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#### Thermal Analysis of 3013/9975 Configuration

#### Narendra K. Gupta <u>nick.gupta@srnl.doe.gov</u>, Ph: 803-725-5300, Fax: 803-725-8829 Savannah River National Laboratory, Aiken, SC 29808

### 1.0 ABSTRACT

The 3013 containers are designed in accordance with the DOE-STD-3013-2004<sup>[1]</sup> and are qualified to store plutonium (Pu) bearing materials for 50 years. The U.S. Department of Energy (DOE) certified Model 9975 shipping package is used to transport the 3013 containers to the K-Area Material Storage (KAMS) facility at the Savannah River Site (SRS) and to store the containers until the plutonium can be properly dispositioned. Detailed thermal analyses to support the storage in the KAMS facility are given in References 2, 3, and 4. The analyses in this paper serve to provide non-accident condition, non-bounding, specific 3013 container temperatures for use in the surveillance activities. This paper presents a methodology where critical component temperatures are estimated using numerical methods over a range of package and storage parameters. The analyses include factors such as ambient storage temperature and the content weight, density, heat generation rate, and fill height, that may impact the thermal response of the packages. Statistical methods are used to develop algebraic equations for ease of computations to cover the factor space. All computations were performed in BTU-FT-Hr-°F units.

#### 2.0 INTRODUCTION

#### 9975 Packaging Configuration

The 9975 package is designed by analysis and testing to meet the requirements of 10 CFR Part 71<sup>[5]</sup> to ensure that the environment and public health are not adversely impacted when the package is used to transport radioactive materials (RAM) under normal conditions of transport (NCT) and under hypothetical accident conditions (HAC). Figure 1 shows the schematic of the 9975 package in a vertical orientation. Only the vertical orientation is analyzed in this paper since this is the orientation for both transportation and storage. The package consists of an outer 35-gallon stainless steel (SS) drum, a primary containment vessel (PCV) for the RAM in the 3013 containers, a secondary containment vessel (SCV) for added protection, a lead shield, and Celotex<sup>TM</sup> as the insulating and energy absorbing material for the protection of containment vessels during accidental impact and fire conditions.

#### 3013 Container Assembly

The 3013 container assembly consists of an outer container, an inner container, and, in most assemblies, a convenience container. The convenience container houses the RAM contents and loosely fits inside the inner container. The inner container in turn loosely fits inside the outer container that goes inside the PCV. The outer container is a standard British Nuclear Fuels

Limited (BNFL) welded design; it is made of 316L SS, one design is 254 mm tall and 125 mm in diameter.<sup>[6]</sup> The inner container designs are DOE site specific but are designed to fit inside the standard BNFL outer container. The inner container is also a welded design: it is made of 304L SS, is 213 mm tall and 117 mm in diameter.<sup>[6]</sup> Figure 2 shows a 3013 container assembly with Rocky Flats inner container and a convenience container inside a PCV.



Figure 1- 9975 Schematic with Key Components

Figure 2 –3013 Container in PCV

### Surveillance Program

The 9975 package was designed as a transportation package and was not qualified for the long term storage of materials. Therefore, a comprehensive surveillance program was set up to assess the material and thermal performance of the 9975 components to ensure that the design limits of the package are not violated under the long term storage conditions.<sup>[7]</sup> In addition, since the outer and inner containers have high residual stresses and contain chlorides and moisture, the stress corrosion potential of these vessels is an important consideration in the surveillance program. The program examines the outer and inner containers, samples for signs of stress corrosion, tests O-rings for leakage rate, and tests Celotex properties at elevated temperatures to ensure that their performance is not degraded over time. The 3013 container assemblies are also examined for gas generation and pressure build up to ensure that the design limits are not violated during the long term storage.

Thermal Output Variables

Thermal output variables required to meet the surveillance needs are the temperatures of the O-rings, Celotex, and the 3013 assembly components at selected locations. This paper covers the 3013 assembly component temperatures. The component temperatures are calculated at three locations (T1, T2, and T3) on the inner container, the outer container, and the convenience container. These locations are shown in Figure 3. T<sub>G</sub> is the average gas/content temperature.



Figure 3 – Output Locations

#### 3.0 DESIGN PARAMETERS

Thermal performance of the 9975 packaging depends upon its content characteristics (i.e. density, weight, and decay heat rate) and the ambient storage conditions. Limits are placed on the maximum decay heat rate (19 watts) and the fill height (17 cm) of the radioactive material inside the convenience containers. Performance also varies to a small extent based on the composition of the fill gases since the thermal properties of the oxide contents vary with the fill gases. The fill gas assumed in this paper is a mixture of 75% He and 25% air at atmospheric conditions to simulate the 'no greater than 5% oxygen limitation' required in the 9975 package SARP.<sup>[5]</sup> The 3013 containers are normally loaded in glove boxes with a helium environment and therefore no air is expected in the fill gases. Since the thermal conductivity of helium is higher than the conductivity of the He-Air mixture, the temperatures reported here are conservative (2°F to 3°F higher). Table 1 gives the <u>expected</u> values of parameters and the limitations for the plutonium oxide (PuO<sub>2</sub>) contents in the Rocky Flats 3013 container assembly.

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Variable	Low	Mid	High			
Fill Height (cm)	? <sup>a</sup>	$?^{a}$	17.0			
Oxide Bulk Density (g/cc)	1.0	3.0	5.0			
Heat Generation (W/kg)	3.0	6.0	12.0			
Total heat load (W)	5.0	10.0	19.0			
Oxide Mass (g)	2000	3000	5000			

Table 1 - 3013 Plutonium Oxide Variables

<sup>a</sup> Height to be calculated to meet the constraints

 $PuO_2$  fill heights and heat rates are calculated based on oxide mass and bulk density, but are never to exceed a fill height of 17.0 cm or a heat rate of 19.0 watts. Table 2 gives the resulting heat loads consistent with the fill height and the powder density.

		<u> </u>			
Density	Rocky Flats Configuration				
	Height	Heat Load			
(g/cc)	(cm/inches)	(kg)	(watts)		
1	17/6.693	1.592	4.78		
3	13.62/5.364	3	10		
5	13.62/5.364	5	19		

Table 2 – Fill Height of PuO<sub>2</sub>

### 4.0 MATHEMATCAL MODEL

The computational thermal model solves the following steady state heat transfer equation in cylindrical coordinates.

$$k_1 \frac{\partial^2 T}{\partial r^2} + \frac{k_1}{r} \frac{\partial T}{\partial r} + k_2 \frac{\partial^2 T}{\partial z^2} + q^{\prime\prime\prime} = 0 \quad (1)$$

Where  $q^{\prime\prime\prime}$  is the volumetric heat generation by the fissile material per unit time,  $k_1$  and  $k_2$  are the thermal conductivities of the materials in the r and z directions, and T is the temperature. The values of  $k_1$  and  $k_2$  are the same since the materials are isotropic. For some materials thermal conductivity is a function of temperature.

#### Statistical Methods

Estimating the 3013 component temperatures for parameter (density, heat load, and storage temperature) values other than used in Table 1 is best accomplished by performing regression analyses. However, regression analysis is a statistical method and certain conditions must be met for the regression equation to be a good predictor.<sup>[8]</sup> These conditions are:

- 1. The errors (residuals) have a zero mean.
- 2. The errors (residuals) have constant variance.
- 3. The errors (residuals) are uncorrelated, i.e. they are independent.
- 4. The errors (residuals) are normally distributed.

A general linear regression equation is of the form:

$$\Gamma = \beta_0 + \beta_1 D + \beta_2 W + \beta_3 T_a + \beta_4 D^2 + \beta_5 W^2 + \beta_6 T_a^2 + \beta_7 DW + \beta_8 DT_a + \beta_9 WT_a + \varepsilon$$

Where:

T is the component temperature, (°F) D is the content density, g/cc W is the content decay heat, watts  $T_a$  is the ambient temperature, DW,  $DT_a$ , and  $WT_a$  are the interaction terms,  $\epsilon$  is the error term, and  $\beta_1$ ,  $\beta_2$ , etc. are the regression parameters that will be calculated from the computed temperature data.

#### 5.0 THERMAL MODELS

The differential equation (1) is solved numerically by a general purpose conduction-radiation computer code MSC/PATRAN/Thermal.<sup>[9]</sup> The data required for creating the thermal models are the component geometries, material properties, thermal loads, and boundary conditions. The inputs and simplifying assumptions made in creating these models are given in detail in the project report in Reference [10]. Since the 9975 and 3013 geometries are cylindrical, two axisymmetric models were created consistent with the fill heights shown in Table 2. These two models with materials depicted as different colors are shown in Figure 4.



Figure 4 - Rocky Flats 9975 Models

#### **Boundary Conditions**

The boundary conditions are the ambient storage temperatures, natural convection losses, and the radiation losses from the 9975 packaging surface. The convection correlations and surface emissivities used in the models are given in Reference [10]. The 9975 package is modeled in an upright configuration with the bottom assumed adiabatic and heat losses occurring only from its cylindrical and top surfaces.

#### Analysis Runs

The two models shown in Figure 4 are analyzed for different values of  $PuO_2$  density, heat rate, and ambient storage temperatures. Additional analyses are also performed to include low probability cases of high density contents with impurities having low heat rates and contents with low density and high heat rates. Table 3 gives the analyses that were performed to cover the entire parameter space. Inclusion of these additional analyses (Analyses 13 to 20 in Table 3) will result in more accurate response surface when regression analyses are performed.

		2	
Analysis No.	Density	Decay Heat Rate	Ambient
	(g/cc)	(Watts)	Temperature (°F)
1	1	4.78	55
2	1	4.78	85
3	1	4.78	120
4	1	4.78	162
5	3	10	55
6	3	10	85
7	3	10	120
8	3	10	162
9	5	19	55
10	5	19	85
11	5	19	120
12	5	19	162
13	1	19	55
14	1	19	85
15	1	19	120
16	1	19	162
17	5	4.78	55
18	5	4.78	85
19	5	4.78	120
20	5	4.78	162

Table 3 – Model Analyses

#### 6.0 RESULTS

The analyses enumerated in Table 3 are run using the MSC/Thermal computer code.<sup>[9]</sup> Temperatures at locations T1, T2, and T3 are picked from the nodes in the models close to the locations shown in Figure 3. Gas temperature is the nodal average of the entire content volume. Regression analyses error tests are performed using the statistical software MINITAB.<sup>[11]</sup>

### 6.1 *Outer Container*

#### **Temperatures**

The temperatures at the indicated locations in the outer 3013 container are summarized in Table 4. The highest gas temperature is 281 °F while the highest container temperature is 293 °F.

Density	Decay Heat	Temp.	Location T1	Location T2	Location T3	Gas
D(g/cc)	W (watts)	$T_a (^{\circ}F)$	(°F)	(°F)	(°F)	(°F)
1	4.78	55	84.47	87.35	83.14	85.18
1	19	55	162.78	173.62	159.49	165.72
3	10	55	126.25	136.09	128.74	129.42
5	19	55	182.75	200.56	188.87	188.51
5	4.78	55	90.62	95.56	91.84	92.15
1	4.78	85	113.18	116.03	112.09	113.92
1	19	85	188.70	199.39	186.07	191.69
3	10	85	153.44	163.07	156.22	156.56
5	19	85	208.2	225.7	214.71	213.87
5	4.78	85	119.12	123.96	120.50	120.65
1	4.78	120	146.8	149.59	145.94	147.55
1	19	120	219.35	229.88	217.41	222.39
3	10	120	185.45	194.84	188.52	188.5
5	19	120	238.38	255.58	245.36	243.98
5	4.78	120	152.51	157.22	154.04	154.03
1	4.78	162	187.34	190.07	186.74	188.11
1	19	162	256.95	267.34	255.82	260.06
3	10	162	224.25	233.39	227.64	227.24
5	19	162	275.69	292.55	283.24	281.21
5	4.78	162	192.81	197.37	194.49	194.31

Table 4 –	Outer	Container	Tem	peratures
I uole l	Outor	Container	1 VIII	perutures

#### **Regression Analyses**

The regression analysis results in terms of  $PuO_2$  density (D), heat rate (W), and storage temperature (T<sub>a</sub>) are given below. The statistical error independence test and normality test results for location T1 are shown in Figures 5 and 6. These figures show that the errors are independent and normally distributed. The errors for location T2, T3, gas temperature T<sub>G</sub> are also independent and are normally distributed.

The regression equations using statistical software MINITAB are:

Temp (T1) = - 9.16 + 0.322 D + 9.038 W + 0.983 T<sub>a</sub> - 0.146 W<sup>2</sup> + 0.237 DW - 0.0058 WT<sub>a</sub> Temp (T2) = - 12.66 + 0.407 D + 10.53 W + 0.981 T<sub>a</sub> - 0.187 W<sup>2</sup> + 0.321 DW - 0.006 WT<sub>a</sub> Temp (T3) = - 13.66 + 0.372 D + 9.73 W + 0.985 T<sub>a</sub> - 0.187 W<sup>2</sup> + 0.353 DW - 0.005 WT<sub>a</sub> Temp (Gas) = - 10.7 + 0.361 D + 9.56 W + 0.983 T<sub>a</sub> - 0.162 W<sup>2</sup> + 0.270 DW -0.006 WT<sub>a</sub>



Figure 5 – Error Independence Test for Outer Container

# Normal Probability Plot



Figure 6 - Error Normality Test for Outer Container

### 6.2 Inner Container

#### Temperatures

The temperatures at the indicated locations in the inner 3013 container are summarized in Table 5. The highest gas temperature is 285 °F while the highest container temperature is 295 °F.

Density	Decay Heat	Temp.	Location T1	Location T2	Location T3	Gas
D(g/cc)	W (watts)	$T_a (^{o}F)$	(°F)	(°F)	(°F)	(°F)
1	4.78	55	84.98	87.92	84.80	86.24
1	19	55	164.70	175.65	169.08	169.60
3	10	55	127.32	137.3	133.06	131.45
5	19	55	184.67	202.74	196.19	192.25
5	4.78	55	91.14	96.18	93.98	93.19
1	4.78	85	113.68	116.57	113.68	114.95
1	19	85	190.59	201.37	195.49	195.47
3	10	85	154.49	164.24	160.36	158.58
5	19	85	210.1	227.82	221.76	217.59
5	4.78	85	119.64	124.56	122.55	121.66
1	4.78	120	147.29	150.12	147.45	148.55
1	19	120	221.21	231.81	226.65	226.07
3	10	120	186.48	195.97	192.46	190.5
5	19	120	240.24	257.65	252.13	247.67
5	4.78	120	153.01	157.80	155.99	155.00
1	4.78	162	187.82	190.57	188.15	189.07
1	19	162	258.76	269.21	264.86	263.63
3	10	162	225.26	234.48	231.38	229.22
5	19	162	277.52	294.56	289.68	284.88
5	4.78	162	193.3	197.29	196.33	195.25

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Table $5 -$	Inner	Container	Temperature	S

#### **Regression Analyses**

The regression analysis results in terms of  $PuO_2$  density (D), heat rate (W), and storage temperature (T<sub>a</sub>) are given below. The statistical error independence and normality test results for location T1 are shown in Figures 7 and 8. These figures show that the errors are independent and normally distributed. The errors for location T2, T3, gas temperature T<sub>G</sub> are also independent and are normally distributed.

The regression equations using statistical software MINITAB are:

 $\begin{array}{l} \text{Temp}\ (T1) = -\ 9.19 + 0.325\ D + 9.16\ W + 0.983\ T_a - 0.146\ W^2 + 0.237\ DW - 0.006\ WT_a \\ \text{Temp}\ (T2) = -\ 12.37 + 0.360\ D + 10.66\ W + 0.978\ T_a - 0.190\ W^2 + 0.326\ DW - 0.006\ WT_a \\ \text{Temp}\ (T3) = -\ 14.8 + 0.726\ D + 10.33\ W + 0.983\ T_a - 0.186\ W^2 + 0.303\ DW - 0.006\ WT_a \\ \text{Temp}\ (Gas) = -\ 10.57 + 0.355\ D + 9.76\ W + 0.983\ T_a - 0.162\ W^2 + 0.270\ DW - 0.006\ WT_a \end{array}$ 



Figure 7 - Error Independence Test for Inner Container

# Normal Probability Plot



Figure 8 - Error Normality Test for Inner Container

## 6.3 *Convenience Container*

#### Temperatures

The temperatures at the indicated locations in the convenience 3013 container are summarized in Table 6. The highest gas temperature is 305 °F while the highest container temperature is 302 °F.

Density	Decay Heat	Temp.	Location T1	Location T2	Location T3	Gas
D(g/cc)	W (watts)	$T_a (^{\circ}F)$	(°F)	(°F)	(°F)	(°F)
1	4.78	55	86.91	89.17	84.05	93.73
1	19	55	171.82	180.30	162.75	199.58
3	10	55	130.5	141.64	131.33	146.48
5	19	55	190.23	210.5	193.45	212.74
5	4.78	55	92.68	98.34	93.17	98.40
1	4.78	85	115.57	117.8	112.96	122.46
1	19	85	197.56	205.94	189.21	225.53
3	10	85	157.6	168.49	158.71	173.57
5	19	85	215.53	235.47	219.14	238.1
5	4.78	85	121.14	126.67	121.77	126.87
1	4.78	120	149.12	151.31	146.77	156.09
1	19	120	228.01	236.30	220.43	256.21
3	10	120	189.51	200.11	190.91	205.47
5	19	120	245.55	265.16	249.63	268.22
5	4.78	120	154.47	159.85	155.26	160.21
1	4.78	162	189.59	191.74	187.52	196.63
1	19	162	265.39	273.61	258.69	293.86
3	10	162	228.19	238.51	229.92	244.17
5	19	162	282.69	301.92	287.32	305.48
5	4.78	162	194.71	199.92	195.65	200.45

Table 6 –	Convenience	Container	Temperatures
	Convenience	Container	remperatures

#### **Regression Analyses**

The regression analysis results in terms of  $PuO_2$  density (D), heat rate (W), and storage temperature (T<sub>a</sub>) are given below. The statistical error independence and normality test results for location T1 are shown in Figures 9 and 10. These figures show that the errors are independent and normally distributed. The errors for location T2, T3, gas temperature T<sub>G</sub> are also independent and are normally distributed.

The regression equations using statistical software MINITAB are:

 $\begin{array}{l} \text{Temp}\ (T1) = -\ 8.51 + 0.326\ D + 9.43\ W + 0.983\ T_a - 0.141\ W^2 + 0.217\ DW - 0.006\ WT_a \\ \text{Temp}\ (T2) = -\ 14.31 + 0.448\ D + 11.33\ W + 0.98\ T_a - 0.208\ W^2 + 0.361\ DW - 0.006\ WT_a \\ \text{Temp}\ (T3) = -\ 14.32 + 0.397\ D + 10.1\ W + 0.984\ T_a - 0.196\ W^2 + 0.369\ DW - 0.005\ WT_a \\ \text{Temp}\ (Gas) = -\ 13.79 + 0.386\ D + 12.31\ W + 0.98\ T_a - 0.198\ W^2 + 0.142\ DW - 0.006\ WT_a \end{array}$ 



Figure 9 - Error Independence Test for Convenience Container

## Normal Probability Plot



Figure 10 - Error Normality Test for Convenience Container

## 7.0 CONCLUSIONS

Detailed finite element analyses are performed to assess the thermal performance of the 3013/9975 container configuration. Temperatures are calculated at specific locations of the 3013 container components. Regression equations are developed for the temperatures in terms of PuO<sub>2</sub> density, heat rate, and the ambient storage temperature. The gas temperatures of a convenience container may exceed 300 °F as may the temperature of the container wall, depending on the regression variables. Although these temperatures are higher than those anticipated in actual containers, it is clear that the predicted temperatures are sufficient to support corrosion induced degradation processes.

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