Hydrogen Concentration in the Inner-Most Container within a Pencil Tank Overpack Packaged in a Standard Waste Box Package

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

CH2MHILL
Plateau Remediation Company

**P.O. Box 1600
Richland, Washington 99352**

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**HYDROGEN CONCENTRATION IN THE
INNER-MOST CONTAINER WITHIN A
PENCIL TANK OVERPACK
PACKAGED IN A STANDARD WASTE BOX
PACKAGE**

January 2012

Prepared by: R. M. Marusich

for

CH2M HILL Plateau Remediation Company
Richland, Washington

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GLOSSARY OF ACRONYMS

Am	americium
DNFSB	Defense Nuclear Facility Board
MMC	Miscellaneous Material Container
NucFil	Nuclear Filter Technology
PFP	Plutonium Finishing Plant
PTO	Pencil Tank Overpacks
Pu	plutonium
PVC	polyvinyl chloride
SWB	Standard Waste Box
TRU	Transuranic
TRUCON	TRU Waste Content
WIPP	Waste Isolation Pilot Plant

1.0 INTRODUCTION AND SUMMARY

1.1 PURPOSE

The purpose of this report is to:

- Answer the initial question by the Defense Nuclear Facility Board (DNFSB) staff requesting an argument for and a technical basis, which supports the position that the twist and tape closure method (a.k.a., “horse-tail”) used on the plastic liners containing Transuranic (TRU) waste, provides a vent path which prevents the accumulation of flammable gas (e.g., hydrogen from radiolytic decomposition);
- Answer the question that arose during the discussions with the DNFSB staff regarding hydrogen concentration in the Plutonium Finishing Plant (PFP)-specific waste package by developing a model to determine the hydrogen diffusion through multiple layers of confinement;
- Use the model to show that the:
 - hydrogen concentration in a waste package for which there are TRU Waste Content (TRUCON) Codes is less than five percent (thus showing that the model reasonably matched the Waste Isolation Pilot Plant [WIPP] calculations), and
 - hydrogen concentration within the Pencil Tank Overpacks (PTO) in a Standard Waste Box (SWB) is below five percent.

1.2 LAYOUT OF THE SECTIONS

A set of steady state diffusion flow equations, for the hydrogen diffusion from one bag to the next bag (or one plastic waste container to another), within a set of nested waste bags (or nested waste containers), are developed and presented. The input data is then presented and justified. Inputting the data for each volume and solving these equations yields the steady state hydrogen concentration in each volume. The input data (permeability of the bag surface and closure, dimensions and hydrogen generation rate) and equations are analyzed to obtain the hydrogen concentrations in the innermost container for a set of containers which are analyzed for the TRUCON code for the general waste containers (RH125) and the TRUCON code for the PTO in an SWB (RH111S/112S).

Chapter 2 provides the diffusion flow equations used in the analysis of the hydrogen transport and the method of solution. The equations and the method solutions were coded into a spreadsheet. (See Appendix A, *Details of the Steps Involved to Calculate the Hydrogen Concentration in the Sonotube using Steady State Diffusion Equations for the Pencil Tank Overpack* and Appendix H, *Equations Shown in the Spreadsheet*).

Chapters 3, 4, and 5 provide the input needed to solve the diffusion equation; the hydrogen generation rate, the permeability of hydrogen through the bag surface and the diffusivity of hydrogen through the twist and tape closures (“horse-tails”).

Chapter 6 provides the results from the spreadsheet analysis. The method is first tested by showing that the hydrogen concentration in the innermost bag within a set of bags, used to package general waste allowed by WIPP for a particular TRUCON code for general debris shipments, is less than 5% of the allowable inventory. The method is then used to show the hydrogen concentration in the PTO/SWB package.

1.3 RESULTS

In the results presented below, it is assumed that the plutonium isotopes are encased in material that results in the greatest hydrogen generation; solidified aqueous or homogeneous inorganic solids or high wattage solid organic materials with absorbed liquids (See Section 3.2).

Section 6.3 describes the design of the PTO/SWB waste package as analyzed by WIPP for the development of the TRUCON code. The WIPP model is based on the information of the PTO/SWB waste package received from PFP. Section 6.3 shows the hydrogen concentration in the sonotube (the inner-most portion of the waste package) in the WIPP analysis is 3.7%, based on an inventory of 325 g of plutonium spread equally between six PTOs.

Section 6.2 shows that there are minor variations between the design WIPP used as compared to that in the present PFP design. The major difference is that WIPP assumed a larger bag existed around the sonotube than is presently in the design. It also assumed a filter in the PTO as having a smaller diffusivity than is presently in the design. Assuming the presence of the PFP designed smaller bag (using the actual sized bag), but using the present PFP designed PTO filter (which has a larger diffusivity), results in a hydrogen concentration of 4.2%.

To assess the sensitivity, the hydrogen concentration in the sonotube was analyzed, for the PFP design of the PTO in a SWB waste package assuming a conservative sized bag around the sonotube, for differing numbers of the PTOs. The inventory in each PTO was chosen so that the hydrogen concentration in the sonotube was 4.7% (i.e., less than 5% with some margin). The results are:

Table 1-1. Results for a number of PTOs (using the actual bag size)

Number of PTOs (number in Cell D15 of the spreadsheet)	1	3	6
Grams of Pu in each PTO (number in Cell D25 of the spreadsheet)	78	70	60
Total grams in the SWB (grams of the Pu mixture shown in Table 3-2)	78	210	360
H ₂ concentration in the Sonotube	4.7%	4.7%	4.7%%

In addition to the inventory considerations, the response to Question 4 in G states that there is also a decay heat consideration. The response states the following:

“As stated in the CH-TRUCON document, CH-TRUCON Code RH 111/211S assumes up to six (6) pencil tank overpacks per standard waste box. The CH-TRUCON code does have gram loading limits in the form of a decay heat limit. A decay heat limit (of 0.3915 watt) is associated with the payload shipping category (10 0160 0077) for RH 111/211S. Compliance with this decay heat limit per SWB is required in addition to the 325 g fissile gram equivalent limit per SWB.”

The decay heat value of 0.3915 W corresponds to 61 g of the >10%Pu-240 plutonium distribution described in Section 3.1. The results of Table 1-1 are not considered to be SWB limits. The further clarification was provided in Appendix G that provides a means to accept waste packages that have inventories that exceed the wattage limits. The clarification reads:

“The decay heat limit can be exceeded if SWB headspace hydrogen gas measurement shows that the flammable gas generation rate is below the limit (calculation done in the WDS software). Headspace measurement is a valid, viable, and approved compliance methodology and has been used to qualify several thousand containers (including containers from Hanford) that have already been shipped to WIPP.”

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2.0 DIFFUSION EQUATIONS

Before the hydrogen concentration located within the PTO in an SWB can be analyzed, a set of equations for the hydrogen diffusion through nested waste containers must be determined. The equations used and the method of the solution of the inter-related equations are developed within this section.

2.1 TIME-VARYING EQUATIONS

Equation 1 and 2 of ICP/CON-04-00563, *High Hydrogen Concentrations Detected In The Underground Vaults For RH-TRU Waste At INEEL Compared With Calculated Values Using The INEEL-Developed Computer Code*, provide the general equations for the hydrogen transport through the nested waste packages. The equations are extended to cover a case in which there is a 6-bag (or 6-container) nested waste package (i.e., Bag 1 is in Bag 2, Bag 2 is in Bag 3, etc.) within a liner in a drum or an SWB. The equations for a nested 6-bag package in a liner within a drum represent the worst-case package for which there is a TRUCON code at Hanford.

The equations are shown below. Subscripts 1-6 denote the nested bags. The bags can be waste bags or other containers (i.e., metal material containers). Subscript "L" denotes the liner and subscript "D" denotes the drum. The terms are defined after the equations are set forth.

The equation for the innermost bag is:

$$\frac{dn_{H2,1}}{dt} = n_{H2,Gen} - L_{R,1 \rightarrow 2} \left(\frac{n_{H2,1}}{n_{T,1}} - \frac{n_{H2,2}}{n_{T,2}} \right)$$

The equations for bags 2 through 5 (i.e., $j = 2$ through 5) are:

$$\frac{dn_{H2,j}}{dt} = \left\{ (L_{R,(j-1) \rightarrow j}) \left(\frac{n_{H2,(j-1)}}{n_{T,(j-1)}} - \frac{n_{H2,j}}{n_{T,j}} \right) \right\} - \left\{ (L_{R,j \rightarrow (j+1)}) \left(\frac{n_{H2,j}}{n_{T,j}} - \frac{n_{H2,(j+1)}}{n_{T,(j+1)}} \right) \right\}$$

The equation for the last bag ($j = 6$ – flow into the Liner) is:

$$\frac{dn_{H2,6}}{dt} = \left\{ (L_{R,(5) \rightarrow 6}) \left(\frac{n_{H2,(5)}}{n_{T,(5)}} - \frac{n_{H2,6}}{n_{T,6}} \right) \right\} - \left\{ (L_{R,6 \rightarrow (L)}) \left(\frac{n_{H2,6}}{n_{T,6}} - \frac{n_{H2,(L)}}{n_{T,(L)}} \right) \right\}$$

The equations for the Liner and the Drum are:

$$\frac{dn_{H2,L}}{dt} = \left\{ (L_{R,(6) \rightarrow L}) \left(\frac{n_{H2,(6)}}{n_{T,(6)}} - \frac{n_{H2,L}}{n_{T,L}} \right) \right\} - \left\{ (L_{R,L \rightarrow (D)}) \left(\frac{n_{H2,L}}{n_{T,L}} - \frac{n_{H2,(D)}}{n_{T,(D)}} \right) \right\}$$

$$\frac{dn_{H2,D}}{dt} = \left\{ (L_{R,(L) \rightarrow D}) \left(\frac{n_{H2,(L)}}{n_{T,(L)}} - \frac{n_{H2,D}}{n_{T,D}} \right) \right\} - \left\{ (L_{R,D \rightarrow \text{atmos}}) \left(\frac{n_{H2,D}}{n_{T,D}} - \frac{n_{H2,\text{atmos}}}{n_{T,\text{atmos}}} \right) \right\}$$

The equation for the hydrogen transport rate from package "I" to package "i+1" is defined as:

$$L_{R,i,(i+1)} = \frac{P \cdot A \cdot C \cdot (76 \text{ cmHg per mole frac.})}{x} \quad (\text{where } i = 1 \text{ to } 6 \text{ or "L" or "D"})$$

Where

- $n_{H2,i}$ = moles of hydrogen in a bag, liner or drum ($i = 1$ to 6 or "L" or "D"),
- $n_{T,i}$ = total moles of gas in a bag, liner or drum ($i = 1$ to 6 or "L" or "D"),
- t = time, seconds,
- $n_{H2,\text{atmos}}$ = hydrogen concentration of the atmosphere = 0.0 ,
- $n_{H2,\text{Gen}}$ = hydrogen generation rate, moles/s,
- $L_{R,i,(i+1)}$ = hydrogen transport rate from package i to $i+1$ (where $i = 1$ to 6 or "L" or "D"), or filter permeability, in units of moles/s-mole frac, if a filter is present rather than diffusion flow through a bag. (See below)
- P = hydrogen gas permeability, $\text{cm}^3(\text{STP})/\text{s-cm-cmHg}$,
(For this paper, the more common and equivalent units are used. The more common units are: $\text{cm}^3\text{-cm/s-cm}^2\text{-cmHg}$).
- A = layer (bag) permeable area, cm^2 ,
- x = bag thickness, cm,
- C = conversion factor for moles/ cm^3 ,
= 4.1×10^{-5} moles/ cm^3 at 298 K and 1 atm per the ideal gas law.

As is shown above, the hydrogen transport rate is a function of the permeability of the material, the material thickness and the area of the material. For a waste package, there are multiple components to the transport rate. Consider a waste bag with a twist and tape closure. There is diffusion through the single layer of the bag surface, through the multiple layers of the bag material used in the twisted portion of the closure, through the multiple layers of the bag material and the tape in the twisted portion of the closure that is taped, etc.

For the purposes of this paper, the waste package is assumed to be comprised of a single layer of material and a closure (e.g., twist and tape). The "area" used in the equation for the transport rate, of the portion of the waste package that is not part of the closure, is the surface area of that portion. The "thickness" is the thickness of the material, which comprises the waste package (e.g., a single layer of the bag material). The "hydrogen gas permeability" is the permeability of the bag material to the hydrogen gas. Tape, which might be placed on the waste package surface outside of the closure, is ignored as the area of the tape plus underlying bag material is assumed to be much smaller than the area of the non-taped area. The transport rate of the closure is assumed to be from the tests (See Section 5).

2.2 STEADY STATE EQUATIONS

In the analyses that follow, the time-varying equations are not used. Instead, since the steady state hydrogen concentration is required, the steady-state equations are used. To obtain the steady state equations, the time-varying equations above are used, but with the term $dn_{H2,i}/dt$, (where $i = 1$ to 6 or "L" or "D") set equal to zero.

Steady-State Equation for innermost bag:

$$n_{H2,Gen} = L_{R,1 \rightarrow 2} \left(\frac{n_{H2,1}}{n_{T,1}} - \frac{n_{H2,2}}{n_{T,2}} \right)$$

Steady-State Equations for bags 2 through 6:

($j = 2$ through 5)

$$\left\{ (L_{R,(j-1) \rightarrow j}) \left(\frac{n_{H2,(j-1)}}{n_{T,(j-1)}} - \frac{n_{H2,j}}{n_{T,j}} \right) \right\} = \left\{ (L_{R,j \rightarrow (j+1)}) \left(\frac{n_{H2,j}}{n_{T,j}} - \frac{n_{H2,(j+1)}}{n_{T,(j+1)}} \right) \right\}$$

($j = 6$ - Flow from bag 6 to the Liner):

$$\left\{ (L_{R,(5) \rightarrow 6}) \left(\frac{n_{H2,5}}{n_{T,(5)}} - \frac{n_{H2,6}}{n_{T,6}} \right) \right\} = \left\{ (L_{R,6 \rightarrow (L)}) \left(\frac{n_{H2,6}}{n_{T,6}} - \frac{n_{H2,(L)}}{n_{T,(L)}} \right) \right\}$$

Steady-State Equations for the Liner and Drum:

$$\left\{ (L_{R,(6) \rightarrow L}) \left(\frac{n_{H2,(6)}}{n_{T,(6)}} - \frac{n_{H2,L}}{n_{T,L}} \right) \right\} = \left\{ (L_{R,L \rightarrow (D)}) \left(\frac{n_{H2,L}}{n_{T,L}} - \frac{n_{H2,(D)}}{n_{T,(D)}} \right) \right\}$$

$$\left\{ (L_{R,(L) \rightarrow D}) \left(\frac{n_{H2,(L)}}{n_{T,(L)}} - \frac{n_{H2,D}}{n_{T,D}} \right) \right\} = \left\{ (L_{R,D \rightarrow \text{atmos}}) \left(\frac{n_{H2,D}}{n_{T,D}} - \frac{n_{H2,\text{atmos}}}{n_{T,\text{atmos}}} \right) \right\}$$

2.3 METHOD OF SOLUTION FOR STEADY-STATE EQUATIONS

The steady-state equations are solved as follows: (See also Appendix A for a step-by-step method of solution for the particular case of hydrogen flow through the components on the Pencil Tank Overpack into the Standard Waste Box.)

Let the term " $i \rightarrow j$ " stand for the term in the braces. For example:

$$2 \rightarrow 3 \equiv \left\{ (L_{R,2 \rightarrow (3)}) \left(\frac{n_{H2,2}}{n_{T,2}} - \frac{n_{H2,(3)}}{n_{T,(3)}} \right) \right\}$$

The steady state equations are recast using this shorthand. The result is:

$$\begin{aligned}
 n_{H2,Gen} &= 1 \rightarrow 2 \\
 1 \rightarrow 2 &= 2 \rightarrow 3 \\
 2 \rightarrow 3 &= 3 \rightarrow 4 \\
 3 \rightarrow 4 &= 4 \rightarrow 5 \\
 4 \rightarrow 5 &= 5 \rightarrow 6 \\
 5 \rightarrow 6 &= 6 \rightarrow 7 \\
 6 \rightarrow 7 &= 7 \rightarrow 8 \\
 7 \rightarrow 8 &= 8 \rightarrow \text{atmos}
 \end{aligned}$$

Solving this set of equations yields:

$$n_{H2,Gen} = 8 \rightarrow \text{atmos}$$

Substituting the term that “8 → atmos” stands for, one obtains:

$$n_{H2,Gen} = L_{R,D \rightarrow \text{atmos}} \left(\frac{n_{H2,D}}{n_{T,D}} - \frac{n_{H2,\text{atmos}}}{n_{T,\text{atmos}}} \right)$$

Where, the subscript “D” stands for the drum.

Since $n_{H2,\text{atmos}} = 0.0$ and $n_{T,\text{atmos}}$ is very large, the last term in the parenthesis is 0.0. Using this fact,

$$n_{H2,Gen} = L_{R,D \rightarrow \text{atmos}} \left(\frac{n_{H2,D}}{n_{T,D}} - 0.0 \right)$$

or

$$\frac{n_{H2,Gen}}{L_{R,D \rightarrow \text{atmos}}} = \left(\frac{n_{H2,D}}{n_{T,D}} \right)$$

The term in parenthesis is the mole fraction of the hydrogen in the drum. It is evaluated by putting in the numerical values for $n_{H2,Gen}$ and $L_{R,D \rightarrow \text{atmos}}$, which, in this case, is the filter diffusivity.

The mole fraction in the next to the last barrier (the Liner), is found using the value of the mole fraction of the drum. The general equation for the drum (where “D” stands for the last package or the drum) is:

$$\left\{ (L_{R,(L) \rightarrow D}) \left(\frac{n_{H2,(L)}}{n_{T,(L)}} - \frac{n_{H2,D}}{n_{T,D}} \right) \right\} = \left\{ (L_{R,D \rightarrow (atmos)}) \left(\frac{n_{H2,D}}{n_{T,D}} - \frac{n_{H2,atmos}}{n_{T,(atmos)}} \right) \right\}$$

Solving for the mole fraction of the liner, yields:

$$\frac{n_{H2,(L)}}{n_{T,(L)}} = \frac{\left\{ (L_{R,D \rightarrow (atmos)}) \left(\frac{n_{H2,D}}{n_{T,D}} - 0 \right) \right\} + (L_{R,(L) \rightarrow D}) \left(\frac{n_{H2,D}}{n_{T,D}} \right)}{L_{R,(L) \rightarrow D}}$$

or,

$$\frac{n_{H2,(L)}}{n_{T,(L)}} = \frac{n_{H2,D}}{n_{T,D}} + \left\{ \left(\frac{L_{R,D \rightarrow (atmos)}}{L_{R,(L) \rightarrow D}} \right) \left(\frac{n_{H2,D}}{n_{T,D}} - \frac{n_{H2,atmos}}{n_{T,(atmos)}} \right) \right\}$$

The hydrogen mole fractions for the other bags are found using the general equation for the remainder of the packages. The general equation is:

The mole fraction within the outer-most of the 6 bags liner is found from the following:

$$\left\{ (L_{R,(K) \rightarrow L}) \left(\frac{n_{H2,(K)}}{n_{T,(K)}} - \frac{n_{H2,L}}{n_{T,L}} \right) \right\} = \left\{ (L_{R,L \rightarrow (D)}) \left(\frac{n_{H2,L}}{n_{T,L}} - \frac{n_{H2,(D)}}{n_{T,(D)}} \right) \right\} \text{ where } K = 6$$

Solving yields,

$$\frac{n_{H2,(K)}}{n_{T,(K)}} = \frac{n_{H2,L}}{n_{T,L}} + \left\{ \left(\frac{L_{R,L \rightarrow (D)}}{L_{R,(K) \rightarrow L}} \right) \left(\frac{n_{H2,L}}{n_{T,L}} - \frac{n_{H2,D}}{n_{T,D}} \right) \right\}$$

The mole fraction in any of the other 5 bags is found using the following equation:

$$\left\{ (L_{R,(K-1) \rightarrow K}) \left(\frac{n_{H2,(K-1)}}{n_{T,(K-1)}} - \frac{n_{H2,K}}{n_{T,K}} \right) \right\} = \left\{ (L_{R,K \rightarrow (K+1)}) \left(\frac{n_{H2,K}}{n_{T,K}} - \frac{n_{H2,(K+1)}}{n_{T,(K+1)}} \right) \right\}$$

Solving yields

$$\frac{n_{H2,(K-1)}}{n_{T,(K-1)}} = \frac{n_{H2,K}}{n_{T,K}} + \left\{ \left(\frac{L_{R,K \rightarrow (K+1)}}{L_{R,(K-1) \rightarrow K}} \right) \left(\frac{n_{H2,K}}{n_{T,K}} - \frac{n_{H2,K+1}}{n_{T,K+1}} \right) \right\}$$

To solve the above equations, the hydrogen generation rate and the hydrogen gas transport rate $L_{R,(K-1) \rightarrow K}$ are needed. These parameters are found in the next three sections.

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3.0 HYDROGEN GENERATION RATE

To solve the diffusion equations, developed in Section 2, the hydrogen generation rate is needed. This parameter is found within this section.

The hydrogen generation rate is found from the energy released during the decay and the ability of the material to release the hydrogen from the molecular structure as a result of the absorption of the released energy. The energy released is a function of the curies contained in the inventory and the energy released applies to each disintegration. The hydrogen release is obtained from an experimentally derived parameter called the "G value" or $G(H_2)$. The units are "molecules of hydrogen per 100 ev absorbed".

The equation for hydrogen generation is:

$$n_{H_2,gen} = \frac{(\# \text{ of Ci}) * (3.7 \times 10^{10} \frac{\text{dis}}{\text{s-Ci}}) * (\text{energy released, } \frac{\text{ev}}{\text{dis}}) * [G(H_2), \frac{\text{molecules } H_2}{100\text{ev}}]}{(6.02E+23 \frac{\text{molecules}}{\text{mole}})} \text{ moles/s}$$

Note in the equation above, the value of $[G(H_2), \frac{\text{molecules } H_2}{100\text{ev}}]$ is found by dividing the value of $G(H_2)$ by 100. For example, Section 3.2 will show that $G(H_2)$ equals 1.6 molecules per 100 ev. Given this, the term $[G(H_2), \frac{\text{molecules } H_2}{100\text{ev}}]$ equals 1.6/100 or 0.016.

3.1 NUMBER OF CURIES AND ENERGY RELEASED

The term "# of Ci", in the equation for hydrogen generation rate, is the number of curies of alpha emitting isotopes in the package. While gamma and betas also produce hydrogen, for the packages containing transuranic isotopes (e.g., plutonium and americium), only the contribution from the alphas need to be included. This is discussed in a paragraph just above Table 3-1 (next page).

The equation for the hydrogen generation requires the number of curies and the average energy released for disintegration. For the packages of interest in this analysis, these parameters are found from the "worst-case" plutonium in the PFP DSA (HNF-15500, *Plutonium Finishing Plant Deactivation and Decommissioning Documented Safety Analysis*). This isotopic distribution is taken from Table 4-2, Section 4.2.3 of Revision 6 to HNF-15500. It is known as the ">10% Pu-240 distribution". This is a mass weighted average of the results of several thousand non-destructive sample analyses from eight and one-half years of PFP inventory records. This isotopic distribution conservatively includes a maximum Am-241 buildup. The isotopic distribution is shown in the second column in Table 3-2, *Calculation of the Average Energy per Disintegration*.

The specific activity (Curies/gram) came from rounding the values found in RADIDOSE (HNF-26181, *User's Guide and Model Description for RADIDOSE Version 3.0*). RADIDOSE is the code used to determine the onsite and offsite consequences for the Documented Safety

Analysis performed for the Hanford facilities. The comparison of the values used vs. those in RADIDOSE is shown below. The comparison also includes a comparison to the values for a specific activity from LA-12846-MS, *Specific Activities and DOE-STD-1027-92 Hazard Category 2 Thresholds – LANL Fact Sheet* which is used by the DOE for Hazard Categorization and from HNF-EP-0063, 2011, *Hanford Site Solid Waste Acceptance Criteria*, the document used at Hanford to determine if the waste is acceptable.

The information presented in Table 3-1, *Search Results for Specific Activity* below shows that, with the exception of the specific activity of Pu-239 in LA-12846, the values from the three references are very close to the value used in this analysis. An Internet search was performed to check the specific activity of Pu-239 used in the analysis (0.062 Ci/g). The specific activity of Pu-239 found from a number of authoritative references (including a 2003 Los Alamos DSA for the waste tanks located at TA-21 given in LA-UR-03-6520, *the General's Tanks Characterization Activities Documented Safety Analysis*) and a later version of the radionuclide decay charts, all show a specific activity of Pu-239 of 0.062 Ci/g. The search results show that the use of a specific activity of Pu-239 of 0.062 Ci/g is a good choice.

Table 3-1. Search Results for Specific Activity

	Specific activity, Ci/g used in this analysis	Specific Activity, Ci/g used in RADIDOSE (HNF-26181)	Specific Activity, Ci/g used in LA-12846-MS, Table 1	Specific Activity, Ci/g used in HNF EP-0063, Table A-1
Pu-238	17.1	17.13	17.13	17.12
Pu-239	0.062	0.06207	0.06133	0.06202
Pu-240	0.23	0.2278	0.2268	0.2269
Pu-241	100	103.0	103.1	103
Pu-242	0.004	0.003929	0.00393	0.003954
Am-241	3.43	3.43	3.428	3.427
HNF-26181, <i>User's Guide and Model Description for RADIDOSE Version 3.0</i> , Fluor Hanford, Inc., Richland, Washington.				
LA-12846-MS, <i>Specific Activities and DOE-STD-1027-92 Hazard Category 2 Thresholds – LANL Fact Sheet</i> , Los Alamos National Laboratory, Los Alamos New Mexico. This reference refers to the Seventh edition (1978) of the <i>Table of Isotopes</i> .				
HNF-EP-0063, <i>Hanford Site Solid Waste Acceptance Criteria</i> , Rev 16, CH2M HILL Plateau Remediation Company, Richland, Washington.				

Table 3-2, *Calculation of the Average Energy per Disintegration*, presents the calculation of the curies in the drum and the average energy. The data on energy per disintegration was taken from the *Radiological Health Handbook*.

In calculations such as these, the contribution from Pu-241 and the gamma from Am-241 are neglected. This is because the energy given off by Pu-241 is a weak beta (energy = 0.021 Mev, max and 0.007 Mev average [using the fact that the average beta energy is about 1/3 of the maximum energy]). The maximum energy given off from the gamma emission from Am-241 is

0.06 Mev 36% of the time (See Note 1 of Table 3-2). The hydrogen generation rate is a function of the curies present and the energy per disintegration. The last column in Table 3-2 shows the contribution of Pu-241 beta and the Am-241 gamma to the generation rate is about 1%. This shows that the contribution of the gammas is negligible. This is confirmed by Section 3.1 of the *CH-TRU Payload Appendices*, which states: "For the CH-TRU wastes, alpha irradiation is the only significant contributor to gas generation."

Table 3-2. Calculation of the Average Energy per Disintegration

	Grams ($>10\%$ ^{240}Pu)	Specific activity, Ci/g	Curies	Mev/dis	Ci*(Mev/dis)
Pu-238	0.00205	17.1	0.0351	5.49 (from 5.50, 72% of the time and 5.46, 28% of the time)	0.193
Pu-239	0.794	0.062	0.0492	5.15 (from 5.16, 88% of the time and 5.11, 12% of the time)	0.253
Pu-240	0.159	0.23	0.0366	5.16 (from 5.17, 76% of the time and 5.12, 24% of the time)	0.189
Pu-241	0.0137	100	1.37	0.007 (beta)	0.01
Pu-242	0.00654	0.004	2.6E-5	4.9	~0
Am-241	0.0241	3.43	0.0827	5.48 (alpha) (from 5.49, 85% of the time and 5.44, 13% of the time)	0.453
				0.06 (gamma) (36% of the time – See Note 1)	0.002
	Total grams 1.0		Total Ci, not including Pu-241 0.2036	Average alpha energy 5.34 Mev/dis	
<p>Average alpha energy = $\frac{\sum Ci_i * Mev_i}{\sum Ci_i}$, not including Pu-241.</p> <p>The average energy per gram is found from:</p> $\frac{0.2036 \text{ Ci}}{g} * \frac{3.7E + 10 \text{ dis}}{s - Ci} * \frac{5.34 \text{ Mev}}{dis} * \frac{1E6 \text{ ev}}{Mev} * \frac{1.6E - 19 \text{ J}}{ev} * \frac{1W}{J/s} = \frac{0.0064 \text{ W}}{g}$					
<p>Note 1: Am-241 decays to Np-237 via alpha emission. Most of the time, the alpha emission leads to a ground state Np-237 atom. About half of the time, alpha emission leads to an excited Np-237 atom which decays to the ground state by gamma emission, 36% of the time the gamma emission is 0.06 Mev. 14% of the time it is via much lower gamma energies. There are greater gamma energies given off, but the frequency is many orders of magnitude smaller than 36%.</p>					

The inventory is assumed to be located such that all of the released energy is absorbed by the hydrogenous material. It is assumed that these radionuclides are absorbed in or encased in the hydrogenous material.

3.2 DETERMINATION OF $G(H_2)$

The effective radiolytic hydrogen G value is a measure of the number of hydrogen molecules generated through radiolysis per 100 ev of ionizing energy deposited into a waste matrix. The value is both waste type and time dependent. Generally, the more hydrogenous material available, the higher the G number and as the absorbed dose increases, the G value may decrease to an approximate steady state condition. Increasing the dose (defined as the product of the decay heat and elapsed time from waste generation to date of compliance evaluation and expressed in units of watt*year) decreases the flammable gas generation rate of the hydrogenous materials (such as plastics and combustibles) due to the depletion of the hydrogen in the target material in the vicinity of the alpha-emitting sources. Both G values and the matrix-depletion criterion of >0.012 watt*year per container are provided in Section 3.2, Table 3.2-1 of the *CH-TRU Payload Appendices*. A summary of this information is provided in Table 3-3, *Summary of G Values for alpha-emitting radionuclides from CH-TRU Payload Appendices*. The values are based on alpha radiation.

Table 3-3. Summary of G Values for alpha-emitting radionuclides from CH-TRU Payload Appendices

Waste Material Type	Effective G Values - Flammable Gas, i.e., $G(H_2)$
I. Solidified aqueous or homogeneous inorganic solids (that contain water)	
I.1 Absorbed, adsorbed, or solidified inorganic liquids (nuclides may be in solution and energy transfer may occur between the liquid and the inorganic binder).	1.6
I.2 Soils, solidified particulates, or sludges formed from precipitates.	1.3
I.3 Concreted inorganic particulate waste having a maximum of 30 weight percent unbound water.	0.4
II. Solid inorganic materials	
II.1 Solid inorganic materials packaged in organic materials.	1.7 (watt*year ≤ 0.012) 0.32 (watt*year > 0.012)
II.2 Solid inorganic materials packaged in metal cans.	0
II.3 Homogeneous solid inorganic materials with unbound absorbed ambient moisture (≤ 6 percent by weight) in metal cans.	0.08
III. Solid organic materials	
III.1 Solid organic materials (including some absorbed liquids and cemented organics).	3.4 (watt*year ≤ 0.012) 1.09 (watt*year > 0.012)
III.2 Homogeneous mixed organic (10 percent by weight) and inorganic (90 percent by weight) materials packaged in metal cans.	0.34 (watt*year ≤ 0.012) 0.11 (watt*year > 0.012)
III.3 Homogeneous mixed organic (10 percent by weight) and inorganic (90 percent by weight) materials packaged in organic materials.	1.85 (watt*year ≤ 0.012) 0.4 (watt*year > 0.012)

Given the high decay heat of the maximum PFP drum (1.6 watts based on 250 g of the “ $>10\%$ Pu-240” mixture), it is apparent that the matrix depletion criteria will be met in a short time (under three days). Section 6 shows a pencil tank overpack may have about 50 g in it. For this package, the heat rate is 0.32 W. The matrix-depletion value of $G(H_2)$ can be used after about two weeks (14 days).

For this analysis, two G values are selected for evaluation from Table 3-3. The first is 0.4 molecules per 100 ev which bounds the highest wattage inorganic (Type II) and solid organic waste materials (Type III.2 and III.3). The second is 1.6 molecules per 100 ev which bounds the solidified aqueous or homogeneous inorganic solids (Type I) and high wattage solid organic materials with absorbed liquids (Type III.1).

The hydrogen generation rate in the package is determined next.

3.3 HYDROGEN GENERATION RATE

Substituting the values for “# of Ci”, average energy per disintegration and $G(H_2)$ for an inventory of 250 g of plutonium having a radionuclide distribution equal to the rate in the PFP DSA (“>10% Pu-240”) yields the hydrogen generation rate. For 250 g of plutonium having the isotopic distribution given in Table 3-3, the number of curies and energy released are:

$$\begin{aligned}\text{\# of Ci} &= 250 \text{ g} * 0.2036 \text{ Ci/g} \\ &= 50.9 \text{ Ci} \\ \text{Energy released} &= 5.34 \text{ Mev/dis} \\ &= 5.34 \times 10^6 \text{ ev/dis}\end{aligned}$$

Substituting these two values and the two values of $G(H_2)$ of interest (1.6 molecules /100 ev and 0.4 molecules/100 ev) into the equation for the hydrogen generation rate presented in Section 3.0,

$$n_{H_2, \text{gen}} = \frac{(\text{\# of Ci}) * \left(3.7 \times 10^{10} \frac{\text{dis}}{\text{s} - \text{Ci}}\right) * \left(\text{Energy released, } \frac{\text{ev}}{\text{dis}}\right) * \left[G(H_2), \frac{\text{molecules } H_2}{100\text{ev}}\right]}{\left(6.02E + 23 \frac{\text{molecules}}{\text{mole}}\right)}$$

yields:

$$\begin{aligned}6.7 \times 10^{-8} \text{ mole/s} &\text{ for a value of } G(H_2) \text{ of 0.4 and an inventory of 250 g of “>10\% Pu-240”} \\ &\text{plutonium mixture,} \\ 2.7 \times 10^{-7} \text{ mole/s} &\text{ for a value of } G(H_2) \text{ of 1.6 and an inventory of 250 g of “>10\% Pu-240”} \\ &\text{plutonium mixture.}\end{aligned}$$

The hydrogen generation rate for the analysis shown in Section 6.0 is calculated in the same way, using the specified inventory in the waste package.

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4.0 PERMEABILITY

To solve the diffusion equations developed in Section 2, the hydrogen gas transport rate $L_{R,(K-1) \rightarrow K}$ is needed. This parameter is broken into two parts; permeability of the surface of the plastic waste package and diffusion through the closure (e.g., "horse-tail"). The permeability of the surface is found in this section.

The hydrogen transport rate ($L_{R,i \rightarrow j}$) includes hydrogen transport through the bag walls (permeation), through a filter or opening in the package (filter on a drum or open bung hole in the liner).

Permeation (hydrogen diffusion through solid layer of plastic) is discussed in this section. Section 5 will discuss diffusion through "twist and tape" closures. Diffusion through open air-filled pathways is discussed in Section 6.

For plastic bags that are the same size as those used in WIPP testing, the values developed by the WIPP tests are used in the analysis.

The permeability values are used for those plastic bags (or plastic waste containers), which are of a different size or material than those analyzed or tested by WIPP. An Internet search was conducted to find the values of permeability of PVC and other plastics. The results of the search are shown in Appendix B, *Literature Search for Values for Permeability of Plastics*. In each section of Appendix B, the paper or Journal article is cited, followed by the value for the permeability.

The permeability value used in the analysis in Section 6, for diffusion through the surface of PVC bags, comes from the WIPP tests. Appendix B shows the permeability derived from the WIPP test results averages the values shown in Appendix B and, therefore, is a reasonable value to use. It is also a reasonable value to use since it is the value, which WIPP used to determine the allowable inventory for the TRUCON code requirements.

Table 6.8-5 of Section 6.8 of Rev. 1 (Rev. 2 is the latest) of *CH-TRU Payload Appendices* provides the permeability of a PVC bag of $4.94 \text{ E-7 moles/s-mole-fraction}$ based on a heat sealed 14-mil thick PVC bag having a surface area of 6.3 ft^2 (per Table 6.8-1 of the reference).

Using the following conversion factors:

At 25°C (298 K), 1 moles occupies $24,450 \text{ cm}^3$,

14 mil = 0.014 in or 0.0356 cm,

$6.3 \text{ ft}^2 = 5,861 \text{ cm}^2$,

1 mole frac = 76 cmHg (see paragraph 1 of Appendix B).

The permeability of the PVC bag is:

$$\frac{4.94E-7 \text{ moles}}{s - \text{mole frac.}} * \frac{24,450 \text{ cm}^3}{\text{mole}} * \frac{0.0356 \text{ cm}}{5861 \text{ cm}^2} * \frac{\text{mole frac.}}{76 \text{ cmHg}} =$$

$$9.6E-10 \frac{\text{cm}^3}{s} \frac{\text{cm}}{\text{cm}^2 - \text{cmHg}}$$

$$\left(\text{Rounded to } 10E-10 \text{ or } 1E-9 \frac{\text{cm}^3}{s} \frac{\text{cm}}{\text{cm}^2 - \text{cmHg}} \right)$$

Where the bag used in the waste package is the same size as this bag (surface area of 6.3 ft²), a value of 4.94 x 10⁻⁷ moles/s-mole fraction is used.

For the cases where the bag is a PVC bag having a different thickness or surface area, the permeability of 1 x 10⁻⁹ cm³-cm/s-cm²-cmHg is used. Appendix B shows the permeability of 1 x 10⁻⁹ cm³-cm/s-cm²-cmHg is a reasonable value.

5.0 PERMEABILITY OF "HORSE-TAILED" OR "TWIST AND WRAP" CLOSURES

To solve the diffusion equations developed in Section 2, the hydrogen gas transport rate $L_{R,(K-1) \rightarrow K}$ is needed. This parameter is broken into two parts; permeability of the surface of the plastic waste package and diffusion through the closure (e.g., "horse-tail"). The diffusivity of the closure is found in this section.

Bags can be closed by twisting and taping the opening (also called a "horse-tail"). Other closure mechanisms are discussed at the end of this section. For these bags, there is hydrogen transport out of the surface of the bag and out of the opening in the core of the twist. Some twist and tape closures involve folding the twisted portion prior to taping.

The diffusivity for the twist and tape closure is found using the data from the test at WIPP. Appendix C, *A Literature Search for Values for Permeability of the Diffusivity of Twist and Tape Closures on Plastic Bags*, provides the WIPP test data as well as data from two other tests performed at other locations. In each of these tests (described in Appendix C), the method for "twist and tape" (or "horse-tailing") is described as follows:

Securely twist a portion of the bag. Wrap tape around the twisted end. Cut the tape at the midpoint of the taped length. Add a layer of tape to seal off the "open" end (i.e., the end that was just cut).

This is the same method used at PFP, based on Procedure ZSP-003, Page 8 of 15, *Seal Out from Glovebox or Glovebag or Remove Items from Hoods* and as taught in Section 3.3.6 of Chapter 3 entitled "Glovebox Work" of the PFP Student Handbook for Nuclear Chemical Operators for Course 200135.

Section 6.8.7.2.2 of Rev. 1 (Rev 2. is the latest) of *CH-TRU Payload Appendices* states the diffusivity of the twist-and-taped section (the "horse-tail"), alone, is $5.6 \text{ E-7 moles/s-mole-fraction}$. The reference states that the value was obtained by subtracting the diffusivity of Test 9A from Test 9C. In each case, a 14-mil thick PVC bag having a surface area of 6.3 ft^2 (per Table 6.8-1) was used in the test.

The length of the twist and tape portion is approximated as follows. The initial bag dimension is 10 inch by 72 inches. The surface area of the finished bag is 6.3 ft^2 . Assume the bag is essentially flat (that is the configuration in the tests shown in Section 6.8 of *CH-TRU Payload Appendices*). Given a width of 10 inches, the length of the bag to yield a surface area of 6.3 ft^2 is 45 inches. This means that the initially twisted length is about 27 inches. Assuming the twisted portion is cut in half, the twist and tape length is about 13 inches.

Sketches of the Bag around the sonotube show the actual bag is 103 inches long. The lower portion of the bag is 16 inches in diameter and 52 inches long. The diameter then increases to 20 inches over a length of 21 inches. The bag is 20 inches in diameter over the last 30 inches. The 16 inch diameter by 52 inch portion is what is placed into the sonotube. The upper portion is

used in the twist and tape portion. The Pencil Tank Overpack is 45 inches long. The twisted length is about 51 inches long (from 103 inches minus 52 inches). The length is twisted, taped and cut so it will fit into the PTO. As a result, the twist and tape portion of the bag around the sonotube is about the same size as those used in the WIPP tests. Therefore, the WIPP test value for the twist and tape closure ($5.6 \text{ E-7 moles/s-mole-fraction}$) could be used in the analysis.

Waste packages can be closed by heat sealing the top and installing a filter. In this case, the diffusivity is provided by the manufacturer for that particular filter.

Waste packages can have an open pathway that is not filtered (e.g., a loose fitting plug in the top of a waste package or a gap in a waste box). In this case, the waste package is not closed. Typically, it is assumed the waste package is not closed and the hydrogen concentration is the same as in the larger waste package that is closed. However, the ability for hydrogen to diffuse out may be lessened due to the size of the pathway. As a result, a value for diffusivity is needed for this condition. The diffusivity of that pathway is developed in Section 6.2.1.

6.0 RESULTS USING THE SPREADSHEET

Section 2 provided the set of equations that had to be solved to determine the hydrogen concentration in the waste package of interest. Section 2 also provided the method of solutions of these equations. Sections 3, 4 and 5 provided the method used to determine the input to the equations. The analysis to follow uses the equations developed in Section 2 and either the input, or the method to develop the input from Sections 3, 4 and 5 to determine the hydrogen concentration in the waste packages containing the debris and in the PTO in an SWB.

In the sections to follow, terms having units of $\frac{cm^3-cm}{s-cm^2-cmHg}$ are called permeability. Terms having units of $\frac{moles}{s-mole\ fraction}$ are called diffusivity. This is in keeping with the term "diffusivity" used by Nuclear Filter Technology for their filters (See Appendix A of HNF-16166).

6.1 THE 6-BAG SPREADSHEET USED FOR THE TRUCON CODES

A spreadsheet was developed to solve the six bag equations, the liner equation, and the drum equation. The results from this spreadsheet were used to compare the hydrogen concentration in the inner bag for the TRUCON codes, RH 125/225. The results are provided in Appendix E, *Sensitivity Analysis Performed with 6-Bag Spreadsheet Modeling the TRUCON Code Configurations*. The spreadsheet used is similar to the one shown in Appendix H. The only difference is the spreadsheet contains 8 volumes (or "bags") where as the one in Appendix E contains 5.

The six bags were all assumed to have a thickness of 14 mils. The permeability was chosen so the diffusivity matched the data in Appendix D, *E-Mail From Murthy Devarakonda, WIPP, Giving the Diffusivities Used by WIPP*.

The results in Appendix E show that for each conditions of the TRUCON code studied, the spreadsheet described in Section 2 and Appendix A shows the hydrogen concentration is below 5%. As a result, the spreadsheet described in Section 2, Appendix A and Appendix H, is a reasonable method to use to determine the hydrogen in the innermost portion of the waste package as the results generally match those obtained by WIPP in the development of the allowable inventory for the TRUCON code.

6.2 HYDROGEN DIFFUSION S IN THE PTO/SWB WASTE PACKAGE – PFP DESIGN

The equations described in Section 2 were coded into a spreadsheet using the method of Appendix A. The spreadsheet is shown in Appendix H. The spreadsheet was developed to include a liner for those cases in which, a liner might be used in the future. In the analysis presented in this paper, no liner is used. As a result, the diffusivity of the "Liner" is set equal to 1.0, representing no liner.

6.2.1 Dimensions, Diffusivities and Initial Conditions of the PTO/SWB Waste Package

Pencil tank assemblies will be removed from their wall-mounted location within the PRF Canyon, moved to the maintenance cell and mounted on the wall. The plutonium mass will then be determined. Liquids and packing material (e.g., raschig rings), if present within the pencil tank assemblies, will be removed. The pencil tanks are then size reduced (i.e., cut into smaller lengths). Sections of the pencil tanks are placed inside of an open top Miscellaneous Material Container (MMC). MMCs may also be used to contain the packing material.

The MMC, with the pencil tank sections, are moved from the maintenance cell to the PRF Mezzanine.

The MMC are sealed out of the canyon into a Pencil Tank Overpack (PTO) Assembly. The PTO will have a contamination control liner (PVC bag) inside. The PVC bag will contain a rigid liner (the sonotube). Prior to placement in the PTO, a wood plug is placed within the bottom of the sonotube and nailed in place.

The MMC is placed into the sonotube. A 2-inch thick spacer cushion is placed on top of the MMC within the sonotube. The spacer cushion does not seal the sonotube. There is a gap between the spacer cushion and the sonotube. After the spacer cushion has been placed, the PVC bag is closed around the sonotube with MMC and spacer cushion, using a twist and tape (also called "horse-tail") closure. The remaining end cap is then taped on. (See Figure 6-1, *PTO Loading Diagram*.)

The loaded PTO is then packed into a Standard Waste Box (SWB). Up to two layers of three PTO assemblies per layer can be placed in an SWB. The layer of three PTO assemblies consist of two short PTOs and one long PTO. The total Pu inventory allowed within the SWB is 325 g.

The components of the PTO are as follows:

- The MMC is made of steel. It is 13 inches in diameter and 39 inches long. MMC has an open top and a screen as the base.
- The sonotube is a 14-inch diameter cardboard-like container. The walls are about 1/4-inch thick. The base of the sonotube is a wood plug. The plug is about 3/4-inch thick. The sonotube is nailed to the plug.
- The 2-inch thick spacer cushion is made of AP/Armaflex pipe insulation.
- The contamination control liner is a 12-mil PVC bag. The bag diameter and height are discussed below.
- The Pencil Tank Overpack (PTO) is a 15-inch diameter, Schedule 40 PVC pipe. End caps are glued on the bottom and taped at the top. The short PTO is 15 inches in diameter and 45 inches long. The long PTO is 63 inches long. The PTO has a NucFil-013 filter in the top end-cap. The PTO occupies either 130 L or 182 L. Six PTOs occupy 884 L (four short PTOs and two long PTOs).

Figure 6-1. PTO Loading Diagram

The Standard Waste box (SWB) dimensions are provided in the Engineering Drawing of the SWB. The SWB is 36.19 inches tall (to the top of the body). The SWB is 52.25 inches wide (to the outside of the body panel) and has curved ends 45-69 inches long. The SWB is assumed to be a rectangular solid that is 52.25 inches wide, 60 inches long and 36.19 inches tall. The volume is 1,859 L. The SWB contains two NucFil-019DS filters.

It is assumed 325 g of the plutonium mix shown in Section 3.1 is stored in the SWB. It is assumed the inventory is split equally between 6 PTOs.

It is assumed the hydrogen generation rate is determined using the largest value for $G(H_2)$ shown in Section 3.3, a value of $G(H_2)$ of 1.6, to be conservative.

The allowable hydrogen concentration is 5%, per WIPP (See Appendix G, *Clarification of Data Used by WIPP in the Development of the TRUCON Code for PTO in SWB*).

Hydrogen Transport through the MMC into the sonotube

The MMC is metal and has an open top and screening on the bottom. As a result, the hydrogen concentration within the MMC is the same as the concentration within the sonotube.

Hydrogen diffusion through the sonotube into the bag around the sonotube

Hydrogen diffusion through the sonotube walls is likely small and is ignored. As a result, the path for the hydrogen transport out of the sonotube is by diffusion through the spacer cushion, itself, through the gap between the cushion and the sonotube walls and through the gap between the wood plug at the base of the sonotube and the sonotube wall. Typically, hydrogen diffusion through the gaps, exceeds the diffusion through the cushion, itself.

The sonotube is 14 inches in diameter. The cushion fits loosely in the sonotube. Assume that there is a 1/16th inch gap between the cushion and the wall of the sonotube, all the way around. The cushion is, therefore, 13.875 inches in diameter. The area of the gap is

$$A = \frac{\pi}{4} (14^2 - 13.875^2) * \left(\frac{2.54 \text{ cm}}{\text{inch}} \right)^2 = 17.6 \text{ cm}^2$$

The height of the cushion is 2 inches or 5.08 cm.

Appendix B of HNF-16166, *Required Staging Times for Hydrogen diffusion in Vented Waste Containers*, provides a method to determine the diffusivity through an opening in a container. The method is based on a heat transfer analogy equating one-dimensional heat flow with diffusion flow. The resistance of the opening is found first. The diffusivity is found from the resistance.

Using the equation on page B-1 of Appendix B of HNF-16166, the resistance of the gap around the plug in the sonotube is found to be:

$$R = \frac{x}{AD} = \frac{5.08 \text{ cm}}{(17.6 \text{ cm}^2) * (0.75 \text{ cm}^2/\text{s})} * \frac{1000 \text{ cm}^3}{L} = 385 \text{ s/L}$$

Where

x = length of flow path, cm,
 = 5.08 cm (2 inches),
 A = cross-sectional area of the flow path, cm²,
 = 17.6 cm² (from the area between a 14 inch diameter circle and a
 13.875 inch diameter circle),
 D = diffusivity of hydrogen in air, cm²/s,
 = 0.75 cm²/s.

The diffusivity of hydrogen through the gap between the spacer cushion and the sonotube is found based on the resistance. The subsection of Appendix B of HNF-16166 entitled "Extension of the Model to the Filters" shows the diffusivity (units of moles/s-mole fraction) is found from the following:

Diffusivity of H₂ thru gap in top cushion

$$= \frac{1}{R * 24.45 \text{ L/mole}} \text{ or } \frac{1}{(385 \text{ s/L}) * (24.45 \text{ L/mole})}$$

$$= 1.06 \times 10^{-4} \frac{\text{moles}}{\text{s} - \text{mole fraction}}$$

The method of Appendix B of HNF-16166 is used in the subsection entitled "Manufacturer's Data and the Resistance Calculation" of Appendix C of HNF-16166 to determine the diffusivity of the Nuclear Filter Technology ("NucFil") Model 007LS filter. The calculated diffusivity was found to be 1.06 times greater than the manufacturer's value, a good result for this complicated filter. As a result, the method, shown above, is a reasonable way to determine the diffusivity of an open path.

The wood plug is about 3/4-inch thick. Assume, to cover uncertainties, that it is 1-inch thick. The wood plug is nailed to the sonotube in 8 places. Assume the gap at the nail is zero. Assume the gap increases to 1/8-inch at a location midway between the nails. To model this, a 1/16-inch gap is assumed to exist over 1/2 of the circumference of the wood plug. The area of the gap is:

$$A = \frac{1}{2} * \frac{\pi}{4} (14^2 - 13.875^2) * \left(\frac{2.54 \text{ cm}}{\text{inch}} \right)^2 = 8.8 \text{ cm}^2$$

Using the equation for resistance in Section 3, the resistance is found to be:

$$R = \frac{x}{AD} = \frac{(1.0 \text{ inch}) * (2.54 \text{ cm/in})}{(8.8) * (0.75)} * 1000 = 385 \text{ s/L}$$

The diffusivity of hydrogen through the gap between the wood plug and the sonotube is:

$$\frac{\text{Diffusivity of H}_2 \text{ thru gap in wood plug}}{(385) * (24.45)} = 1.06 \times 10^{-4} \frac{\text{moles}}{\text{s} - \text{mole fraction}}$$

The diffusivity is proportional to the inverse of the resistance. To obtain the resistance for a parallel path, the effective resistance is found from:

$$\frac{1}{R_{eq}} = \frac{1}{R_{cushion}} + \frac{1}{R_{wood \text{ base}}}$$

Or

$$\text{Diffusivity}_{\text{equivalent}} = \text{Diffusivity}_{\text{cushion}} + \text{Diffusivity}_{\text{wood base}}$$

As a result, the total diffusivity out of the sonotube is 2.1×10^{-4} moles/s-mole fraction (from 1.06×10^{-4} plus 1.06×10^{-4}).

The diffusivity of the spacer cushion is found as follows. The spacer cushion is made of AP/Armaflex Pipe Insulation. Based on the manufacturer's data sheet, AP/Armaflex is an elastomeric foam based on a synthetic rubber. The constituents of AP/Armaflex are not provided.

The permeability of AP/Armaflex to water vapor is provided. The value is 0.08 perm-inch or 1.16×10^{-13} kg/s-m-Pa. Transforming the units to the standard units of permeability yields:

$$1.16 \times 10^{-13} \frac{kg}{s-m-Pa} \left(\frac{1000 g}{kg} \right) \left(\frac{mole}{18 g} \right) \left(\frac{24450 cm^3}{mole} \right) \left(\frac{m}{100 cm} \right) \left(\frac{101320 Pa}{76 cm Hg} \right)$$

$$= 2.1 \times 10^{-6} \frac{cm^3-cm}{s-cm^2-cm Hg}$$

No data is provided for the permeability of hydrogen through AP/Armaflex.

The permeability for hydrogen through AP/Armaflex is inferred from a comparison of the permeability of water vapor and hydrogen in various elastomers (rubbers). The data on the permeability of water vapor through elastomers comes from Table 4 of EPA-600/2-79-038, *Liner Materials Exposed to Municipal Solid Waste Leachate – Third Interim Report*. The hydrogen permeability data comes from Table 3-24 (page 3-29) of the *Parker O-Ring Handbook*. Other data comes from Table 2.2 and 2.3 of Chapter 8100 – *Polymers* of the *Technical Reference on Hydrogen Compatibility of Materials*. The data is shown in Table 6-1, below.

The data in Table 6-1 shows the permeability of water vapor through the rubber is about a factor of 1 to 10 times greater than for hydrogen. Recall, from Appendix B that permeability is a function of diffusivity and solubility. So, while the diffusivity of hydrogen is typically higher than most gases or vapors, the combination of diffusivity and solubility can result in the permeability being lower.

To model hydrogen permeation through the spacer cushion, the permeability of water vapor of $2.1 \times 10^{-6} \frac{cm^3-cm}{s-cm^2-cmHg}$ is divided by 10 to obtain the permeability of hydrogen through the material as this, results in the smallest value.

Table 6-1. Data on Water Vapor and Hydrogen Permeability

Material	Data from the EPA on water vapor permeability		Data on hydrogen permeability from <i>Parker O-Ring Handbook</i>		Data on Hydrogen Permeability from <i>Technical Reference...</i>		Water Vapor H_2 (Column 4 divided by Column 6 or Column 8)
	Thickness of sample, cm	Permeability, $\frac{\text{grams-cm}}{\text{d-m}^2\text{-mmHg}}$	Permeability, $\frac{\text{grams-cm}}{\text{s-cm}^2\text{-cmHg}}$	Permeability, $\frac{\text{cm}^3\text{-cm}}{\text{s-cm}^2\text{-bar}}$	Permeability, $\frac{\text{grams-cm}}{\text{s-cm}^2\text{-cmHg}}$	Permeability, $\frac{\text{mol } H_2}{\text{s-m-MPa}}$	Permeability, $\frac{\text{grams-cm}}{\text{s-cm}^2\text{-cmHg}}$
Butyl Rubber	0.185	1.39E-3	2.18E-08	1.61E-07	2.15E-09		10
	0.085	0.15E-3	2.36E-09				
Neoprene							
	0.159	2.89E-3	4.54E-08	1.80E-06	2.40E-08	9.24E-9	1.9 and 15
	0.051	1.22E-3	1.92E-08				
Ethylene-Propylene							
	0.17	2.52E-3	3.96E-08	2.90E-07	3.87E-09	6.96E-9 (From EPDM)	10 and 17.4
	0.051	1.09E-3	1.71E-08				
Hypalon AP/Armaflex							
	0.079	3.97E-3	6.23E-08			3.68E-9	52
		1.16E - 13 $\frac{\text{kg}}{\text{s-m-Pa}}$ (Note 1)	1.5E-9 (Note 2)				
Note 1: Data from manufacturer							
Note 2: Permeability is $2.1\text{E-}6 \frac{\text{cm}^3\text{-cm}}{\text{s-cm}^2\text{-cmHg}}$, using 18 g/mole, 24,450 cm ³ /mole and 101,320 Pa/76 cmHg.							

The cushion is 2 inches (5.08 cm) thick. The area is 975 cm² (based on a diameter of 13.875 inches). Using this, the diffusivity is:

$$2.1 \times 10^{-7} \frac{cm^3 - cm}{s - cm^2 - cm Hg} * \left(\frac{975 cm^2}{5.08 cm} \right) * 76 cm Hg * \left(\frac{moles}{24450 cm^3} \right) \\ = 1.25 \times 10^{-7} \frac{moles}{s - mole fraction}$$

Diffusion through the gaps is much greater than diffusion through the cushion, itself. The reason is that the cushion is so thick. Note, had the permeability of hydrogen been set equal to water vapor, the diffusivity would have been 10 times greater or 1.25×10^{-6} moles/s-mole fraction, which is still 100 times less than the diffusivity through the gaps.

The diffusivity of hydrogen through the sonotube into the bag around the sonotube is 2.1×10^{-4} moles/s-mole fraction and comes from diffusion through the gaps between the cushion and the sonotube walls at the top of the sonotube and through the gaps between the wood plug and the base of the sonotube. The gaps are 1/16-inch or 62.5 mils.

Because the size of the gap is not controlled or assured, and because it is believed that a gap will exist, a sensitivity analysis is performed assuming the diffusivity of the gap is a factor of 10 less or 2.1×10^{-5} moles/s-mole fraction. This is equivalent to a plug diameter of 13.988 inches in a 14 inch diameter sonotube. The gap is 0.006 inches (6 mils).

Hydrogen transport through the bag around the sonotube

Sketches of the Bag around the sonotube show the actual bag is 103 inches long. The lower portion of the bag is 16 inches in diameter and 52 inches long. Then the diameter increases to 20 inches over a length of 21 inches. The bag is 20 inches in diameter over the last 30 inches. The 16 inch diameter by 52 inch portion is what is placed into the sonotube. The upper portion is used in the twist and tape portion. The Pencil Tank Overpack is 45 inches long. The twisted length is about 51 inches long (from 103 inches minus 52 inches). The length is twisted, taped and cut so it will fit into the PTO.

To be conservative, the PVC bag placed around the sonotube is assumed to be tight fitting around the sonotube. This differs from the looser fitting bag, which is currently in the design. The tight fitting bag is assumed to be 14.5 inches in diameter and 44.5 inches long. The area of the bag, excluding the top and base, is 13,080 cm². The bag thickness is 12 mil or 0.03 cm. The permeability of the bag is assumed to be 1×10^{-9} cm³-cm/s-cm²-cm Hg per Section 4.7, above. The diffusivity, found using the bag surface area and thickness, is

$$\frac{10^{-9} cm^3 - cm}{s - cm^2 - cm Hg} * \frac{13,080 cm^2}{0.03 cm} * \frac{76 cm Hg}{24,450 cm^3 / mole} = 1.35E-6 \text{ moles/s-mole fraction.}$$

As described above, the twist and tape portion of the bag around the sonotube is about the same size as the one used in the WIPP tests (about 13 inches). Therefore, the WIPP test value for the twist and tape closure ($5.6 \text{ E-}7$ moles/s-mole-fraction from Appendix C) could be used in the

analysis. To be conservative, the diffusivity of a shorter twist and tape closure described in Appendix C of 2.7×10^{-7} moles/s-mole fraction could also be used.

The total diffusivity is the sum of these two or 1.62×10^{-6} moles/s-mole fraction. This diffusivity will be modeled in the spreadsheet by an artificially increased permeability (1.215×10^{-9}). This is the minimum diffusivity of the bag around the sonotube.

A more reasonable value is obtained by determining the diffusivity of the bag surface using the actual bag diameter of 16 inches and actual length of 52 inches. Using these values, the area is $16,900 \text{ cm}^2$ rather than $13,080 \text{ cm}^2$. The diffusivity, using a permeability of $1 \times 10^{-9} \text{ cm}^3\text{-cm/s-cm}^2\text{-cm Hg}$ and a bag thickness of 12 mil (0.03 cm), is 1.75×10^{-6} moles/s-mole fraction. Adding the diffusivity of the twist and tape portion of 5.6×10^{-7} moles/s-mole fraction yields 2.3×10^{-6} moles/s-mole fraction.

Hydrogen transport through the PTO

The PTO has a NucFil -013 filter in it. The diffusivity of the filter is 1.1×10^{-5} moles/s-mole fraction per HNF-16166, Appendix A and the Manufacturers datasheet.

Hydrogen transport through the SWB

The SWB contains two NucFil-019DS filters. The diffusivity of the -019DS filter is 1.5×10^{-5} moles/s-mole fraction. The total diffusivity of the two filters is 3×10^{-5} moles/s-mole fraction.

6.2.2 Hydrogen Concentration in the Components of the PTO/SWB Package – PFP Design

Appendix A provides the method of solution of the steady state diffusion equations.

The base case input and results are shown in the tables below. The general model contains a liner. Since, there is no liner in this analysis, the diffusivity of the liner is set equal to 1.0.

Table 6-2a, *Input for the Case with Liner using PFP data (conservative Base Case data)* provides the input for the conservative base case. Table 6-2b, *Results for the case with liner using PFP data* presents the results. Tables 6-2c, *Results for the case with liner using PFP data (Base Case data with smaller diffusivity for gap around cushion in sonotube)*, 6-2d, *Results for the case with liner using PFP data (Base Case data based on actual size of the bag around sonotube) – The Realistic case*, and 6-2e, *Results for the case with liner using PFP data (Base Case data based on actual size of the bag around sonotube and lowered diffusivity for gap around cushion in sonotube)*, present the results for variations on the base case.

Table 6-2a. Input for the Case with Liner using PFP data (conservative Base Case data)

	Sonotube	Bag around sonotube	PTO	SWB Liner	SWB
Permeability, cm ³ -cm/s-cm ² -cmHG		1.22E-09			
Bag thickness, mil		12			
Bag thickness, cm		0.0305			
Bag height, in	44	44.5	45		
Bag height, cm	111.76	113.03	114.30		
Bag diameter, in	14	14.5	15		
Bag diameter, cm	35.56	36.83	38.1		
Bag surface area, cm ²		13078.11			
cmHg/mole frac		76			
cm ³ /mole at 298 K (25 °C)		24450			
Diffusivity, moles/s-mole frac	2.10E-04	1.62 E-06	1.10E-05	1.0	3.00E-05
Number of PTOs	6				
Total SWB Liner volume, L	0				
Total SWB volume, L	1859				
volume of 1 PTO, L	130				
From bag X to Bag Y	1 to 2	2 to 3	3 to 4	4 to 5	5 to 6
Bag free volume, L	110.99	9.42	9.90	0.00	1077.13
moles of air in bag at 298 K (25 °C)	4.542	0.386	0.405	0.000	44.079
Hydrogen generation rate					
G(H ₂)	1.6				
grams Pu in inner pkg.	54				
curies in inner package	10.99				
Alpha energy, Mev	5.34				
H ₂ generation rate, moles/s	5.77E-08				

Table 6-2b. Results for the case with liner using PFP data

0.0115	SWB
0.0115	SWB Liner
0.0168	PTO
0.0524	Bag around sonotube
0.0527	Sonotube
Diffusivity of gap around sonotube plug = 2.1E-4 (represents a 1/16-inch gap)	
Diffusivity of bag around sonotube = 1.62E-6	

Table 6-2c. Results for the case with liner using PFP data (Base Case data with smaller diffusivity for gap around cushion in sonotube)

0.0115	SWB
0.0115	SWB Liner
0.0168	PTO
0.0524	Bag around sonotube
0.0552	Sonotube
Diffusivity of gap around sonotube cushion = 2.1E-5 (represents a 6 mil gap)	
Diffusivity of bag around sonotube = 1.62E-6	

Table 6-2d. Results for the case with liner using PFP data (Base Case data based on actual size of the bag around sonotube) – The Realistic case

0.0115	SWB
0.0115	SWB Liner
0.0168	PTO
0.0419	Bag around sonotube
0.0422	Sonotube
Diffusivity of gap around sonotube cushion = 2.1E-4 (represents a 1/16-inch gap)	
Diffusivity of bag around sonotube = 2.3E-6 (modeled with permeability increased from 1E-9 to 1.725E-9)	

Table 6-2e. Results for the case with liner using PFP data (Base Case data based on actual size of the bag around sonotube and lowered diffusivity for gap around cushion in sonotube)

0.0115	SWB
0.0115	SWB Liner
0.0168	PTO
0.0419	Bag around sonotube
0.0446	Sonotube
Diffusivity of gap around sonotube plug = 2.1E-5 (represents a 6 mil gap)	
Diffusivity of bag around sonotube = 2.3E-6 (modeled with permeability increased from 1E-9 to 1.725E-9)	

Summary of the Diffusion through the PFP designed PTO in an SWB waste package

The results of the sensitivity analysis are shown in Table 6-3, *Results of the Sensitivity Analysis*.

Table 6-3. Results of the Sensitivity Analysis

Case or Sensitivity	Hydrogen concentration in the Sonotube. %
Conservative Base Case (assumed a close-fitting bag around the sonotube and a 1/16-inch gap between the sonotube cushion and the sonotube sides)	5.3
Gap between the sonotube cushion and the sonotube sides is assumed to be 6 mils, rather than 1/16-inch	5.5
Realistic Case Bag size is assumed to be the actual bag size, not a close-fitting bag (16 inch diameter, 52 inches long, not 14.5 inch diameter, 44.5 inches long)	4.2
Actual bag size, but with the smaller gap size	4.5

The results show that:

- The plug in the sonotube has no significant effect on the hydrogen concentration. That is, the hydrogen concentration is the same with or without the plug being present.
- Use of the actual size of the bag around the sonotube results in a hydrogen concentration below 5%, whereas, use of a conservative tight fitting bag results in a hydrogen concentration of just over 5%.

The spreadsheet was run with the conservative base case input (Table 6-2a) for differing numbers of the PTOs. The inventory in each PTO was chosen so that the hydrogen concentration in the sonotube was 4.7% (i.e., less than 5% with some margin). The results are shown in Table 6-4, *Results for a Number of PTOs*, for both the conservative bag size and the realistic bag size.

Table 6-4a. Results for a number of PTOs (using conservative bag size)

Number of PTOs (Number in Cell D15 of the spreadsheet)	1	3	6
Grams of Pu in each PTO (number in Cell D25 of the spreadsheet)	59	54	54
Total grams in the SWB	59	162	325
H ₂ concentration in the Sonotube	4.7%	4.7%	5.3% (4.2% using the actual bag size)

Table 6-4b. Results for a number of PTOs (using the actual bag size)

Number of PTOs (number in Cell D15 of the spreadsheet)	1	3	6
Grams of Pu in each PTO (number in Cell D25 of the spreadsheet)	78	70	60
Total grams in the SWB (grams of the Pu mixture shown in Table 3-2)	78	210	360
H ₂ concentration in the Sonotube	4.7%	4.7%	4.7%%

This shows that if less than 6 PTOs are included in the waste package, the allowed plutonium inventory in a PTO is greater, but the total inventory in the SWB is less. This is also confirmed by the response to Question 4 shown in Appendix G. Question 4 asked about the inventory limits for the TRUCON code associated with PTOs in an SWB. The response states:

“As stated in the CH-TRUCON document, CH-TRUCON Code RH 111/211S assumes up to six (6) pencil tank overpacks per standard waste box. The CH-TRUCON code does have gram loading limits in the form of a decay heat limit. A decay heat limit (of 0.3915 watt) is associated with the payload shipping category (10 0160 0077) for RH 111/211S. Compliance with this decay heat limit per SWB is required in addition to the 325 g fissile gram equivalent limit per SWB.

The decay heat value of 0.3915 W corresponds to 61 g of the >10%Pu-240 plutonium distribution described in Section 3.1. The results of Table 6-4a and 6-4b are not considered to be SWB limits. The further clarification was provided in Appendix G that provides a means to accept waste packages that have inventories that exceed the wattage limits. The clarification reads:

“The decay heat limit can be exceeded if SWB headspace hydrogen gas measurement shows that the flammable gas generation rate is below the limit (calculation done in the WDS software). Headspace measurement is a valid, viable, and approved compliance methodology and has been used to qualify several thousand containers (including containers from Hanford) that have already been shipped to WIPP.”

6.3 PTO IN AN SWB – WIPP DIFFUSIVITIES AND ASSUMED DESIGN

The same case was analyzed with the same spreadsheet. In this case, rather than setting the “Liner” diffusivity to 1.0, the liner diffusivity was not provided as no liner exists in the

TRUCON code. The hydrogen concentration for the “liner” is set equal to that within the SWB to model a case where there is no liner. The diffusivities from the TRUCON code were used.

Rev. 40 of CH-TRUCON (DOE/WIPP-0103194) shows the following for the Pencil Tank Overpack Package (RH 111S/112S):

“Size reduced sections of pencil tank waste are placed inside a cardboard tube. The cardboard tube is packaged inside of a twist-and-tape plastic bag, which is then placed in a PVC pipe with caps at each end. The PVC pipe is vented with a filter with a minimum hydrogen diffusivity value of $3.7\text{E-}06$ moles/s-mole fraction. Up to six “pencil tank overpacks” are packaged in a direct-load SWB. The SWB is vented such that it has a minimum total hydrogen diffusivity value of $3.7\text{E-}06$ moles/s-mole fraction.”

Personnel at WIPP take the contractor data for the design of the waste package, analyze it with a computer code (or spreadsheet) described in *CH-TRU Payload Appendices* (code is conceptually similar to that of ICP/CON-04-00563), and from the results, determine the allowable inventory in the waste package.

Since the maximum inventory of an SWB is 325 g of plutonium and since the revision to the TRUCON code for this waste package did not have a limit on the inventory, it is assumed WIPP performed their analysis using 325 g of plutonium.

WIPP used a value of $G(\text{H}_2)$ of 1.6 to be conservative.

Based on the above, the following diffusivity values are used.

- Sonotube – 1.0. A value of 1.0 is used since there is no mention of a plug in the sonotube in the TRUCON code description. A sensitivity analysis will be run to see if the value of 2.1×10^{-4} , used in Section 6.2, affects the results.
- Bag around sonotube – The TRUCON code information did not specify the diffusivity of the bag. This was provided by Jennifer Biedscheid, Advisory Engineer, Washington TRU Solutions LLC (WIPP Site Contractor). She sent an e-mail (see Appendix G) stating that “based on the information (bag dimensions) provided by Hanford, a “drum liner bag” ($4.67\text{E-}06$ mol/s/mf as specified in CH-TRU Payload Appendix 2.2) was used in the calculation of payload shipping categories”.

The corresponding bag area is now found. Using the diffusivity of the twist and tape portion of 5.6×10^{-7} moles/s-mole fraction from Table 6.8-5 of *CH-TRU Payload Appendices*, the diffusivity of the bag itself is 4.11×10^{-6} moles/s-mole fraction (from 4.67×10^{-6} minus 5.6×10^{-7}). Assuming a 14-mil bag (0.0356 cm) and a permeability of 1×10^{-9} cm³-cm/s-cm²cmHg, the bag area is 47,100 cm² or 51 ft². This is about 3 times the surface area of the short PTO, about 2.5 times the area of the actual bag (16,900 cm² per Section 6.2.1) and about double the diffusivity of the actual bag (2.3×10^{-6} moles/s-mole fraction) and about 3.5 times the area and about 3 times the diffusivity of the tight-fitting bag (See Section 6.2.1).

A sensitivity analysis will be run to see the effect.

- PTO filter – 3.7×10^{-6} per CH-TRUCON, and
- SWB – 3.7×10^{-5} per CH-TRUCON.

The spreadsheet used in the section above was also used for this analysis. The only difference is the mole fraction of the liner is coded to be the same as the SWB to model a case where there is no liner. The inputs are shown in Table 6-5a, *Input for the Case with TRUCON Code inputs for Diffusivity*.

Table 6-5a. Input for the Case with TRUCON Code inputs for Diffusivity

	Sonotube	Bag around sonotube	PTO	SWB Liner	SWB
Permeability, cm ³ -cm/s-cm ² -cmHG					
Bag thickness, mil					
Bag thickness, cm					
Bag height, in	44	44.5	45		
Bag height, cm	111.76	113.03	114.30		
Bag diameter, in	14	14.5	15		
Bag diameter, cm	35.56	36.83	38.1		
Bag surface area, cm ²					
cmHg/mole frac					
cm ³ /mole at 298 K (25 °C)					
Diffusivity, moles/s-mole frac (All are input values, not calculated)	1.0	4.67E-06	3.70E-06		3.70E-05
Number of PTOs	6				
Total SWB Liner volume, L	1833				
Total SWB volume, L	1859				
volume of 1 PTO, L	130				
From bag X to Bag Y	1 to 2	2 to 3	3 to 4	4 to 5	5 to 6
Bag free volume, L	110.99	9.42	9.90	1051.13	26.00
moles of air in bag at 298 K (25 °C)	4.542	0.386	0.405	43.015	1.064
Hydrogen generation rate					
G(H ₂)	1.6				
grams Pu in inner pkg.	54				
curies in inner package	10.99				
Alpha energy, Mev	5.34				
H ₂ generation rate, moles/s	5.77E-08				

Table 6-5b. Results for the Case with TRUCON Code inputs for Diffusivity

0.0094	SWB
0.0094	SWB Liner – value set equal to that of the SWB
0.0250	PTO
0.0373	Bag around sonotube
0.0376	Sonotube

With the WIPP data, the hydrogen concentration is below 5%.

There are four differences between the WIPP data on which the TRUCON code is based:

- The diffusivity of the sonotube differs as in the PFP design, there is a loosely fitting cushion in the top of the sonotube.

- The diffusivity of the bag around the sonotube in the TRUCON Code (4.67×10^{-6}) is about 2 times larger than used for the case where the actual bag size is used at PFP (2.3×10^{-6}).
- The diffusivity, assumed by WIPP for the PTO filter (3.7×10^{-6}) is less than that assumed by PFP (1.075×10^{-5}).
- The diffusivity of the SWB filter (3.7×10^{-5}) is greater than the combined diffusivity of the two filters PFP is using in the SWB (3.0×10^{-5}).

If the diffusivities are changed, one by one, the following is obtained.

The hydrogen concentration in the sonotube is:

- 3.73% for the base case (all WIPP data),
- 3.76% for the case where the calculated diffusivity of the cushion in the sonotube is used, rather than assuming no cushion as WIPP does.
- 5.0% for the case where the diffusivity of the bag around the sonotube is set equal to 2.3×10^{-6} (see above for the basis of the PFP bag diffusivity) based on the size of the bag used in the PFP design, instead of 4.76×10^{-6} used in the WIPP analysis.
- 2.7% for the case where the diffusivity of the PTO filter is used in the PFP design (1.075×10^{-5}), instead of the value of 3.7×10^{-6} used in the WIPP analysis.
- 4% for the case where the diffusivity of the SWB filter is used in the PFP design (3.0×10^{-5}) instead of the value of 3.7×10^{-5} assumed by WIPP.
- 4.0% for the case where
 - the diffusivity of the PTO filter is used in the PFP design (1.075×10^{-5}), instead of the value of 3.7×10^{-6} used in the WIPP analysis, and
 - the diffusivity of the bag around the sonotube is set equal to 2.3×10^{-6} (see above for the basis of the PFP bag diffusivity) based on the size of the bag used in the PFP design, instead of 4.76×10^{-6} used in the WIPP analysis.

From the above, one can conclude:

- The fact that the PFP design has a plug in the sonotube, does not affect the results. The hydrogen concentration throughout the waste package is the same as the case using WIPP data.
- The size of the bag around the sonotube has some effect. However, using the actual bag dimensions, the hydrogen concentration does not exceed 5%.
- The larger hydrogen concentration found by using a more correct size for the bag around the sonotube is offset by the fact a filter having a larger diffusivity is used in the PFP design.

As a result, the minor differences in the determination of the diffusivity of the component parts of the waste package as determined by WIPP and as determined in this paper does not result in hydrogen concentration exceeding 5%.

7.0 REFERENCES

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APPENDIX A

**DETAILS OF THE STEPS INVOLVED TO CALCULATE THE HYDROGEN
CONCENTRATION IN THE SONOTUBE USING STEADY STATE DIFFUSION
EQUATIONS FOR THE PENCIL TANK OVERPACK**

Hydrogen flow path:

- From Sonotube (S) to Bag around the sonotube (BAS),
- From Bag around sonotube to PTO,
- From up to 6 PTOs to SWB Liner,
- From SWB Liner to SWB,
- From SWB to atmosphere.

Subscripts:

S	Sonotube
BAS	Bag around sonotube
PTO	Pencil Tank Overpack (PTO)
SWBL	SWB Liner
SWB	Standard Waste Box (SWB)
H ₂	hydrogen
T	total (hydrogen + air)

Variables:

n_A	number of moles in Enclosure A
$L_{R,A \rightarrow (B)}$	Diffusivity (hydrogen removal) from Enclosure A to Enclosure B
$n_{H_2, Gen}$	hydrogen generation rate
N_{PTO}	Number of PTOs in the SWB Liner

- A. Hydrogen in the sonotube (hydrogen generation in the sonotube minus flow out of sonotube to bag around sonotube):

$$n_{H_2, Gen} = L_{R,S \rightarrow BAS} \left(\frac{n_{H_2,S}}{n_{T,S}} - \frac{n_{H_2,BAS}}{n_{T,BAS}} \right) \quad (1)$$

- B. Hydrogen in the bag around the sonotube (flow from the sonotube into the bag and flow out of the bag into the PTO):

$$\left\{ (L_{R,(S) \rightarrow BAS}) \left(\frac{n_{H_2,(S)}}{n_{T,(S)}} - \frac{n_{H_2,BAS}}{n_{T,BAS}} \right) \right\} = \left\{ (L_{R,BAS \rightarrow (PTO)}) \left(\frac{n_{H_2,BAS}}{n_{T,BAS}} - \frac{n_{H_2,(PTO)}}{n_{T,(PTO)}} \right) \right\} \quad (2)$$

- C. Hydrogen in the PTO (flow from the bag into the PTO and flow out of the PTO into the SWB Liner):

$$\left\{ (L_{R,(BAS) \rightarrow PTO}) \left(\frac{n_{H_2,BAS}}{n_{T,(BAS)}} - \frac{n_{H_2,PTO}}{n_{T,PTO}} \right) \right\} = \left\{ (L_{R,PTO \rightarrow (SWBL)}) \left(\frac{n_{H_2,PTO}}{n_{T,PTO}} - \frac{n_{H_2,(SWBL)}}{n_{T,(SWBL)}} \right) \right\} \quad (3)$$

D. Hydrogen in the SWBL (flow from the PTO into the SWB Liner and flow out of the SWB Liner into the SWB):

$$N_{PTO} \left\{ (L_{R,(PTO) \rightarrow SWBL}) \left(\frac{n_{H2,(PTO)}}{n_{T,(PTO)}} - \frac{n_{H2,SWBL}}{n_{T,SWBL}} \right) \right\} = \left\{ (L_{R,SWBL \rightarrow (SWB)}) \left(\frac{n_{H2,SWBL}}{n_{T,SWBL}} - \frac{n_{H2,(SWB)}}{n_{T,(SWB)}} \right) \right\} \quad (4a)$$

OR,

$$\left\{ (L_{R,(PTO) \rightarrow SWBL}) \left(\frac{n_{H2,(PTO)}}{n_{T,(PTO)}} - \frac{n_{H2,SWBL}}{n_{T,SWBL}} \right) \right\} = \frac{1}{N_{PTO}} (L_{R,SWBL \rightarrow (SWB)}) \left(\frac{n_{H2,SWBL}}{n_{T,SWBL}} - \frac{n_{H2,(SWB)}}{n_{T,(SWB)}} \right) \quad (4b)$$

E. Hydrogen in the SWB (Flow from the SWB Liner into the SWB and flow out of the SWB to the atmosphere):

$$\left\{ (L_{R,(SWBL) \rightarrow SWB}) \left(\frac{n_{H2,(SWBL)}}{n_{T,(SWBL)}} - \frac{n_{H2,SWB}}{n_{T,SWB}} \right) \right\} = \left\{ (L_{R,SWB \rightarrow \text{atmos}}) \left(\frac{n_{H2,SWB}}{n_{T,SWB}} - \frac{n_{H2,\text{atmos}}}{n_{T,\text{atmos}}} \right) \right\} \quad (5)$$

Method of solution:

Step 1

Add Equations 1-3. This yields Equation 6:

$$n_{H2,Gen} = \left\{ (L_{R,PTO \rightarrow (SWBL)}) \left(\frac{n_{H2,PTO}}{n_{T,PTO}} - \frac{n_{H2,(SWBL)}}{n_{T,(SWBL)}} \right) \right\} \quad (6)$$

Step 2

Add Equation 6 to Equation 4b. This yields Equation 7a and Equation 7b:

$$n_{H2,Gen} = \frac{1}{N_{PTO}} (L_{R,SWBL \rightarrow (SWB)}) \left(\frac{n_{H2,SWBL}}{n_{T,SWBL}} - \frac{n_{H2,(SWB)}}{n_{T,(SWB)}} \right) \quad (7a)$$

OR,

$$n_{H2,Gen} * N_{PTO} = (L_{R,SWBL \rightarrow (SWB)}) \left(\frac{n_{H2,SWBL}}{n_{T,SWBL}} - \frac{n_{H2,(SWB)}}{n_{T,(SWB)}} \right) \quad (7b)$$

Step 3

Add Equation 7b and Equation 5. This yields Equation 9, the mole fraction of hydrogen in the SWB (since $\frac{n_{H2,\text{atmos}}}{n_{T,\text{atmos}}} = 0.0$):

$$n_{H2,Gen} * N_{PTO} = \left\{ (L_{R,SWB \rightarrow \text{atmos}}) \left(\frac{n_{H2,SWB}}{n_{T,SWB}} - \frac{n_{H2,\text{atmos}}}{n_{T,\text{atmos}}} \right) \right\} \quad (9)$$

Step 4

Equation 9 is solved for the mole fraction in the SWB.

$$\frac{n_{H2,Gen} * N_{PTO}}{L_{R,SWB \rightarrow \text{atmos}}} = \frac{n_{H2,SWB}}{n_{T,SWB}}$$

Step 5

The value obtained for the mole fraction in the SWB is used in Equation 7b to obtain the mole fraction in the SWB Liner.

$$\frac{n_{H2,Gen} * N_{PTO}}{L_{R,SWBL \rightarrow (SWB)}} + \frac{n_{H2,(SWB)}}{n_{T,(SWB)}} = \left(\frac{n_{H2,SWBL}}{n_{T,SWBL}} \right)$$

Step 6

The value obtained for the mole fraction in the SWBL is used in Equation 6 to obtain the mole fraction in the PTO.

$$\frac{n_{H2,Gen}}{L_{R,PTO \rightarrow (SWBL)}} + \frac{n_{H2,(SWBL)}}{n_{T,(SWBL)}} = \frac{n_{H2,PTO}}{n_{T,PTO}}$$

Step 7

The value obtained for the mole fraction in the PTO is used in Equation 3 to obtain the mole fraction in the bag around the sonotube.

$$\frac{n_{H2,BAS}}{n_{T,(BAS)}} = \frac{n_{H2,PTO}}{n_{T,PTO}} + \left\{ \left(\frac{L_{R,PTO \rightarrow (SWBL)}}{L_{R,(BAS) \rightarrow PTO}} \right) \left(\frac{n_{H2,PTO}}{n_{T,PTO}} - \frac{n_{H2,(SWBL)}}{n_{T,(SWBL)}} \right) \right\}$$

Step 8

The value obtained for the mole fraction in the bag around the sonotube is used in Equation 2 to obtain the mole fraction in the sonotube.

$$\frac{n_{H2,(S)}}{n_{T,(S)}} = \frac{n_{H2,BAS}}{n_{T,BAS}} + \left\{ \left(\frac{L_{R,BAS \rightarrow (PTO)}}{L_{R,(S) \rightarrow BAS}} \right) \left(\frac{n_{H2,BAS}}{n_{T,BAS}} - \frac{n_{H2,(PTO)}}{n_{T,(PTO)}} \right) \right\}$$

APPENDIX B

LITERATURE SEARCH FOR VALUES FOR PERMEABILITY OF PLASTICS

A literature search was performed to determine the permeability of PVC and other plastics for use in determining the hydrogen concentration in waste packages. The results are shown below.

Chapter 8100, entitled "Polymers" of the reference *Technical Reference on Hydrogen Compatibility of Materials* (SAND2006-1163), states the permeability of gases through polymers is assumed to be independent of pressure and is defined as:

$$P = DS$$

Where P = permeability, moles H_2 /m-s-MPa or cm^3 -cm/s- cm^2 -cmHg,
 D = diffusivity, m^2 /s or cm^2 /s, and
 S = solubility, (moles/ m^3)/MPa or ($cm^3 H_2/cm^3$)/cmHg.

In this section, the units are changed from what is in the reference to $\frac{cm^3-cm}{s-cm^2-cmHg}$. The pressure term in the permeability (MPa) is the partial pressure of the gas in the volume. In the cases to be studied, the volumes (containers or bags) are initially filled with air at atmospheric pressure. Air remains within the volumes. Hydrogen generated with a volume or as diffused into a volume increases the pressure above atmospheric. Therefore, the term "MPa" is really the "over pressure" in the volume. Since the volume and temperature are assumed to be constant, the ideal gas law would show the over pressure is proportional to the mole fraction of hydrogen in the volume. For example, assume a volume contains air and is at atmospheric pressure. Assume, enough hydrogen is added to the sealed volume such that the mole fraction of hydrogen in the volume = 0.02. Given this, the pressure in the volume is now 1.0204 atm. (Consider a 1 L volume at 1 atm and 298 K, there is 0.0409 moles of air. Adding 0.000835 moles of hydrogen yields a mole fraction of hydrogen of 0.02.). The pressure differential is 0.0204 atm or 1.55 cmHg. As a result, a mole fraction is related to the pressure differential. To change the pressure term to a mole fraction (in doing units conversion), 1 mole fraction = 76 cmHg

THE PAPER: *HIGH HYDROGEN CONCENTRATIONS DETECTED IN THE UNDERGROUND VAULTS FOR RH-TRU WASTE AT INEEL COMPARED WITH CALCULATED VALUES USING THE INEEL-DEVELOPED COMPUTER CODE*

Page 14 of ICP/CON-04-00563, *High Hydrogen Concentrations Detected In The Underground Vaults For RH-TRU Waste At INEEL Compared With Calculated Values Using The INEEL-Developed Computer Code*, used a value for permeability for a "polyethylene" bag of

$$7.6 \times 10^{-10} \frac{cm^3-cm}{s-cm^2-kPa} \quad \text{or} \quad 10.1 \times 10^{-10} \frac{cm^3-cm}{s-cm^2-cmHg} \quad (\text{using } 101 \text{ kPa} = 76 \text{ cmHg}).$$

THE PAPER: MEASUREMENT OF HYDROGEN DIFFUSION RATES THROUGH BOTH "TWIST AND TAPE" AND HEAT-SEALED POLYURETHANE AND POLYVINYL CHLORIDE BAGS

The paper provides diffusion rates through a layer of polyurethane (PU) and a layer of polyvinyl chloride (PVC). In the test, the PU and PVC layer (separately) are wrapped over the outlet of a 10-inch diameter pipe. The layer is wrapped over the top opening of the pipe. The sides of the layer are taped to the side of the pipe. There is extra material over the top of the pipe (i.e., the layer is not wrapped tightly across the pipe opening). The extra material makes the effective shape of the layer resemble a cylinder with no base. The layer is estimated to have a height of 1 inch. The effective surface area of the layer is comprised of the area of the circular top of the layer (10 inches or 25.4 cm diameter for an area of 507 cm²) and the area of the sides of the cylinder (10 inches in diameter and 1 inch tall for an area of 203 cm²). The total area for diffusion is 710 cm².

Table 2 of the paper *Measurement Of Hydrogen Diffusion Rates Through Both "Twist And Tape" and Heat-Sealed Polyurethane and Polyvinyl Chloride Bags*, shows the following values of hydrogen diffusivity through polyurethane (PU) and polyvinyl chloride (PVC) bags with heat-sealed ends, corrected to 25 °C:

2.32 x 10⁻⁷ Moles/s-mole-fraction for Polyurethane (PU) 6-mil thick PVC bag having an area of 0.71 ft² (710 cm²) for a bag that is 10 inches in diameter and 1 inch tall (estimate) wrapped over a 10-in. diameter pipe.

1.71 x 10⁻⁷ Moles/s-mole-fraction for a 14-mil thick PVC bag having an area of 0.71 ft² (710 cm²) for a bag that is 10 inches in diameter and 1 inch tall (estimate) wrapped over a 10-in diameter pipe.

Using the following conversion factors:

At 25 °C (298 K), 1 moles occupies 24,450 cm³ (using a value for the gas constant as 0.08206 L-atm/mole-K),

14 mil = 0.014 in or 0.0356 cm, and

1 mole frac = 76 cmHg.

The permeability of the PVC bag is:

$$\frac{1.71 \times 10^{-7} \text{ moles}}{\text{s} - \text{mole frac.}} * \frac{24,450 \text{ cm}^3}{\text{mole}} * \frac{0.0356 \text{ cm}}{710 \text{ cm}^2} * \frac{\text{mole frac.}}{76 \text{ cmHg}} =$$

$$28 \times 10^{-10} \frac{\text{cm}^3}{\text{s} \text{ cm}^2 - \text{cmHg}}$$

The permeability of the PU bag is found in the same way, except that the bag thickness is 6 mils, not 14 mils. The permeability of the PU bag is 16 x 10⁻¹⁰ cm³-cm/s-cm²-cmHg.

THE PAPER: *IMPROVED HYDROGEN GAS GETTERS FOR TRU WASTE TRANSURANIC AND MIXED WASTE FOCUS AREA – PHASE 2 FINAL REPORT*

The paper *Improved Hydrogen Gas Getters for TRU Waste Transuranic and Mixed Waste Focus Area –Phase 2 Final Report* (INEL/EXT-02-00564) provides the results of tests performed to determine which polymers are the best to coat a hydrogen getter particle. The first task of Phase 1 was to select potentially useful polymers. Membranes having thicknesses in the range of 50 to 200 microns (2 mils to 8 mils) were tested in a pure (single) gas facility at the INEEL (Figure 3). The primary focus of the pure gas test screening has been to determine if the polymers being considered have a H₂ permeability high enough to allow H₂ to pass through the polymer at the same rate as it is produced, $\sim 5 \times 10^{-10} \text{ cm}^3\text{-cm/sec-cm}^2\text{-cmHg}$. Each polymer was initially tested using six gases that might be seen in a container: He, H₂, N₂, O₂, CH₄, and CO₂. All of the pure gas tests were performed at 30 °C and 30 psi feed gas pressure.

Table 3 of the reference presents the results. The permeability of hydrogen through various polymers, in units of $10^{-10} \text{ cm}^3\text{-cm/s-cm}^2\text{-cmHg}$, is:

- 6.4 for unplasticized PVC,
- 4.6 for PVC having a viscosity of 0.62,
- 5.3 for PVC having a viscosity of 1.02,
- 17.3 for polyethylene bag,
- 2.4 for PMMA (poly-methyl-methacrylate), and
- 25.4 for polystyrene.

THE PAPER: *TECHNICAL REFERENCE ON HYDROGEN COMPATABILITY OF MATERIALS*

Table 2-1 of Chapter 8100 – Polymers of the reference *Technical Reference on Hydrogen Compatibility of Materials* (SAND2006-1163) provides the permeability of hydrogen through various polymers. The units are $10^{-9} \text{ Mole/s-m-MPa}$ or $10^{-9} \text{ Mole-m/s-m}^2\text{-MPa}$. The values are:

- Low density polyethylene (LDPE) – 3.3,
- Unplasticized PVC – 0.58,
- PMMA – 1.24, and
- Polystyrene – 7.58.

For PVC, the permeability, using more standard units is:

$$\frac{0.58 \times 10^{-9} \text{ moles}}{\text{s} - \text{m} - \text{MPa}} * \frac{\text{m}}{100 \text{ cm}} * \frac{24,450 \text{ cm}^3}{\text{mole}} * \frac{0.101 \text{ MPa}}{76 \text{ cmHg}} =$$

$$1.9 \times 10^{-10} \frac{\text{cm}^3}{\text{s} \text{ cm}^2 - \text{cmHg}} \text{ for PVC}$$

Table 2.4 gives the temperature dependence of the values. The temperature dependence follows the following equation:

$$P(T) = P_{T,base} \left[\exp \left(-\frac{E}{RT} \right) \right]$$

Where $P_{T,base}$ = the permeability at the base temperature T_{base}

Tables 2.2 and 2.4 provide the data for the equation.

Material	T_{base} , K	E, kJ/mole
Unplasticized PVC	298	34.5

THE PAPER: *CH-TRU PAYLOAD APPENDICES*

Table 6.8-5 of Section 6.8 of Rev. 1 (Rev. 2 is the latest) of *CH-TRU Payload Appendices*, provides the permeability of a PVC bag of $4.94 \text{ E-}7$ moles/s-mole-frac based on a heat sealed 14-mil thick PVC bag having a surface area of 6.3 ft^2 (per Table 6.8-1).

The reference also provided a value of $5.6 \text{ E-}7$ moles/s-mole-frac for a "horse-tailed" (i.e., twist and taped), 14-mil thick PVC bag having a surface area of 6.3 ft^2 (per Table 6.8-1).

Using the following conversion factors:

At 25°C (298 K), 1 moles occupies $24,450 \text{ cm}^3$,
 14 mil = 0.014 in or 0.0356 cm,
 $6.3 \text{ ft}^2 = 5861 \text{ cm}^2$, and
 1 mole frac = 76 cmHg.

The permeability of the PVC bag is:

$$\frac{4.94 \text{ E-}7 \text{ moles}}{\text{s-mole frac.}} * \frac{24,450 \text{ cm}^3}{\text{mole}} * \frac{0.0356 \text{ cm}}{5861 \text{ cm}^2} * \frac{\text{mole frac.}}{76 \text{ cmHg}} =$$

$$9.6 \text{ E-}10 \frac{\text{cm}^3}{\text{s}} \frac{\text{cm}}{\text{cm}^2 \text{ - cmHg}}$$

THE PAPER: *HYDROGEN VENTING CHARACTERISTICS OF COMMERCIAL CARBON COMPOSIT FILTERS AND APPLICATIONS TO TRU WASTE*

The paper *Hydrogen Venting Characteristics of Commercial Carbon-Composite Filters and Applications to TRU Waste*, shows 2.9×10^{-7} moles/s-mole-fraction for a heat-sealed 14-mil thick PVC bag having an area of $2,800 \text{ cm}^2$

Using the following conversion factors:

At 25 °C (298 K), 1 moles occupies 24,450 cm³,
 14 mil = 0.014 in or 0.0356 cm, and
 1 mole frac = 76 cmHg.

The permeability of the PVC bag is:

$$\frac{2.9 \times 10^{-7} \text{ moles}}{s - \text{mole frac.}} * \frac{24,450 \text{ cm}^3}{\text{mole}} * \frac{0.0356 \text{ cm}}{2800 \text{ cm}^2} * \frac{\text{mole frac.}}{76 \text{ cmHg}} =$$

$$12 \times 10^{-10} \frac{\text{cm}^3}{s} \frac{\text{cm}}{\text{cm}^2 - \text{cmHg}}$$

SUMMARY OF BAG SURFACE PERMEABILITY DATA

Table B-1 provides the summary of the permeability data for the bag surface. For PVC bags, the analysis to following Section 6 will use the value of $10 \times 10^{-10} \text{ cm}^3\text{-cm/s-cm}^2\text{-cmHg}$ or $1 \times 10^{-9} \text{ cm}^3\text{-cm/s-cm}^2\text{-cmHg}$ as this value results in the diffusivity matching the test performed at WIPP (See Section 4.5).

Table B-1. Permeability Data

Section	Material	Permeability, 10 ⁻¹⁰ cm ³ -cm/s-cm ² -cmHg
Polyvinyl chloride (PVC)		
4.2	PVC	28.0
4.3	Unplasticized PVC	6.4
4.3	PVC having a viscosity of 0.62	4.6
4.3	PVC having a viscosity of 1.02	5.3
4.4	Unplasticized PVC	1.9
4.5	PVC bag	9.6
4.6	Heat-sealed PVC bag	12.0
	Average for PVC	10
Polyethylene (PE)		
4.1	Polyethylene bag	10.1
4.3	PE (polyethylene) bag	17.3
4.4	Low density PE	10.8
Poly-methyl-methacrylate (PMMA)		
4.3	PMMA (poly-methyl-methacrylate)	2.4
4.4	PMMA	4.1
Other		
4.2	PU (polyurethane)	16
4.3	PS (polystyrene)	24.8

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APPENDIX C

**A LITERATURE SEARCH FOR VALUES FOR PERMEABILITY OF THE
DIFFUSIVITY OF TWIST AND TAPE CLOSURES ON PLASTIC BAGS**

A literature search was performed to determine the diffusivity for twist and tape closures for plastic bags. The results are shown below. In addition, Section 3.5 proposed a theory as to the pathway for hydrogen escape from the closure that explains the relatively high values of diffusivity coming from a relatively small surface.

THE PAPER: MEASUREMENT OF HYDROGEN DIFFUSION RATES THROUGH BOTH "TWIST AND TAPE" AND HEAT-SEALED POLYURETHANE AND POLYVINYL CHLORIDE BAGS

Table 2 of the paper *Measurement of Hydrogen Diffusion Rates through both "Twist And Tape" and Heat-Sealed Polyurethane And Polyvinyl Chloride Bags*, shows the values of hydrogen diffusivity through PU and PVC bags with twist and taped ends, corrected to 25 °C. The bags were 14 mil PVC or 6 mil PU bags that are sealed at one or two ends by securely twisting a portion of the bag, wrapping tape around the twisted end, cutting the tape at the midpoint of the taped length and adding a layer of tape to seal off the "open" end (i.e., the end that was just cut).

The bag end was cut to fit onto a 10-inch diameter PVC pipe (called the test vessel). A photo of the set-up showed a relatively flat bag surface stretched across the 10-inch pipe with a 4-inch long, twisted and taped, closure laying on the bag surface. Hydrogen diffused through the bag surface and the twist.

The two-run average hydrogen diffusion rate through the twisted and taped bag ends was

$$5.2 \times 10^{-7} \text{ Moles/s-mole-fraction for Polyurethane (PU), and} \\ 4.4 \times 10^{-7} \text{ Moles/s-mole-fraction for PVC.}$$

The fraction of the diffusion rate, hydrogen diffusing through the surface, is found as follows:

The permeability from Section 4.2 is used. Section 4.2 provides the permeability of PVC bags from the same test. It is:

$$28 \times 10^{-10} \frac{\text{cm}^3}{\text{s}} \frac{\text{cm}}{\text{cm}^2 - \text{cmHg}}$$

Assume that the hydrogen diffuses through the surface.

Using the following conversion factors:

At 25 °C (298 K), 1 moles occupies 24,450 cm³,

14 mil = 0.014 in or 0.0356 cm,

1 mole frac = 76 cmHg,

Area = 507 cm² (top) + 203 cm² (the side) = 710 cm² (The bag is assumed to be a cylinder that is 1-inch tall and 10 inches in diameter. The cylinder is presumed to have some height because of the folds shown in Figure 1. The bag is not flat on the surface of the 10-inch diameter pipe. The surface area is the top surface and the sides of the bag).

The diffusivity is:

$$28 \times 10^{-10} \frac{\text{cm}^3}{\text{s}} \frac{\text{cm}}{\text{cm}^2 - \text{cmHg}} * \frac{\text{mole}}{24,450 \text{ cm}^3} * \frac{710 \text{ cm}^2}{0.0356 \text{ cm}} * 76 \text{ cmHg}$$

$$= 1.74 \times 10^{-7} \frac{\text{moles}}{\text{s} - \text{molefrac}}$$

This shows that about 40% of the diffusion goes through the surface and the remainder through the twisted and taped closure. (Note that Section 4.2 shows that the diffusivity of the heat sealed bag is 1.71×10^{-7} . This is essentially the same as that calculated above).

The diffusivity of the twist and taped section is 2.7×10^{-7} moles/s-mole fraction. This is found by obtaining the difference between the diffusivity of the bag with the twist and tape section (4.4×10^{-7}) and the diffusivity of the bag, alone (1.7×10^{-7}).

THE PAPER: *HYDROGEN VENTING CHARACTERISTICS OF COMMERCIAL CARBON-COMPOSITE FILTERS AND APPLICATIONS TO TRU WASTE*

Table 2-3 of the paper *Hydrogen Venting Characteristics of Commercial Carbon-Composite Filters and Applications to TRU Waste* shows a diffusion coefficient of 7.6×10^{-7} moles/s-mole fraction for PVC bags closed with "horse-tails". The values ranged from 6.63×10^{-7} moles/s-mole-fraction to 12×10^{-7} moles/s-mole-fraction. The bag was 14-mil thick. The "horse-tail" involved a 25 cm (10 inch) length of bag that was tightly twisted, taping the twist and then cutting through the center of the twist and taping over the cut end. The bag had an area of $2,800 \text{ cm}^2$.

Section 4.6 showed that the diffusivity through a sealed bag of this size was 2.9×10^{-7} moles/s-mole fraction. The diffusivity of the twist and taped section is the difference between the diffusivity of the bag with the twist and tape section and the diffusivity of the bag, alone, or 4.7×10^{-7} moles/s-mole fraction. Using the diffusivity of the bag and twist, and the taped portion of 7.6×10^{-7} , about 40% of the diffusion goes through the surface area, with the remainder through the twist.

THE PAPER: *CH-TRU PAYLOAD APPENDICES*

Section 6.8.7.2.2 of Rev. 1 (Rev. 2 is the latest) of *CH-TRU Payload Appendices* states that the diffusivity through the bag surface, alone, is 4.97×10^{-7} moles/s-mole-fraction. This is shown in Table 6.8-3 for Test 9B and in Table 6.8-5. Section 6.8.7.2.2, states that the diffusivity of the twist-and-taped section (the "horse-tail"), alone, is $5.6 \text{ E-}7$ moles/s-mole-fraction. This value is obtained by subtracting the diffusivity of Test 9A from Test 9C. In each case, a 14-mil thick PVC bag having a surface area of 6.3 ft^2 (per Table 6.8-1) was used in the test. In this case, about 50% of the hydrogen flow goes through the bag walls. This fraction is much larger than it was in the cases shown in Sections 5.1 and 5.2 because the surface area is much greater ($5,860 \text{ cm}^2$ for this case, $2,800 \text{ cm}^2$ for Section 5.2 and 710 cm^2 for Section 5.1).

The length of the twist and tape portion is approximated as follows. The initial bag dimension is 10 inch by 72 inches. The surface area of the finished bag is 6.3 ft^2 . Assume that the bag is essentially flat (that is the configuration in the tests shown in Section 6.8 of CH-TRU Payload Appendices). Given a width of 10 inches, the length of the bag to yield a surface area of 6.3 ft^2 is 45 inches. This means that the initially twisted length is about 27 inches. Assuming that the twisted portion is cut in half, the twist and tape length is about 13 inches.

SUMMARY OF DIFFUSIVITY OF TWIST AND TAPED (“HORSE-TAILED”) CLOSURES

The diffusivity of twist and taped closures, alone, of PVC bags was measured and found to be:

- 2.2×10^{-7} moles/s-mole-fraction for a relatively flat bag surface stretched across the 10 inch pipe (710 cm^2 area) with a 4-inch long, twisted and taped, closure laying on the bag surface,
- 4.7×10^{-7} moles/s-mole fraction for a 14-mil thick, $2,800 \text{ cm}^2$ bag having a “horse-tail” that involved a 25 cm (10 inch) length of bag that was tightly twisted, taping the twist and then cutting through the center of the twist and taping over the cut end.
- 5.6×10^{-7} moles/s-mole fraction for a “horse-tailed” (i.e., twist and taped), 14-mil thick PVC bag having a surface area of 6.3 ft^2 ($5,860 \text{ cm}^2$). The twist and tape portion is about 13 inches long.

Note that there is a linear relationship between the length of the twist and tape portion and the diffusivity.

HYDROGEN TRANSPORT PATH OUT THE TWIST AND TAPE CLOSURE

Sections A3.1 to A3.3 show that the large fraction (around 40%) of hydrogen is transported out of the twist and tape closure. The surface area of the twist and tape enclosure is much smaller than the surface of the bag. The thickness of the plastic in the twist and tape closure is much greater than that of the bag. As a result, the diffusivity of the twist and tape region should be much smaller. Hydrogen diffusion flow out the sides of the twist and tape portion is much smaller than it is out of the bag, simply because the area of the twist and tape portion is much less than the bag and the thickness of the plastic in the twist and tape portion is thicker than the bag itself. As a result, hydrogen transport out of the sides, due to diffusion, is quite small. The same is true for diffusion out of the taped end. In this case, the area for the flow is very small (the area of the core), while the thickness across which hydrogen diffuses is likely is about the same as the bag. However, the tests show that the diffusivity through the twist and tape portion is about the same magnitude as the diffusivity of the bag surface.

To achieve a high diffusivity, the twist and tape portion must contain a “core” region which has the same concentration of hydrogen as does the remainder of the bag. The core region is not necessarily cylindrical or straight, but is present as a path of some dimension through the twist and tape region. Most of the hydrogen transported out of the twist and tape region, flows out through this core and out to the atmosphere via open pathways under the tape.

To show the size of the core, consider the following. Appendix B of HNF-16166, *Required Staging Times for Hydrogen diffusion in Vented Waste Containers*, provides a method to determine the diffusivity through an opening in a container (like an opening in a drum liner or in the shaft of a filter). The method is based on a heat transfer analogy equating one-dimensional heat flow with diffusion flow. The resistance of the opening is found first. The diffusivity is found from the resistance.

Using the equation on page B-1 of Appendix B of HNF-16166, the resistance of the opening is found to be:

$$R = \frac{x}{AD} * \frac{1000 \text{ cm}^3}{L}$$

The subsection of Appendix B of HNF-16166 entitled "Extension of the Model to the Filters" shows the diffusivity (units of moles/s-mole fraction) is found from the following:

$$\text{Diffusivity} = \frac{1}{R * 24.45 \text{ L/mole}}$$

The method of Appendix B of HNF-16166 is used in the subsection entitled "Manufacturer's Data and the Resistance Calculation" of Appendix C to determine the diffusivity of the Nuclear Filter Technology ("NucFil") Model 007LS filter. The calculated diffusivity was found to be 1.06 times greater than the manufacturer's value, a good result for this complicated filter.

Of the three cases discussed in Sections A3.1 – A3.3, the data from Section A3.1 is discussed here for illustration of the concept. In the case to be studied here (diffusion through a small diameter channel through the twist and tape closure and out under the tape to the environment), assume that the twisted and taped portion is 4 inches (10 cm). The equation for diffusivity will be solved for the area of the channel, knowing the path length and the diffusivity.

From above, the diffusivity of an open pathway is obtained from

$$\text{Diffusivity, } \frac{\text{moles}}{\text{s} - \text{mole fraction}} = \left[\frac{x}{AD} * \frac{24,450 \text{ cm}^3}{\text{mole}} \right]^{-1}$$

Where

x = length of the path, cm,
 = 10 cm (or 4 inches), in this case,
 A = cross-sectional area of the path, cm², and
 D = diffusion constant of hydrogen, cm²/s,
 = 0.75 cm²/s (per HNF-16166, Appendix C).

Section A3.1 shows the diffusivity of the 4-inch long twist and tape is 2.7×10^{-7} moles/s-mole fraction. Given this, the area must be 0.09 cm². This is equal to a circle having a diameter of 0.13 inches or about 1/8 inch. That is, an equivalent of a 1/8 inch core through the twist and tape and the equivalent of a 1/8 inch diameter opening underneath the tape will yield the hydrogen flows seen through the tape. Since the cut end is jagged and the tape is wrapped over the cut

end, a number of small open pathways exist from the core, under the taped portion (that are not tightly bound to the plastic) and out to the atmosphere. This is why the diffusion is so great out of the closure.

Section A3.2 shows a diffusivity of the 13 inch long twist and tape portion is 5.6×10^{-7} moles/s-mole fraction. Using the equation above, the area is found to be 0.6 cm^2 . The equivalent diameter of the opening is 0.34 inches. The equivalent diameter of the open channel is greater for this longer twist and tape portion. This could be because:

- it is more difficult to twist a longer length of bag to the same tightness as is possible for a smaller length,
- the procedures for twisting differ,
- the operator's attention to twist tightness differed, or
- the tape was applied more loosely (or the top of the twist and tape portion was more "lumpy").

The point is that the only way the diffusivity of the twist and tape portion can be the value found in the tests is for hydrogen to diffuse through an open channel in the twist and tape portion and out through the openings under the tape.

Bending the twist and tape portion over will not completely close off the inner open core, but it might restrict flow to some extent, possibly resulting in a lower diffusivity.

The diffusivity out of the twist and tape portion is a function of the length of the twist and tape portion. It is also likely from a function of the tightness of the twist, the method and the extent to which the end is taped.

However, since an opening existed for three different tests of a twist and tape portion involving three different operators, it is assumed that the diffusivity of the twist and tape portion of a waste package is non-zero. In the analysis that follows, the diffusivity of the twist and tape portion is chosen to be from Section 5.3, or, 5.6×10^{-7} moles/s-mole fraction. A sensitivity analysis will be performed using a factor of 10 less than this 5.6×10^{-8} moles/s-mole fraction. This is 20% of the lowest value found in the tests (2.7×10^{-7} moles/s-mole fraction).

REFERENCES

Measurement Of Hydrogen Diffusion Rates Through Both "Twist And Tape" And Heat-Sealed Polyurethane And Polyvinyl Chloride Bags, 2000, Paper given at the Waste Management 2000 conference, held Feb 27 – March 2, 2000 in Tucson, Arizona. Authors TJ Wickland and Don Dustin. Found at: <http://www.wmsym.org/archives/2000/pdf/31/31-41.pdf>

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CH-TRU Payload Appendices, Sept 2004, found at:
<http://pbadupws.nrc.gov/docs/ML0430/ML043000139.pdf>

HNF-16166, 2006, *Required Staging Times for Hydrogen diffusion in Vented Waste Containers*, Revision 7, Fluor Hanford, Inc., Richland, Washington.

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APPENDIX D

**E-MAIL FROM MURTHY DEVARAKONDA, WIPP, GIVING THE DIFFUSIVITIES
USED BY WIPP**

Marusich, Robert M

Subject: FW: Regarding Data needed to determine H2 concentration in inner bags - Hanford
Attachments: ConfinementLayerReleaseRates.docx

From: Devarakonda, Murthy - WTS [mailto:Murthy.Devarakonda@wipp.ws]
Sent: Tuesday, August 02, 2011 2:17 PM
To: Marusich, Robert M; Brown, Mike - DOE
Cc: Colburn, Alan J.; Danna, Marc; Ploetz, David - WTS; Percy, Mark - WTS; Bledscheid, Jennifer - WTS
Subject: RE: Regarding Data needed to determine H2 concentration in inner bags - Hanford

Bob:

Attached is a summary of the release rates for the different confinement layers used in the CH-TRAMPAC calculations.

Attachment to Email

Release Rates for Confinement Layers

From CH-TRU Payload Appendices

Layer	Waste Types II and III (mol/s/mf)
Small twist-and-tape inner bag	5.58E-7
Large twist-and-tape liner bag	4.67E-6
Filtered inner bag	1.074E-5
Filtered liner bag	1.486E-5
Rigid drum liner (0.3"-dia hole)	5.076E-5
Drum filter (1X)	3.70E-6
Drum Filter (5X)	1.85E-5

APPENDIX E

**SENSITIVITY ANALYSES PERFORMED WITH 6-BAG SPREADSHEET MODELING
THE TRUCON CODE CONFIGURATIONS**

The inventories shown in Table E-1 (next page) applies only to the debris waste streams (RH 125/225 TRUCON Code). This table came from Appendix F, *Attachment From E-Mail Regarding Gram Limit Guidance for Debris Waste Streams*. The debris waste streams consist of: surgical gloves, plastic bags and sheets, paper products, cloth, tape, rubber, leaded glass, lead-lined hood gloves, lead blankets, light bulbs, flashlight batteries, piping, conduit, wiring, glass and metal portions of gloveboxes, pumps, motors, standard laboratory equipment and various other debris.

Per the guidance of the TRUCON manual, the following values are assumed:

- Each filtered plastic bag has a diffusivity of $1.075\text{E-}05$ moles per second per mole fraction,
- Each filtered metal can has a diffusivity of $1.9\text{E-}06$ moles per second per mole fraction,
- Each pipe component has a diffusivity of $1.9\text{E-}06$ moles per second per mole fraction,
- Each 55-gallon drum has a rigid liner punctured with a 0.3-inch diameter hole,
- Each 85-gallon drum used to overpack a 55-gallon drum has a diffusivity of $3.7\text{E-}06$ moles per second per mole fraction, and
- Each standard waste box (SWB) used to overpack 55-gallon drums (SWB overpack) has a diffusivity of $7.4\text{E-}06$ moles per second per mole fraction.

Other data shown in Appendix D is also used.

The Pu limit for the package configurations is shown in the table below.

In each case, the bag dimensions are arbitrary. Section 2, of the main body of this report, shows that the hydrogen concentration, for the steady state case, is not a function of bag size just the diffusivity of the bag. For the analysis, the bag diffusivity comes from WIPP.

**Table E-1. Pu limit for Various Package Configurations from TRUCON Code RH 125/225
("Gram Limit Guidance for Debris Waste Streams")**

Package Configuration	Gram Limit Weapons Grade (typically <7% ²⁴⁰ Pu)	Gram Limit Fuel Grade (typically 7% to 19% ²⁴⁰ Pu)	Gram Limit Reactor Grade (typically >19% ²⁴⁰ Pu)
55 Gal Drum 3 Filtered Layers (0.2634 w)	83	36	25
55 Gal Drum 1 Filtered Layer (0.3131 w)	99	40	28
SWB 3 Filtered Layers (0.6383 w)	198	84	58
SWB 1 Filtered Layer (0.9763 w)	325*	127	91
55 Gal Drum 3 Non-Filtered Layers (0.0690 w)	27	9	4.5
55 Gal Drum 3 Non-Filtered Layers (0.0221 w)	6	3.1	2.7
55 Gal Drum 6 Non-Filtered Layers (0.0326 w)	12	4	3
55 Gal Drum 6 Non-Filtered Layers (0.0104 w)	3.1	1.2	0.9

*Fissile Gram Equivalent

A number of these cases will be checked using the model. In each case, the Pu quantity is based on the "fuels grade" value. Since PFP does not, typically, package with non-filtered, heat sealed bags, only the "filtered" cases and the non-filtered cases assuming that twist and tape closure is used.

The data required is shown in Table E-2.

Table E-2. Data used for the TRUCON Code Comparison

Layer	Diffusivity for Waste Types II and III (mol/s/mole-fraction), from Appendix 2	Other references
Small twist-and-tape closure (just the closure, not the bag surface) (Note 1)	5.6E-7	Table 6.8.5 of CH-TRU Payload Appendices
Non-filtered and non-twist-and-taped bag (i.e., the bag surface)	4.94E-7	Table 6.8.5 of CH-TRU Payload Appendices
Small bag with a twist and tape closure	1.054E-6	Obtained by adding the diffusivity for the twist and tape closure to that for the bag surface.
Filtered inner bag	1.074E-5 (shown in WIPP 90-045, Rev 4)	DOE/WIPP 01-3194, Table 2C, Content code ID 1120, (Page 2-23) and other ID-XXX codes
Rigid drum liner (0.3"-dia hole)	5.076E-5	Calculated as 6.0×10^{-5} in Section 5.1
Drum filter (1X)	3.70E-6	DOE/WIPP 01-3194, Table 2A,
Note 1: Bag area is 6.3 ft ² per Table 6.8-1 of Chapter 6.8 of the CH-TRU Payload Appendices.		

Case 1

Case 1 presents the results using the model for the TRUCON Code case of 3 filtered bags. The input data is shown in Table E-3.

Table E-3. Input for the 3-Filtered Bag Case in the TRUCON code comparison

	Bag 1	Bag 2	Bag 3	Bag 4	Bag 5	Bag 6	Liner	Drum
Permeability, cm ³ -cm/s-cm ² -cmHG								
Bag thickness, mil								
Bag thickness, cm								
Bag height, in								
Bag height, cm								
Bag diameter, in								
Bag diameter, cm								
Bag surface area, cm ²								
cmHg/mole frac								
cm ³ /mole at 298 K (25 C)								
Diffusivity, moles/s-mole frac	1.07E-05	1.07E-05	1.07E-05	1.00E+00	1.00E+00	1.00E+00	5.08E-05	3.70E-06
Hydrogen transport	1 to 2	2 to 3	3 to 4	4 to 5	5 to 6	6 to 7	7 to 8	8 to atmos.

Parameter	Value
Power used in the calculation, Watts	0.2624
G(H ₂), molecules/100 ev	1.6
Hydrogen generation rate obtained using the power, moles/s	4.359E-8

Results from the spreadsheet

The generation rate was from 0.2624 watts. This equates to a generation rate of $4.375\text{E-}8$ moles/s using a value of $G(\text{H}_2)$ of 1.6 from Appendix 3.2 of the CH-TRU Payload Appendices (the worst case condition). This same generation rate occurs with 40.6 g of the >10% Pu-240 mixture having a curie-weighted average alpha energy of 5.34 Mev.

Using the steady state model, the following results were obtained:

Bag number (starting with the inner bag as bag 1)	Hydrogen fraction (steady state)
n,8/n,t (Drum)	0.0118
n,7/n,T (Liner)	0.0126
n,6/n,T (bag 6)	0.0126
n,5/n,T (Bag 5)	0.0126
n,4/n,T (Bag 4)	0.0126
n,3/N,T (bag 3)	0.0167
n,2/n,T (Bag 2)	0.0208
n,1/n,T (Inner Bag)	0.0248

The steady state Pu concentration in the inner bag is 2.5%. This is less than 4%.

Case 2

Case 2 presents the results using the model for the TRUCON Code case of 1 filtered bag. The input data is shown in Table E-4.

Table E-4. Input for the 1-Filtered Bag Case in the TRUCON code comparison

	Bag 1	Bag 2	Bag 3	Bag 4	Bag 5	Bag 6	Liner	Drum
Permeability, cm ³ -cm/s-cm ² -cmHg								
Bag thickness, mil								
Bag thickness, cm								
Bag height, in								
Bag height, cm								
Bag diameter, in								
Bag diameter, cm								
Bag surface area, cm ²								
cmHg/mole frac								
cm ³ /mole at 298 K (25 C)								
Diffusivity, moles/s-mole frac	1.07E-05	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	5.08E-05	3.70E-06
Hydrogen transport	1 to 2	2 to 3	3 to 4	4 to 5	5 to 6	6 to 7	7 to 8	8 to atmos.

Parameter	Value
Power used in the calculation, Watts	0.3131
G(H ₂), molecules/100 ev	1.6
Hydrogen generation rate obtained using the power, moles/s	5.201E-8

Results from the spreadsheet

The generation rate was from 0.3131 watts (40 g of fuels grade Pu per the table above). This equates to a generation rate of $5.2\text{E-}8$ moles/s using a value of $G(\text{H}_2)$ of 1.6 from Appendix 3.2 of the *CH-TRU Payload Appendices* (the worst case). This same generation rate occurs with 49 g of the >10% Pu-240 mixture having a curie-weighted average alpha energy of 5.34 Mev.

Using the steady state model, the following results were obtained:

Bag number (starting with the inner bag as bag 1)	Hydrogen fraction (steady state)
n,8/n,t (Drum)	0.0141
n,7/n,T (Liner)	0.0151
n,6/n,T (bag 6)	0.0151
n,5/n,T (Bag 5)	0.0151
n,4/n,T (Bag 4)	0.0151
n,3/N,T (bag 3)	0.0151
n,2/n,T (Bag 2)	0.0151
n,1/n,T (Inner Bag)	0.0199

The steady state Pu concentration in the inner bag is 2%. This is less than 4%.

Case 3

Case 3 presents the results using the model for the TRUCON Code case of 6 non-filtered bags. It is assumed that the bags have twist and tape closures on each. The input data is shown in Table E-5. The permeability for the inner bag (Bag 1) was adjusted so that the diffusivity is as close as possible to those in Table 11 ($1.054\text{E-}6$ moles/s-mole fraction). The permeability for the other bags was set equal to those from the inner bag. The diffusivities for the other bags change as the surface area changes.

Table E-5. Input for the 6 Non-Filtered Bag Case in the TRUCON code comparison (With “Horse-tails”)

	Bag 1	Bag 2	Bag 3	Bag 4	Bag 5	Bag 6	Liner	Drum
Permeability, cm ³ -cm/s-cm ² -cmHg	2.06E-09	2.06E-09	2.06E-09	2.06E-09	2.06E-09	2.06E-09		
Bag thickness, mil	14	14	14	14	14	14		
Bag thickness, cm	0.0356	0.0356	0.0356	0.0356	0.0356	0.0356		
Bag height, in	17	17.5	18	18.5	19	19.5		
Bag height, cm	43.18	44.45	45.72	46.99	48.26	49.53		
Bag diameter, in	17	17.5	18	18.5	19	19.5		
Bag diameter, cm	43.18	44.45	45.72	46.99	48.26	49.53		
Bag surface area, cm ²	5857.53	6207.16	6566.92	6936.82	7316.85	7707.01		
cmHg/mole frac	76	76	76	76	76	76		
cm ³ /mole at 298 K (25 C)	24454	24454	24454	24454	24454	24454		
Diffusivity, moles/s-mole frac (note 1)	1.055E-06	1.118E-06	1.182E-06	1.249E-06	1.317E-06	1.388E-06	5.08E-05	3.70E-06

Parameter	Value
Power used in the calculation, Watts	0.0326
G(H ₂), molecules/100 ev	1.6
Hydrogen generation rate obtained using the power, moles/s	5.415E-9

Results from the spreadsheet

Using the steady state model, the following results were obtained:

Bag number (starting with the inner bag as bag 1)	Hydrogen fraction (steady state)
n,8/n,t (Drum)	0.0015
n,7/n,T (Liner)	0.0016
n,6/n,T (bag 6)	0.0055
n,5/n,T (Bag 5)	0.0096
n,4/n,T (Bag 4)	0.0139
n,3/N,T (bag 3)	0.0185
n,2/n,T (Bag 2)	0.0233
n,1/n,T (Inner Bag)	0.0285

Since in all three cases the hydrogen concentration was well below 4%, the model matches the data from the WIPP TRUCON data.

APPENDIX F

**ATTACHMENT FROM E-MAIL REGARDING GRAM LIMIT GUIDANCE FOR
DEBRIS WASTE STREAMS**

Marusich, Robert M

Subject: FW: Gram Guidance Table

From: Greager, Eric M
Sent: Monday, July 18, 2011 11:17 AM
To: Clinton, Richard (Rich)
Cc: Arrenholz, Daniel A; DeRosa, David C; Danna, Marc; Greager, Eric M
Subject: FW: Gram Guidance Table

Rich:

This might be the table you were asking me about last week.

Eric

From: Smith, Kathryn A
Sent: Wednesday, November 19, 2003 1:16 PM
To: Greager, Eric M; Roberts, Kay J
Cc: Clark, Travis
Subject: Gram Guidance Table

Here's the latest and greatest gram guidance table. Removed days to matrix depletion...

Kathryn A. Smith
Site Transportation Certification Official
(309) 372-3300

Attachment to Email

Gram Limit Guidance for Debris Waste Streams

Note: This information is for guidance only and is not a waste packaging instruction. All waste is to be packaged in accordance with an approved waste profile sheet.

These tables apply only to debris waste streams (RH 125/225 TRUCON Code). This consists of: surgical gloves, plastic bags and sheets, paper products, cloth, tape, rubber, leaded glass, lead-lined hood gloves, lead blankets, light bulbs, flashlight batteries, piping, conduit, wiring, glass and metal portions of gloveboxes, pumps, motors, standard laboratory equipment and various other debris. For questions regarding "debris", contact the TRU Program.

Package Configuration	Gram Limit Weapons Grade	Gram Limit Fuel Grade	Gram Limit Reactor Grade
55 Gal Drum 3 Filtered Layers (0.2634 w)	83 grams	36 grams	25 grams
55 Gal Drum 1 Filtered Layer (0.3131 w)	99 grams	40 grams	28 grams
SWB 3 Filtered Layers (0.6383 w)	198 grams	84 grams	58 grams
SWB 1 Filtered Layer (0.9763 w)	325 FGE*	127 grams	91 grams
55 Gal Drum 3 Non-Filtered Layers (0.0690 w)	27 grams	9 grams	4.5 grams
55 Gal Drum 3 Non-Filtered Layers (0.0221 w)	6 grams	3.1 grams	2.7 grams
55 Gal Drum 6 Non-Filtered Layers (0.0326 w)	12 grams	4 grams	3 grams
55 Gal Drum 6 Non-Filtered Layers (0.0104 w)	3.1 grams	1.2 grams	0.9 gram
SWB 3 Filtered Layers Option 2 see note** (0.9764)	325 FGE*	127 grams	91 grams
SWB 1 Filtered Layer Option 2 see note** (1.3832)	325 FGE*	200 grams	135 grams

* TRAMPAC limit – Includes actual plus 2 times measurement uncertainty

** Option 2 Includes 2 filters per inner bag and 4 filters on SWB.

For percentages of Am-241 or Pu-238 greater than those listed below, contact the TRU Program for gram limits. The gram limits will be greatly affected by higher percentages of Am-241 or Pu-238.

Am-241		Pu-238	
Weapons Grade:	0.16%	Weapons Grade:	0.01%
Fuel Grade:	1.46%	Fuel Grade:	0.15%
Reactor Grade:	2.45%	Reactor Grade:	0.27%

For waste with only Americium-241 present see below. This table is not to be combined or used with the table above.

Package Configuration	Gram Limit Am-241 Only
55 Gal Drum 3 Filtered Layers (0.2634 w)	2 grams
55 Gal Drum 1 Filtered Layer (0.3131 w)	2.5 grams
SWB 3 Filtered Layers (0.6383 w)	5 grams
SWB 1 Filtered Layer (0.9764 w)	8.4 grams
55 Gal Drum 3 Non-Filtered Layers (0.0637 w)	0.5 gram
55 Gal Drum 3 Non-Filtered Layers (0.0204 w)	0.15 gram
55 Gal Drum 6 Non-Filtered Layers (0.0326 w)	0.25 gram
55 Gal Drum 6 Non-Filtered Layers (0.0104 w)	0.08 gram
SWB 3 Filtered Layers Option 2 see note** (0.9764)	8.4 grams
SWB 1 Filtered Layer Option 2 see note** (1.3832)	11.8 grams

** Option 2 Includes 2 filters per inner bag and 4 filters on SWB.

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APPENDIX G

**CLARIFICATION OF DATA USED BY WIPP IN THE DEVELOPMENT OF THE
TRUCON CODE FOR PTO IN SWB**

From: Biedscheid, Jennifer - WTS [<mailto:Jennifer.Biedscheid@wipp.ws>]
Sent: Tuesday, November 29, 2011 10:17 AM
To: Marusich, Robert M
Cc: Rhoades, James - DOE; Brown, Mike - DOE; Sellmer, Todd - WTS; Devarakonda, Murthy - WTS; Sinisa M Djordjevic; Morrison, Cindy - WTS
Subject: RE: Clarification added to question 2 - Need your help in interpreting WIPP TRUCON code data for Hanford

Robert:

Responses to your specific questions (of 11/18/11; clarified on 11/20/11) are provided below (in blue font).

Please let us know if you have additional questions or if any of the responses require clarification.

Thank you,

Jennifer

Jennifer Biedscheid
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Question 1: The TRUCON code data made no mention of a liner (Rev 40 of CH-TRUCON for RH-111S/112S). The Pencil Tank Overpacks (PTO) in a Standard Waste Box configuration has a liner in it. Does the TRUCON data include a liner that has openings large enough that the hydrogen concentration in the liner is the same as in the SWB or was it based on no liner being present? If a liner was assumed to be present, what is the diffusivity of the liner.

Response to Question 1: All CH-TRUCON codes are developed using information provided by the requesting site. The approved packaging configuration description for CH-TRUCON Code RH 111S/211S is based on information provided by Hanford, which did not specify a liner in the SWB. RH 111S/211S payload shipping categories assume no liner is present in the SWB. The confinement layers consist only of the drum liner bag (twist-and-tape closure), the filtered PVC pipe (3.7E-06 mol/s/mf), and the SWB (3.7E-05 mol/s/mf total). Correspondence with Eric Greager during the code development process that confirmed the accuracy of the description for RH 111S/211S is attached. I am copying Eric on this message so that any discrepancies can be addressed internally at Hanford.

Question 2: Regarding the plastic bag around the cardboard tube (we call it the sonotube). What diffusivity was used for the plastic bag in the WIPP development of the TRUCON code? Not having that data, I considered using the WIPP data you sent to me for a "large twist and tape liner bag" - a diffusivity of 4.67×10^{-6} moles/s-mole fraction. One could also use the diffusivity of the twist and tape bag from the tests performed in the *CH-TRU Payload Appendices*, Section 6.8, Table 6.8-5 of around $1.054\text{E-}6$ moles/s-mole fraction (adding the diffusivity of the bag and the diffusivity of the closure). Which was used in the analysis for the TRUCON code? There are indications that the bag we will use may be in-between the sizes of the bags used in the analysis. How would you accommodate that?

Response to Question 2: Based on the information (bag dimensions) provided by Hanford, a "drum liner bag" ($4.67\text{E-}06$ mol/s/mf as specified in CH-TRU Payload Appendix 2.2) was used in the calculation of payload shipping categories. As stated above, the generator site information is used in the development of the CH-TRUCON code and resulting shipping category. If there are any discrepancies in the packaging description provided by Hanford (versus the information being presented now), these need to be resolved internally at Hanford and a new code requested if applicable.

Regarding the hypothetical question as to how bag sizes in between those defined in the CH-TRU Payload Appendices are addressed, the lower diffusivity value is used. Note that any site-specific analyses Hanford is performing can presumably use actual values.

Question 3: Do the equations for WIPP use, as a maximum allowable H₂ concentration limit within a package, a 4% hydrogen or 5% hydrogen?

Response to Question 3: The NRC requirements specify a limit of 5% hydrogen concentration in all regions of the payload/package. If flammable volatile organic compounds are present in concentrations greater than 500 ppm, the allowed hydrogen concentration is proportionately reduced to keep the concentrations of the mixture below a mixture lower explosive limit.

Question 4: For TRUCON code RH 111S/112S, how many PTOs were assumed to be in the standard waste box? I assume that since the TRUCON code does not have any gram load limits, the limit is the standard value for SWBs (325 g).

Response to Question 4: As stated in the CH-TRUCON document, CH-TRUCON Code RH 111/211S assumes up to six (6) pencil tank overpacks per standard waste box. The CH-TRUCON code does have gram loading limits in the form of a decay heat limit. A decay heat limit (of 0.3915 watt) is associated with the payload shipping category (10 0160 0077) for RH 111/211S. Compliance with this decay heat limit per SWB is required in addition to the 325 g fissile gram equivalent limit per SWB. Based on the decay heat limit and assuming weapons-grade plutonium, you cannot put 325 g FGE per PTO. However, if hydrogen is measured in the SWB headspace and found to be low, higher FGE quantities (exceeding the decay heat limit) per SWB may be compliant. (See clarification on next page)

Clarificataion to Question 4 was supplied by Murthy Devarakonda, Senior Technical Advisor Washington TRU Solutions LLC. The reply is shown in the e-mail below.

From: Devarakonda, Murthy - WTS [mailto:Murthy.Devarakonda@wipp.ws]
Sent: Wednesday, January 18, 2012 10:10 AM
To: Marusich, Robert M
Cc: Biedscheid, Jennifer - WTS; Rhoades, James - DOE; Brown, Mike - DOE; Sellmer, Todd - WTS
Subject: A clarification, please on the Hanford calculation of hydrogen in waste packages.

Bob:

I am responding to your e-mail to Jennifer Biedscheid. Please see the embedded responses below.

Please contact Jennifer or me if you have any questions.

Regards,

Murthy Devarakonda
Senior Technical Advisor
Washington TRU Solutions LLC
Contractor for the US Department of Energy
505-878-1344

From: Marusich, Robert M [mailto:Robert_M_Marusich@RL.gov]
Sent: Tuesday, January 10, 2012 12:20 PM
To: Biedscheid, Jennifer - WTS
Cc: Marusich, Robert M
Subject: A clarification, please on the Hanford calculation of hydrogen in waste packages.

First Question that needs clarification:

You replied to an earlier questions by telling me that there is a decay heat limit besides a gram limit. The decay heat limit was 0.3915 W. Is this limit a "per PTO" limit or an "SWB-as-a-whole" limit?

Reply from Murthy Devarakonda: *The decay heat limit is per SWB (not per pencil tank overpack – several pencil tank overpacks may be present per SWB).*

Second question that needs clarification:

In my calculations, using fuels grade Pu, I get that 0.3915 W is equal to about 60 g. If the decay heat limit is an SWB limit, then one could only put 60 g in an SWB.

Reply from Murthy Devarakonda: *Concluding that the decay heat limit will limit the gram loading of the SWB to 60g is incorrect – as discussed during our phone call a few months back, the decay heat limit can be exceeded if SWB headspace hydrogen gas measurement shows that the flammable gas generation rate is below the limit (calculation done in the WDS software). Headspace measurement is a valid, viable, and approved compliance methodology and has been used to qualify several thousand containers (including containers from Hanford) that have already been shipped to WIPP.*

Bob Marusich
Safety Analysis Group
376-8081
Pager 85-7426
PFP, MO-273, Room C-108

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APPENDIX H
EQUATIONS SHOWN IN THE SPREADSHEET

With the exception of a few variables, the “variable names” (the variables are in Column A) are obvious. The ones that are not are defined below.

Cell		
A32	n,5/N,T	Mass fraction in the SWB.
A33	n,4/N,T	Mass fraction in the SWB Liner.
A34	n,3/N,T	Mass fraction in the PTO.
A35	n,2/N,T	Mass fraction in the bag around the sonotube.
A36	n,1/N,T	Mass fraction within the sonotube.
E26	watts	Input value – the watts in the waste package.
E27	Moles/s	The hydrogen generation rate, in units of moles/s, based on the watts.
A25	Grams Pu in inner package	Grams Pu in the sonotube.
F30 – F36	grams	Reading down, the values are the grams of that plutonium (or americium) isotope in a gram of plutonium mix (Cell D25).
G30 – G36	Ci/gram	Reading down, these are the values for specific activity for the plutonium and americium isotopes.
H30-H36	Curies	Reading down, these are the values of the curies of the plutonium and americium isotopes in a gram of the plutonium mix.
I30-I36	Mev/dis	Reading down, the values are the energy of the radiation given off by the plutonium (or americium) isotope.
G29,I29	Average Mev	I29 is the average energy of the radiation given off by the mixture of plutonium and americium isotopes.
F38 and H38	Total minus Pu-241	Cell H38 provides the curies per gram of the alpha emitting isotopes in the plutonium and americium mix.

The next page shows the layout of the spreadsheet. The three pages after that show the equations used for each cell within the spreadsheet.

	A	B	C	D	E	F	G	H	I
1				Sonotube	Bag around sonotube	PTO	SWB Liner	SWB	
2	Permeability, cm ³ -cm/s-cm ² -cmHG				1.22E-09				
3	Bag thickness, mil				12				Pu in PTOs in SWBs
4	Bag thickness, cm				0.0305				With liner included
5	Bag height, in			44	44.5	45			
6	Bag height, cm			111.76	113.03	114.30			
7	Bag diameter, in			14	14.5	15			
8	Bag diameter, cm			35.56	36.83	38.1			
9	Bag surface area, cm ²				13078.11				
10									
11	cmHg/mole frac				76				
12	cm ³ /mole at 298 K (25 C)				24454				
13									
14	Diffusivity, moles/s-mole frac			2.10E-04	1.62E-06	1.10E-05	1.80E-05	3.00E-05	
15	Number of PTOs			6					
16	Total SWB Liner volume, L			1833					
17	Total SWB volume, L			1859					
18	volume of 1 PTO, L			130					
19	From bag X to Bag Y			1 to 2	2 to 3	3 to 4	4 to 5	5 to 6	
20	Bag free volume, L			110.99	9.42	9.90	1051.13	26.00	
21	moles of air in bag at 298 K (25 C)			4.542	0.386	0.405	43.015	1.064	
22	Hydrogen generation rate								
23									
24	G(H ₂)			1.6					
25	grams Pu in inner pkg.			54	<u>Calc using Watts</u>				
26	curies in inner package			9.21	Watts	0.26			
27	Alpha energy, Mev			5.34	moles/s	4.319E-08			
28									
29	H ₂ generation rate, moles/s			4.84E-08			Average Mev		5.37989927
30						grams	Ci/gram	curies	Mev/dis
31						0.00205	17.1	0.0351	5.49
32	n,5/n,T				Pu-238	0.794	0.062	0.0492	5.15
33	n,4/n,T			0.0097 SWB	Pu-239	0.159	0.023	0.0037	5.16
34	n,3/n,T			0.0258 SWB Liner	Pu-240	0.0137	100	1.3700	0
35	n,2/n,T			0.0302 PTO	Pu-241				
36	n,1/n,T			Bag around					
37				0.0601 sonotube	Pu-242	0.00654	0.004	0.0000	4.9
38				0.0603 Sonotube	Am-241	0.0241	3.43	0.0827	5.48
						total	total	1.5406	
						total minus Pu-241		0.17062916	Ci/g for >10%

	A	B	C	D
1				
2	Permeability, cm ³ -cm/s-cm ² -cmHg			Sonotube
3	Bag thickness, mil			
4	Bag thickness, cm			
5	Bag height, in			44
6	Bag height, cm			=D5*2.54
7	Bag diameter, in			14
8	Bag diameter, cm			=D7*2.54
9	Bag surface area, cm ²			
10				
11	cmHg/mole frac			
12	cm ³ /mole at 298 K (25 C)			
13				
14	Diffusivity, moles/s-mole frac			0.00021
15	Number of PTOs			6
16	Total SWB Liner volume, L			1833
17	Total SWB volume, L			1859
18	volume of 1 PTO, L			=(3.14159/4)*F8*F8*F6/1000
19	From bag X to Bag Y			1 to 2
20	Bag free volume, L			=(3.14159/4)*D8*D8*D6/1000
21	moles of air in bag at 298 K (25 C)			=1*D20/(0.082*298)
22	Hydrogen generation rate			
23				
24	G(H ₂)			1.6
25	grams Pu in inner pkg.			54
26	curies in inner package			=H38*D25
27	Alpha energy, Mev			5.34
28				
29	H ₂ generation rate, moles/s			=D26*3700000000000*D27*1000000*D24/(6.02E+23*100)
30				
31				
32	n, 5/N, T		= (D15*D29)/H14	SWB
33	n, 4/n, T		= ((D29*D15)/G14) + (C32)	SWB Liner
34	n, 3/n, T		= (D29/F14) + (C33)	PTO
35	n, 2/n, T		= ((SF\$14/E14)*(C34-C33))+(C34)	Bag around sonotube
36	n, 1/n, T		= ((SE\$14/D14)*(C35-C34))+(C35)	Sonotube
37				
38				
39				

	E	F	G
1	Bag around sonotube	PTO	SWB Liner
2	0.00000000144		
3	12		
4	$=(E3/1000)*2.54$		
5	44.5	45	
6	$=E5*2.54$	$=F5*2.54$	
7	14.5	15	
8	$=E7*2.54$	$=F7*2.54$	
9	$=3.14159*E8*E6$		
10			
11	76		
12	$=298*0.08206*1000$		
13			
14	$=(E2)*(E9/E4)*(E11/E12)$	0.000011	0.000121
15			
16			
17			
18			
19	2 to 3	3 to 4	4 to 5
20	$=(3.14159/4)*E8*E8*E6/1000) - D20$	$=(3.14159/4)*F8*F8*F6/1000) - D20 - E20$	$=D16-(D15*D18)$
21	$=1*E20/(0.082*298)$	$=1*F20/(0.082*298)$	$=1*G20/(0.082*298)$
22			
23			
24			
25	<u>Calc using Watts</u>		
26	Watts	0.26	
27	moles/s	$=(F26/(1.6E-19))*(D24/100)/(6.02E+23)$	
28			
29			Average Mev
30		grams	Ci/gram
31	Pu-238	0.00205	17.1
32	Pu-239	0.794	0.062
33	Pu-240	0.159	0.023
34	Pu-241	0.0137	100
35	Pu-242	0.00654	0.004
36	Am-241	0.0241	3.43
37		total minus Pu-241	total
38			
39			

	H	I	J
1	SWB	Pu in PTOs in SWBs With liner included	
2			
3			
4			
5			
6			
7			
8			
9			
10			
11			
12			
13			
14	0.00003		
15			
16			
17			
18			
19	5 to 6		
20	=D17-D16		
21	=1*H20/(0.082*298)		
22			
23			
24			
25			
26			
27			
28			
29		=J37/H38	
30	curies	Mev/dis	Ci*(Mev/dis)
31	=F31*G31	5.49	=H31*131
32	=F32*G32	5.15	=H32*132
33	=F33*G33	5.16	=H33*133
34	=F34*G34	0	=H34*134
35	=F35*G35	4.9	=H35*135
36	=F36*G36	5.48	=H36*136
37	=(SUM(H31:H36))		=SUM(J31:J36)
38	=H37-H34	Ci/g for >10% Pu-240	
39	Ci/g	Mev	

APPENDIX I
PEER REVIEW SHEET

Peer Review Checklist

CHPRC REVIEW CHECKLIST			
Document Reviewed: HYDROGEN CONCENTRATION IN THE INNER-MOST CONTAINER WITHIN A PENCIL TANK OVERPACK (PTO) PACKAGED IN A STANDARD WASTE BOX (SWB) PACKAGE			
Scope of Review: Complete document was reviewed along with calculations and appendices.			
Yes	No	N/A	
☐	☐	☒	* Previous reviews complete and cover analysis, up to scope of this review, with no gaps.
☒	☐	☐	Problem completely defined.
☐	☐	☒	Accident scenarios developed in a clear and logical manner.
☒	☐	☐	Necessary assumptions explicitly stated and supported.
☒	☐	☐	Computer codes and data files documented.
☒	☐	☐	Data used in calculations explicitly stated in document.
☒	☐	☐	Data checked for consistency with original source information as applicable.
☒	☐	☐	Mathematical derivation checked including dimensional consistency of results.
☒	☐	☐	Models appropriate and used within range of validity or use outside range of established validity justified.
☒	☐	☐	Hand calculations checked for errors. Spreadsheet results should be treated exactly the same as hand calculations.
☒	☐	☐	Software input correct and consistent with document reviewed.
☒	☐	☐	Software output consistent with input and with results reported in document reviewed.
☒	☐	☐	Limits/criteria/guidelines applied to analysis results are appropriate and referenced.
☐	☐	☒	Safety margins consistent with good engineering practices.
☒	☐	☐	Conclusions consistent with analytical results and applicable limits.
☒	☐	☐	Results and conclusions address all points required in the problem statement.
☒	☐	☐	* Format consistent with appropriate NRC Regulatory Guide or other standards.
☒	☐	☐	Review calculations, comments, and/or notes are attached.
☐	☐	☒	For calculations in which codes/spreadsheets (e.g., RADDOSE, GENII, etc) are used, is the latest revision used? Is the User Authorized?
☐	☐	☒	Hazard controls established are appropriate for the hazards including selection using the appropriate hierarchy (e.g., engineered over administrative).
☐	☐	☒	The preventive or mitigative credit assigned to hazard controls are appropriate, and the basis is documented.
☒	☐	☐	Document approved.
Michael E. Johnson			12/06/2011
Reviewer (Printed Name and Signature)			Date
*Any calculations, comments, or notes generated as part of this review should be signed, dated and attached to this checklist. Such material should be labeled and recorded in such a manner as to be intelligible to a technically qualified third party.			