installation:	Threaded into ¾" pipe thread bung typical
Type of Seal:	Neoprene gasket .125" thick, 50-70 durometer

In conformance to the following Standards or Specifications:

ASME-NQA-1, DOT 7A, Trampac Rev.19 Appendix 2.5

Identification markings: (All items will be marked with the following information at a minimum)

Model Number: NucFil®013
 Date of Manufacture: (mm/yy)
 Unique Serial Number:

741 Corporate Circle, Suite R Golden, Colorado 80401

Product Specification Data Sheet

Model: NucFil®019
 Specification #: NFT-019
 Engineering
 Drawing #: 05190000

Date: 03/18/04
 Revision: 2

Usage:

Advanced design for Control VOC release and ventilation of hydrogen gas generated in 55-gallon drums, overpack drums, and Standard Waste Boxes containing TRU, Low Level, Hazardous or Mixed Wastes. Installed into 3/4" flange of newly generated waste drum lids with 10-foot pounds torque. Maximum hydrogen permeability without loss of integrity.

Performance Characteristics:

Particle Removal Efficiency:	Tested at greater than 99.97% of 0.3 μ to 0.5 μ poly-dispersed (DOP) aerosol.
Resistance to Flow:	Less than 1.0" W.C. DP @200 ml/min
Hydrogen Diffusivity:	2.4 E -05 Mol/sec/mol fraction
Notes:	

Physical Characteristics:

Filter Media:	Carbon-bonded-carbon
Size:	Overall Height: 0.72"
	Diameter: 1.50" Hex
	Profile: 0.4"
Material of Construction:	Type 304 Stainless steel
Type of Installation:	Threaded into 3/4"-14 NPS
Type of Seal:	Neoprene gasket 0.125" thick 50-70 Durometer

In conformance to the following Standards or Specifications:

ASME-NQA-1

Identification markings:

(All items will be marked with the following information at a minimum)

Model Number: NucFil®019
 Date of Manufacture: (MM/YY)
 Unique Serial Number:

Engineering:

(303) 384-9785

Quality:

Fax (303) 384-9979

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7.2 Piglets in the 55-Gallon Drum (Ref. 22)

7.3 Piglets Vented Lid (Ref. 3)

7.4 Bottle's Vented Bag, with BOP Filter (Ref. 18)

7.5 BOP Filter Sample Test Report (2 pages total)

October 9, 2008

Mr. Joe Lechmann
LANCS Industries Inc.
12704 NE 124th St. #36
Kirkland, WA 98034

Subject: Test Report for Filter Diffusivity, Efficiency and Flow Rate of BOP 3CPU-1.5"-2PU Filters for LANC's PO # 19127

The 3CPU-1.5"-2PU filters manufactured by BOP Filter/Barriers LLC (BOP) and further identified by serial numbers recorded on the filters have been tested for flow and efficiency as described in this report. Separate tests performed at Jacksonville University tested the diffusivity of this filter design. All filters provided meet the requirements as stated below.

- Filters are manufactured by BOP and the filtering material is made from split (melt blown) polypropylene fibers.
- The flow rate of these filters is approximately 4.0 L/min of air at 1" of water column differential pressure uncorrected to STP conditions. This flow rate is approximately 100 times the required flow rate of 35 mL/min of air at standard temperature and pressure with a 1" water column pressure differential.
- The hydrogen diffusivity of this filter design has been tested at Jacksonville University and is $1.12 \pm 0.04 \times 10^{-4}$ mole/second/mole fraction that is approximately 10 times the requested value of 1.075×10^{-5} mole/second/mole fraction. A copy of this report is available upon request from BOP Filter/Barriers LLC.
- Filter efficiency is tested to be 99.98% or higher with a monodispersed DOP aerosol of 0.3micron particles in a penetrometer test. This test exceeds the requirements for filter efficiency of 99.97% with particles of 0.3 to 0.5 microns of DOP.
- The filters are welded to two 1.5" ID x 4.0" OD discs of 6 mil yellow polyester polyurethane to facilitate mounting into similar plastic membranes.
- Background

This test report documents the methodology for testing of BOP's 3CPU-1.5"-2PU filters to ensure they meet their specified design criteria and that they perform to, or exceed, the

www.bopfilters.com

office	208-523-1996
fax	208-523-7470
hq	2997 S. Boulevard Idaho Falls, ID 83404

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requirements for a HDBF5X filter specification in Table 2.5-1 of Appendix 2.5 of the WIPP TRAMPAC document. The filter supplied has twice the diffusivity required for the HDBF5X filter.

Test Methodology

The system used for testing is a customized TDA-100, monodispersed aerosol penetrometer, produced by Air Techniques Inc. The test is performed in accordance with ASTM D 2986-71, Standard Practice for Evaluation of Air Assay Media by the Monodisperse DOP (Diocetyl Phthalate) Smoke Test. BOP maintains a Test Program in accordance with SNT-TC-1A that is administered by our ASNT NDT Level III Certified Tester, Paul Pinson.

Test Procedure

BOP's detailed written procedure utilizes calibrated instruments for all data that is reported in our test reports. A constant flow rate of 4.0L/min is set as the controlling parameter for these tests. This is approximately equivalent to 1" of water column differential pressure.

Test Data

Original test data is recorded in BOP's hardbound test data logbooks that are retained as Quality Records in our files. Data are recorded in chronological order by date and by the unique serial number on each filter. Data recorded includes the differential pressure from the delta pressure meter, flow from the rotometer setting and penetration from our penetration meter.

3CPU-1.5-2PU Filters Delivery Schedule

Date Shipped to LANCIS Industries Inc	Quantity Shipped	Filter Serial Numbers	Test Date
10/02/08	100	75101 to 75200	8/22/08
10/02/08	400	75201 to 75600	8/27/08
10/09/08	100	75601 to 75700	10/07/08
10/09/08	50	75701 to 75750	10/09/08

I certify that the S/N filters identified above have been tested as described in this report and that they have a minimum efficiency of 99.98% with a 0.3micron DOP Smoke Test.

Certified by: Paul Pinson, Date: 10/09/2008
Paul Pinson ASNT NDT Level III Certificate Number 148298

7.6 Sample Bottle (2 pages total)

Nominal Capacity	Description	Catalog Number	Approx. Brim Cap, ml	Material	I.D. Neck, mm/in.	Hgt. w/ Closure, mm/in.	Hgt. w/o Closure, mm/in.	O.D. Bottle, mm/in.
4 L (1 gal)	Bottle, Heavy Duty	2126-4000	4,100	PP	65 / 2 9/16	338 / 13 5/16	327 / 12 7/8	155 / 6 1/6

From Bottle Specifications in Thermo Scientific Nalgene Plastics Technical Guide at the NALGENE® website, www.NALGENElabware.com.

7.7 Sample Bottle Source Term and H₂ Generation from Radiolysis

Radcalc 4.1 was used for this report. The sample bottle source term was determined as follows:

- 1) The sludge source data is taken from Ref. 9, Table 2-2a *Sludge Radionuclide Inventories (Decayed to 5-31-1998)*. The data was decayed to 1/1/2010, including January 1, the duration is 4234 days. The data was also decayed a nominal 15 days. The worst case H₂ generation resulting from these two results was used in this report.
- 2) The volume in the 4.1 L bottle that is not sludge is conservatively assumed to be KE canister water, from Ref. 12, Table 4-1 *Nominal Inventory for K Basin Water Associated with Sludge*, i.e., ¹³⁷Cs concentration an order of magnitude greater than that in KW canister water. The "nominal" water source term from this table is used for the design basis inventory.

An Excel spreadsheet was used to determine the specific inventory for an arbitrary volume of sludge with the remaining volume water, as discussed above. The results from the spreadsheet were used as inputs for Radcalc 4.1 which resulted in the H₂ generation results from radiolysis used in this report.

The source inventory for 600 mL of sludge (with the remaining volume water) is shown below in Table 7.7.1. The Table 7.7.1 column titled Design Total is the combinations of the water and Design Basis sludge. It is these totals that are input into Radcalc 4.1.

Section 7.7.1 and 7.7.2 contains the Design Basis Radcalc 4.1 output for the two decay times.

The Radcalc 4.1 program was obtained from <https://www.radcalc.energy.gov/dnnradweb>, and the author and checker of this report are authorized and registered Radcalc users. As required by the Radcalc authorization instructions, the "download" menu was checked for Problem Report/Change Request (PR/CR) information. Two PR/CR reports were found as of the date of this report: PR/CR-68 and PR/CR-64. Both PR/CR's were read and found to not impact the Radcalc results used in this report. The Radcalc installation verification report, showing "Verification Status: Passed" is on file in the Transportation Safety organization.

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Table 7.7.1 Source Inventory for 600 mL Sludge (Radcalc 4.1 Input)

Isotope	Design	Water	Design
	Sludge		Total
	Ci	Ci	Ci
Co-60	6.30E-03	5.50E-05	6.35E-03
Sr-90	2.40E+00	5.81E-02	2.46E+00
Y-90	2.40E+00	5.81E-02	2.46E+00
Tc-99	9.30E-04		9.30E-04
Cs-134	0.00E+00	1.49E-04	1.49E-04
Cs-137	1.44E+00	4.62E-02	1.49E+00
Ba-137m	1.36E+00	4.37E-02	1.40E+00
Eu-152	0.00E+00	2.06E-04	2.06E-04
Eu-154	1.91E-02	1.44E-04	1.93E-02
Eu-155	9.06E-03	5.85E-04	9.64E-03
U-234	3.01E-04		3.01E-04
U-235	1.03E-05		1.03E-05
U-236	3.40E-05		3.40E-05
U-238	2.10E-04		2.10E-04
Np-237	1.32E-05	3.22E-06	1.64E-05
Pu-238	2.35E-02	7.32E-06	2.35E-02
Pu-239	8.40E-02	7.32E-06	8.40E-02
Pu-240	4.59E-02	7.32E-06	4.59E-02
Pu-241	2.63E+00		2.63E+00
Pu-242	2.07E-05		2.07E-05
Am-241	1.12E-01	5.29E-04	1.13E-01
Total	1.05E+01	2.08E-01	1.07E+01

0.6-L 50/50 KE/KW Canister Sludge, Table 2-2a, HNF-41051 Rev. 5

3.5-L KE Canister Water, Table 4-1, HNF-SD-TI-009, Vol 2, Rev 4

4.1-L Size of the poly bottle for sludge

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7.7.1 600 mL Design Basis Radcalc 4.1 Results Decayed to 1/1/2010

Radcalc 4.1: D:\Hanford\2009\H2GEN\rad files\original_0_6L_Design_4234day_rev.rad

Performed By:

Checked By:

Don Riley

Alvia Bridges

228 3/24/10

===== Input Information =====

Comments:

0.6L Sludge, Design Basis

Decayed from 5/31/1998 to 1/1/2010.

Sludge: HNF-41051 Rev. 5, Table 2-2a Settler Source Term (50/50 KE/KW)

Water: KE Canister Water, Table 4-1, HNF-SD-SNF-TI-009, Vol 2, Rev 4

Initial Source Data:

Isotope	Cl	Gm	TBq
Co-60	6.350E-03	5.611E-06	2.350E-04
Sr-90	2.460E+00	1.781E-02	9.102E-02
Y-90	2.460E+00	4.524E-06	9.102E-02
Tc-99	9.300E-04	5.506E-02	3.441E-05
Cs-134	1.490E-04	1.153E-07	5.513E-06
Cs-137	1.490E+00	1.714E-02	5.513E-02
Ba-137m	1.400E+00	2.601E-09	5.180E-02
Eu-152	2.060E-04	1.184E-06	7.622E-06
Eu-154	1.930E-02	7.140E-05	7.141E-04
Eu-155	9.640E-03	1.986E-05	3.567E-04
U-234	3.010E-04	4.842E-02	1.114E-05
U-235	1.030E-05	4.766E+00	3.811E-07
U-236	3.400E-05	5.320E-01	1.258E-06
U-238	2.100E-04	6.248E+02	7.770E-06
Np-237	1.640E-05	2.327E-02	6.068E-07
Pu-238	2.350E-02	1.372E-03	8.695E-04
Pu-239	8.400E-02	1.354E+00	3.108E-03
Pu-240	4.590E-02	2.023E-01	1.698E-03
Pu-241	2.630E+00	2.541E-02	9.731E-02
Pu-242	2.070E-05	5.235E-03	7.659E-07
Am-241	1.130E-01	3.298E-02	4.181E-03

Total Activity: 1.074E+01

3.975E-01

* Radionuclides with an A1/A2 fraction of less than 0.001 will not be shown in the output.

Container Data:

Container Void Volume:	0.0542	m^3
Container Mass:	5806	kg
Mass of solid beryllium, lead, graphite, and hydrogenous material enriched with deuterium:	0	kg
Gross Mass:	5816	kg

Waste Data:

Waste Form:	Normal	
Waste State:	Solid	
Waste Volume:	0.0041	m^3
Waste Mass:	10.1	kg
Mass of solid lead:	0	kg
Mass of solid beryllium, graphite, and hydrogenous material enriched with deuterium:	0	kg
Waste Void Volume:	0	m^3

Decay Time Data:

Time to decay source before sealing:	4234	day
Time container is sealed:	0	day

Gamma Absorption Model:

Gamma Abs Model:	100% Gamma Absorption
------------------	-----------------------

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G Value Data:

G Alpha	G Beta	G Gamma
0.24	0.072	1.64
G values entered by the user.		

===== Radioactive Decay Results =====

Decayed Source:

Isotope	Ci	Gm	TBq
Co-60	1.383E-03	1.222E-06	5.116E-05
Sr-90	1.861E+00	1.347E-02	6.885E-02
Y-90	1.861E+00	3.423E-06	6.887E-02
Tc-99	9.300E-04	5.506E-02	3.441E-05
Xe-134	8.220E-26	3.387E-13	3.041E-27
Cs-134	3.043E-06	2.354E-09	1.126E-07
Cs-137	1.140E+00	1.312E-02	4.219E-02
Ba-137m	1.076E+00	2.000E-09	3.983E-02
Nd-144	2.179E-48	2.008E-36	8.062E-50
Sm-148	1.778E-33	5.887E-21	6.580E-35
Eu-152	1.137E-04	6.536E-07	4.208E-06
Eu-154	7.576E-03	2.803E-05	2.803E-04
Eu-155	1.778E-03	3.662E-06	6.578E-05
Gd-152	3.224E-18	1.480E-07	1.193E-19
Hg-206	1.686E-19	1.505E-27	6.238E-21
Tl-206	1.182E-17	5.442E-26	4.374E-19
Tl-207	4.044E-10	2.123E-18	1.496E-11
Tl-208	2.157E-15	7.285E-24	7.982E-17
Tl-209	9.524E-15	2.329E-23	3.524E-16
Tl-210	1.685E-14	2.447E-23	6.236E-16
Pb-209	4.409E-13	9.565E-20	1.631E-14
Pb-210	8.873E-12	1.155E-13	3.283E-13
Pb-211	4.055E-10	1.643E-17	1.500E-11
Pb-212	6.004E-15	4.321E-21	2.221E-16
Pb-214	8.025E-11	2.448E-18	2.969E-12
Bi-209	6.093E-32	6.767E-16	2.254E-33
Bi-210	8.829E-12	7.116E-17	3.267E-13
Bi-211	4.055E-10	9.874E-19	1.500E-11
Bi-212	6.004E-15	4.098E-22	2.221E-16
Bi-213	4.409E-13	2.277E-20	1.631E-14
Bi-214	8.026E-11	1.818E-18	2.970E-12
Bi-215	3.320E-16	2.810E-24	1.229E-17
Po-210	7.716E-12	1.717E-15	2.855E-13
Po-211	1.107E-12	1.068E-23	4.096E-14
Po-212	3.846E-15	2.154E-32	1.423E-16
Po-213	4.315E-13	3.421E-29	1.596E-14
Po-214	8.024E-11	2.492E-25	2.969E-12
Po-215	4.055E-10	1.376E-23	1.500E-11
Po-216	6.006E-15	1.725E-26	2.222E-16
Po-218	8.026E-11	2.883E-19	2.970E-12
At-215	1.622E-15	3.091E-30	6.002E-17
At-217	4.410E-13	2.740E-25	1.632E-14
At-218	1.525E-14	4.420E-25	5.642E-16
At-219	3.423E-16	3.588E-25	1.267E-17
Rn-217	5.292E-17	5.497E-31	1.958E-18
Rn-218	1.525E-17	1.031E-29	5.642E-19
Rn-219	4.055E-10	3.118E-20	1.500E-11
Rn-220	6.006E-15	6.536E-24	2.222E-16
Rn-222	8.026E-11	5.217E-16	2.970E-12
Fr-221	4.410E-13	2.540E-21	1.632E-14
Fr-223	5.705E-12	1.475E-19	2.111E-13
Ra-223	4.055E-10	7.917E-15	1.500E-11
Ra-224	6.006E-15	3.751E-20	2.222E-16
Ra-225	4.441E-13	1.133E-17	1.643E-14
Ra-226	8.047E-11	8.140E-11	2.977E-12
Ra-228	8.971E-15	3.290E-17	3.319E-16
Ac-225	4.410E-13	7.600E-18	1.632E-14

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Ac-227	4.134E-10	5.716E-12	1.530E-11
Ac-228	8.970E-15	4.014E-21	3.319E-16
Th-227	4.028E-10	1.311E-14	1.490E-11
Th-228	6.021E-15	7.346E-18	2.228E-16
Th-229	4.486E-13	2.110E-12	1.660E-14
Th-230	3.211E-08	1.558E-06	1.188E-09
Th-231	1.030E-05	1.938E-11	3.811E-07
Th-232	1.945E-14	1.774E-07	7.196E-16
Th-234	2.100E-04	9.067E-09	7.770E-06
Pa-231	2.525E-09	5.346E-08	9.343E-11
Pa-233	1.689E-05	8.140E-10	6.250E-07
Pa-234	3.150E-07	1.595E-13	1.165E-08
Pa-234m	2.100E-04	3.058E-13	7.770E-06
U-233	8.316E-10	8.633E-08	3.077E-11
U-234	3.017E-04	4.853E-02	1.116E-05
U-235	1.030E-05	4.767E+00	3.811E-07
U-235m	8.392E-02	2.728E-09	3.105E-03
U-236	3.402E-05	5.323E-01	1.259E-06
U-237	3.698E-05	4.531E-10	1.368E-06
U-238	2.100E-04	6.248E+02	7.770E-06
Np-237	1.690E-05	2.398E-02	6.252E-07
Pu-238	2.144E-02	1.252E-03	7.934E-04
Pu-239	8.397E-02	1.354E+00	3.107E-03
Pu-240	4.584E-02	2.020E-01	1.696E-03
Pu-241	1.501E+00	1.451E-02	5.554E-02
Pu-242	2.070E-05	5.235E-03	7.659E-07
Am-241	1.479E-01	4.317E-02	5.473E-03
Total Activity:	7.836E+00		2.899E-01
w/o Daughters:	4.898E+00		1.812E-01

Decay Heat:

Heat Generated at Time Zero:	0.03226	W
Heat Generated When Sealed:	0.02754	W
Heat Generated When Opened:	0.02754	W

===== Regulatory Requirements Warning =====

Radcalc utilizes numerically based criteria to classify packages against the regulations. Many regulations also include subjective criteria that Radcalc does not consider. The user must check to ensure that all requirements in the regulations are met.

===== DOT Classification Results =====

- * DOT classification calculations are made at the end of the user-specified decay time.

Radioactive Determination:

Radioactive:	Yes		(ACEMs and ALECs > 1.0)
ACEM Limit Fraction:	1671000	ACEMs	(Number of ACEMs)
ALEC Limit Fraction:	14610000	ALECs	(Number of ALECs)

- * This package is not exempt from 49 CFR Subchapter C.

Effective A2s for Mixture: 1.455E+10 Bq

Type Determination:

Type:	B		(A2s > 1.0)
A2 Limit Fraction:	12.45	A2s	(Number of A2s)

Limited Quantity Determination:

Limited Quantity:	No		(Solid, activity > 0.001 A2)
Activity:	12.45	A2	
	7.836	Ci	
	0.2899	TBq	

Fissile: Yes
Fissile Excepted: Yes (b)

LSA Determination:

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LSA-I:	No		(Fissile excepted, ACEMs > 30 x rad limits)
LSA-II:	No		(A2s/gm > 0.0001)
LSA-III:	Yes		(A2s/gm <= 0.002)
Specific Activity:	0.001233	A2/gm	
	0.0007759	Ci/gm	

HRCQ Determination:			
HRCQ:	No		(A2s <= 3000, Activity <= 1000 TBq)
A2 Limit Fraction:	12.45	A2s	
Activity:	7.836	Ci	
	0.2899	TBq	

Fissile Determination:			
Fissile:	Yes		(Contains fissile isotopes per 49 CFR 173.403)

Fissile Excepted Determination:			
Fissile Excepted:	Yes (b)		(Fissile isotopes <= 15 grams, container + contents)
solid non-fissile > = 1.227E+03 grams)			
Fissile Mass:	6.135	gm	
Container beryllium, lead, graphite, and hydrogenous material enriched with deuterium:	0	gm	
Container Mass:	5806000	gm	
Waste lead:	0	gm	
Waste beryllium, graphite, and hydrogenous material enriched with deuterium:	0	gm	
Waste Mass:	10100	gm	
Solid Non-Fissile Mass:	5816000	gm	
Total Uranium Mass:	630.1	gm	
U-233 Mass:	8.633E-08	gm	
U-235 Mass:	4.767	gm	
Uranium Enrichment:	0.7564	%	
Total Plutonium Mass:	1.577	gm	
Pu-239 Mass:	1.354	gm	
Pu-241 Mass:	0.01451	gm	

Reportable Quantity Determination:			
Reportable Quantity:	Yes		(RQs > = 1.0)
RQ Limit Fraction:	52.53	RQs	(Number of RQs)

Shipping Papers and Labels:				
Isotope	Number of A2s	Fraction of A2s	Cumulative A2s	Cumulative Fraction of A2s
+ Am-241	5.473	0.4394	5.473	0.4394
+ Pu-239	3.107	0.2495	8.58	0.6889
+ Pu-240	1.696	0.1362	10.28	0.8251
+ Pu-241	0.9257	0.07433	11.2	0.8994
+ Pu-238	0.7934	0.0637	12	0.9632
Sr-90	0.2295	0.01843	12.22	0.9816
U-235m	0.1553	0.01247	12.38	0.994
Cs-137	0.07032	0.005646	12.45	0.9997

- + Contains 95% of the total A2s and must be included per 49 CFR 173.433.
- * Radionuclides comprising less than 0.1% of the total A2s are not shown in the list.

===== DOE Classification Results =====

- * DOE classification calculations are made at the end of the user-specified decay time.

DOE-STD-1027 Category Determination:		
Category:	< Cat 3	(Cat3s <= 1.0)
Cat 2 Limit Fraction:	0.005979	
Cat 3 Limit Fraction:	0.7525	

- * The DOE-STD-1027 category determination is based on dose-related limits. The user must apply any criticality-related limits separately.

Dose-Equivalent Curies:	
ICRP-72 DE-Ci:	0.3024

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FGR-11 DE-Ci: 0.3373

TRU Waste Determination:

TRU Waste: Yes (TRU activity > 100 nCi/gm)
TRU Activity: 29630 nCi/g

WIPP Quantities:

FGE Value: 4.457
PE-Ci Value: 0.3297

===== NRC Classification Results =====

* NRC classification calculations are made at the end of the user-specified decay time.

NRC Container Category:

Container Category: III
LSA-I: No
LSA-II: No
LSA-III: Yes
Total Activity: 7.836 Ci
A2 Limit Fraction: 12.45 A2s

===== Hydrogen/Helium Gas Results =====

* Hydrogen gas calculations are made at the end of the user-specified seal time.

Hydrogen Gas:

H2 Concentration: 0 %
H2 Moles : 0 moles
H2 Volume : 0 cm³ (0 C, 101.325 kPa)
H2 Rate When Sealed: 0.08154 cm³/hr (0 C, 101.325 kPa)
H2 Rate When Opened: 0.08154 cm³/hr (0 C, 101.325 kPa)

Helium Gas:

He Concentration: 0 %
He Moles : 0 moles
He Volume : 0 cm³ (0 C, 101.325 kPa)
He Rate When Sealed: 1.486E-06 cm³/hr (0 C, 101.325 kPa)
He Rate When Opened: 1.486E-06 cm³/hr (0 C, 101.325 kPa)

Pressure When Opened:

Partial Pressure (H2): 0 kPa
Partial Pressure (He): 0 kPa
Partial Pressure (O2): 0 kPa (if H2O present in waste)
Total Pressure (H2 + He + Air): 101.3 kPa
Total Pressure (H2 + He + O2 + Air): 101.3 kPa (if H2O present in waste)

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7.7.2 600 mL Design Basis Radcalc 4.1 Results Decayed Nominal 15 day

Radcalc 4.1: D:\Hanford\2009\H2GEN\rad files\original_0_6L_Design_15day_rev.rad

Performed By:
Checked By:

DJR 3/24/10
Don Riley
Alvia Bridges
AEA 3/24/10

===== Input Information =====

Comments:

0.6L Sludge, Design Basis

Decayed from 5/31/1998 by 15 days.

Sludge: HNF-41051 Rev. 5, Table 2-2a Settler Source Term (50/50 KE/KW)

Water: KE Canister Water, Table 4-1, HNF-SD-SNF-TI-009, Vol 2, Rev 4

Initial Source Data:

Isotope	Ci	Gm	TBq
Co-60	6.350E-03	5.611E-06	2.350E-04
Sr-90	2.460E+00	1.781E-02	9.102E-02
Y-90	2.460E+00	4.524E-06	9.102E-02
Tc-99	9.300E-04	5.506E-02	3.441E-05
Cs-134	1.490E-04	1.153E-07	5.513E-06
Cs-137	1.490E+00	1.714E-02	5.513E-02
Ba-137m	1.400E+00	2.601E-09	5.180E-02
Eu-152	2.060E-04	1.184E-06	7.622E-06
Eu-154	1.930E-02	7.140E-05	7.141E-04
Eu-155	9.640E-03	1.986E-05	3.567E-04
U-234	3.010E-04	4.842E-02	1.114E-05
U-235	1.030E-05	4.766E+00	3.811E-07
U-236	3.400E-05	5.320E-01	1.258E-06
U-238	2.100E-04	6.248E+02	7.770E-06
Np-237	1.640E-05	2.327E-02	6.068E-07
Pu-238	2.350E-02	1.372E-03	8.695E-04
Pu-239	8.400E-02	1.354E+00	3.108E-03
Pu-240	4.590E-02	2.023E-01	1.698E-03
Pu-241	2.630E+00	2.541E-02	9.731E-02
Pu-242	2.070E-05	5.235E-03	7.659E-07
Am-241	1.130E-01	3.298E-02	4.181E-03

Total Activity: 1.074E+01 3.975E-01

* Radionuclides with an A1/A2 fraction of less than 0.001 will not be shown in the output.

Container Data:

Container Void Volume:	0.0542	m^3
Container Mass:	5806	kg
Mass of solid beryllium, lead, graphite, and hydrogenous material enriched with deuterium:	0	kg
Gross Mass:	5816	kg

Waste Data:

Waste Form:	Normal	
Waste State:	Solid	
Waste Volume:	0.0041	m^3
Waste Mass:	10.1	kg
Mass of solid lead:	0	kg
Mass of solid beryllium, graphite, and hydrogenous material enriched with deuterium:	0	kg
Waste Void Volume:	0	m^3

Decay Time Data:

Time to decay source before sealing:	15	day
Time container is sealed:	0	day

Gamma Absorption Model:

Gamma Abs Model:	100% Gamma Absorption
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G Value Data:

G Alpha G Beta G Gamma
0.24 0.072 1.64
G values entered by the user.

===== Radioactive Decay Results =====

Decayed Source:

Isotope	Ci	Gm	TBq
Co-60	6.316E-03	5.581E-06	2.337E-04
Sr-90	2.458E+00	1.779E-02	9.093E-02
Y-90	2.458E+00	4.521E-06	9.095E-02
Tc-99	9.300E-04	5.506E-02	3.441E-05
Xe-134	1.149E-27	4.733E-15	4.251E-29
Cs-134	1.470E-04	1.137E-07	5.438E-06
Cs-137	1.489E+00	1.712E-02	5.508E-02
Ba-137m	1.405E+00	2.611E-09	5.199E-02
Nd-144	1.116E-55	1.029E-43	4.130E-57
Sm-148	2.693E-38	8.915E-26	9.965E-40
Eu-152	2.056E-04	1.181E-06	7.606E-06
Eu-154	1.924E-02	7.117E-05	7.117E-04
Eu-155	9.582E-03	1.974E-05	3.546E-04
Gd-152	1.513E-20	6.945E-10	5.599E-22
Hg-206	3.482E-27	3.109E-35	1.288E-28
Tl-206	8.126E-26	3.741E-34	3.007E-27
Tl-207	1.425E-16	7.482E-25	5.272E-18
Tl-208	1.037E-22	3.503E-31	3.838E-24
Tl-209	4.017E-22	9.822E-31	1.486E-23
Tl-210	1.088E-19	1.580E-28	4.027E-21
Pb-209	1.753E-20	3.804E-27	6.488E-22
Pb-210	1.836E-19	2.390E-21	6.795E-21
Pb-211	1.431E-16	5.798E-24	5.296E-18
Pb-212	2.934E-22	2.112E-28	1.086E-23
Pb-214	5.201E-16	1.586E-23	1.924E-17
Bi-209	4.523E-42	5.024E-26	1.674E-43
Bi-210	5.900E-20	4.755E-25	2.183E-21
Bi-211	1.431E-16	3.483E-25	5.293E-18
Bi-212	2.889E-22	1.972E-29	1.069E-23
Bi-213	1.861E-20	9.610E-28	6.885E-22
Bi-214	5.184E-16	1.174E-23	1.918E-17
Bi-215	3.818E-21	3.230E-29	1.413E-22
Po-210	8.017E-22	1.784E-25	2.966E-23
Po-211	3.905E-19	3.769E-30	1.445E-20
Po-212	1.851E-22	1.036E-39	6.848E-24
Po-213	1.821E-20	1.444E-36	6.738E-22
Po-214	5.183E-16	1.609E-30	1.918E-17
Po-215	1.445E-16	4.902E-30	5.347E-18
Po-216	3.416E-22	9.810E-34	1.264E-23
Po-218	5.225E-16	1.877E-24	1.933E-17
At-215	5.780E-22	1.102E-36	2.139E-23
At-217	1.888E-20	1.173E-32	6.985E-22
At-218	9.928E-20	2.878E-30	3.673E-21
At-219	3.940E-21	4.130E-30	1.458E-22
Rn-217	2.265E-24	2.353E-38	8.381E-26
Rn-218	9.928E-23	6.715E-35	3.673E-24
Rn-219	1.445E-16	1.111E-26	5.347E-18
Rn-220	3.416E-22	3.717E-31	1.264E-23
Rn-222	5.228E-16	3.399E-21	1.934E-17
Fr-221	1.888E-20	1.087E-28	6.985E-22
Fr-223	6.568E-17	1.698E-24	2.430E-18
Ra-223	1.445E-16	2.821E-21	5.347E-18
Ra-224	3.416E-22	2.134E-27	1.264E-23
Ra-225	1.038E-19	2.647E-24	3.840E-21
Ra-226	1.011E-15	1.023E-15	3.740E-17
Ra-228	1.702E-19	6.244E-22	6.299E-21
Ac-225	1.891E-20	3.258E-25	6.995E-22

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Ac-227	4.774E-15	6.601E-17	1.767E-16
Ac-228	1.621E-19	7.252E-26	5.996E-21
Th-227	7.074E-16	2.302E-20	2.617E-17
Th-228	7.826E-22	9.547E-25	2.896E-23
Th-229	6.645E-19	3.125E-18	2.459E-20
Th-230	1.136E-10	5.513E-09	4.205E-12
Th-231	1.030E-05	1.938E-11	3.811E-07
Th-232	6.889E-17	6.282E-10	2.549E-18
Th-234	7.361E-05	3.178E-09	2.723E-06
Pa-231	8.035E-12	1.701E-10	2.973E-13
Pa-233	5.242E-06	2.526E-10	1.939E-07
Pa-234	1.080E-07	5.467E-14	3.995E-09
Pa-234m	7.360E-05	1.072E-13	2.723E-06
U-233	4.985E-13	5.175E-11	1.844E-14
U-234	3.010E-04	4.842E-02	1.114E-05
U-235	1.030E-05	4.766E+00	3.811E-07
U-235m	8.395E-02	2.728E-09	3.106E-03
U-236	3.400E-05	5.321E-01	1.258E-06
U-237	5.077E-05	6.221E-10	1.878E-06
U-238	2.100E-04	6.248E+02	7.770E-06
Np-237	1.640E-05	2.327E-02	6.069E-07
Pu-238	2.349E-02	1.372E-03	8.692E-04
Pu-239	8.400E-02	1.354E+00	3.108E-03
Pu-240	4.590E-02	2.023E-01	1.698E-03
Pu-241	2.625E+00	2.536E-02	9.712E-02
Pu-242	2.070E-05	5.235E-03	7.659E-07
Am-241	1.132E-01	3.303E-02	4.187E-03
Total Activity:	1.082E+01		4.004E-01
w/o Daughters:	6.959E+00		2.575E-01

Decay Heat:

Heat Generated at Time Zero:	0.03226	W
Heat Generated When Sealed:	0.03227	W
Heat Generated When Opened:	0.03227	W

===== Regulatory Requirements Warning =====

Radcalc utilizes numerically based criteria to classify packages against the regulations. Many regulations also include subjective criteria that Radcalc does not consider. The user must check to ensure that all requirements in the regulations are met.

===== DOT Classification Results =====

* DOT classification calculations are made at the end of the user-specified decay time.

Radioactive Determination:

Radioactive:	Yes		(ACEMs and ALECs > 1.0)
ACEM Limit Fraction:	1749000	ACEMs	(Number of ACEMs)
ALEC Limit Fraction:	18400000	ALECs	(Number of ALECs)

* This package is not exempt from 49 CFR Subchapter C.

Effective A2s for Mixture: 2.139E+10 Bq

Type Determination:

Type:	B		(A2s > 1.0)
A2 Limit Fraction:	12.04	A2s	(Number of A2s)

Limited Quantity Determination:

Limited Quantity:	No		(Solid, activity > 0.001 A2)
Activity:	12.04	A2	
	10.82	Ci	
	0.4004	TBq	

Fissile:	Yes
Fissile Excepted:	Yes (b)

LSA Determination:

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LSA-I:	No		(Fissile excepted, ACEMs > 30 x rad limits)
LSA-II:	No		(A2s/gm > 0.0001)
LSA-III:	Yes		(A2s/gm <= 0.002)
Specific Activity:	0.001192	A2/gm	
	0.001071	Ci/gm	
HRCQ Determination:			
HRCQ:	No		(A2s <= 3000, Activity <= 1000 TBq)
A2 Limit Fraction:	12.04	A2s	
Activity:	10.82	Ci	
	0.4004	TBq	
Fissile Determination:			
Fissile:	Yes		(Contains fissile isotopes per 49 CFR 173.403)
Fissile Excepted Determination:			
Fissile Excepted:	Yes (b)		(Fissile isotopes <= 15 grams, container + contents)
solid non-fissile > = 1.229E+03 grams)			
Fissile Mass:	6.146	gm	
Container beryllium, lead, graphite, and hydrogenous material enriched with deuterium:	0	gm	
Container Mass:	5806000	gm	
Waste lead:	0	gm	
Waste beryllium, graphite, and hydrogenous material enriched with deuterium:	0	gm	
Waste Mass:	10100	gm	
Solid Non-Fissile Mass:	5816000	gm	
Total Uranium Mass:	630.1	gm	
U-233 Mass:	5.175E-11	gm	
U-235 Mass:	4.766	gm	
Uranium Enrichment:	0.7564	%	
Total Plutonium Mass:	1.589	gm	
Pu-239 Mass:	1.354	gm	
Pu-241 Mass:	0.02536	gm	
Reportable Quantity Determination:			
Reportable Quantity:	Yes		(RQs > = 1.0)
RQ Limit Fraction:	57.09	RQs	(Number of RQs)
Shipping Papers and Labels:			
Isotope	Number of A2s	Fraction of A2s	Cumulative A2s
+ Am-241	4.187	0.3479	4.187
+ Pu-239	3.108	0.2582	7.295
+ Pu-240	1.698	0.1411	8.993
+ Pu-241	1.619	0.1345	10.61
+ Pu-238	0.8692	0.07221	11.48
Sr-90	0.3031	0.02518	11.78
U-235m	0.1553	0.0129	11.94
Cs-137	0.0918	0.007626	12.03
+ Contains 95% of the total A2s and must be included per 49 CFR 173.433.			
* Radionuclides comprising less than 0.1% of the total A2s are not shown in the list.			
===== DOE Classification Results =====			
* DOE classification calculations are made at the end of the user-specified decay time.			
DOE-STD-1027 Category Determination:			
Category:	< Cat 3		(Cat3s <= 1.0)
Cat 2 Limit Fraction:	0.005803		
Cat 3 Limit Fraction:	0.7678		
* The DOE-STD-1027 category determination is based on dose-related limits.			
The user must apply any criticality-related limits separately.			
Dose-Equivalent Curies:			
ICRP-72 DE-Ci:	0.2959		

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FGR-11 DE-Ci: 0.3267

TRU Waste Determination:

TRU Waste: Yes (TRU activity > 100 nCi/gm)
TRU Activity: 26400 nCi/g

WIPP Quantities:

FGE Value: 4.482
PE-Ci Value: 0.3182

===== NRC Classification Results =====

* NRC classification calculations are made at the end of the user-specified decay time.

NRC Container Category:

Container Category: III
LSA-I: No
LSA-II: No
LSA-III: Yes
Total Activity: 10.82 Ci
A2 Limit Fraction: 12.04 A2s

===== Hydrogen/Helium Gas Results =====

* Hydrogen gas calculations are made at the end of the user-specified seal time.

Hydrogen Gas:

H2 Concentration: 0 %
H2 Moles : 0 moles
H2 Volume : 0 cm³ (0 C, 101.325 kPa)
H2 Rate When Sealed: 0.1002 cm³/hr (0 C, 101.325 kPa)
H2 Rate When Opened: 0.1002 cm³/hr (0 C, 101.325 kPa)

Helium Gas:

He Concentration: 0 %
He Moles : 0 moles
He Volume : 0 cm³ (0 C, 101.325 kPa)
He Rate When Sealed: 1.325E-06 cm³/hr (0 C, 101.325 kPa)
He Rate When Opened: 1.325E-06 cm³/hr (0 C, 101.325 kPa)

Pressure When Opened:

Partial Pressure (H2): 0 kPa
Partial Pressure (He): 0 kPa
Partial Pressure (O2): 0 kPa (if H2O present in waste)
Total Pressure (H2 + He + Air): 101.3 kPa
Total Pressure (H2 + He + O2 + Air): 101.3 kPa (if H2O present in waste)

7.8 PNNL Supplied Data on Plutonium Dioxide Enthalpies and Free Energies of Reaction

Formula	Compound	kJ/mole		data source
		$\Delta H_{f,298}^0$	$\Delta G_{f,298}^0$	
UO ₂	uraninite	-1084.9	-1031.7	Wagman
PuO ₂	plutonium dioxide	-1055.8	-998.113	Guillaumont
H ₂ O	water	-285.830	-237.129	Wagman

Ref.	Thermo data from:
Wagman	D. D. Wagman, W. H. Evans, V. B. Parker, R. H. Schumm, I. Halow, S. M. Bailey, K. L. Churney, and R. L. Nuttall. 1982. "The NBS Tables of Chemical Thermodynamic Properties - Selected Values for Inorganic and C1 and C2 Organic Substances in SI Units." <i>Journal of Physical and Chemical Reference Data</i> 11 (Supplement 2). Available at: http://www.nist.gov/srd/PDFfiles/jpcrdS2Vol11.pdf
Guillaumont	Guillaumont, Robert, Thomas Fanghänel, Volker Neck, Jean Fuger, Donald A. Palmer, Ingmar Grenthe, Malcolm H. Rand. 2003. <u>Update on the Chemical Thermodynamics of Uranium, Neptunium, Plutonium, Americium, and Technetium</u> . Elsevier, Amsterdam.

Reactions	kJ/reaction as-written		kJ/mole U or Pu	
	ΔH_{rxn}	ΔG_{rxn}	ΔH_{rxn}	ΔG_{rxn}
U + 2 H ₂ O → UO ₂ + 2 H ₂	-513.24	-557.44	-513.24	-557.44
Pu + 2 H ₂ O → PuO ₂ + 2 H ₂	-484.14	-523.86	-484.14	-523.86