

3. THERMAL EVALUATION

The thermal evaluation in this addendum examines the incorporation of plutonium metal as a new payload for the PAT-1 package. The Pu metal is packed in an inner container (*T-Ampoule Assembly*,⁴ Drawing 2A0261, designated the T-Ampoule) that replaces the PC-1 inner container. The T-Ampoule and associated Pu metal contents packing configurations are described in Section 1.2.1 and Section 1.2.2 of this addendum, respectively.

The thermal evaluations documented in Chapter 3 of the Safety Analysis Report (SAR)¹ for the Plutonium Air Transportation Package, Model PAT-1, NUREG-0361¹ (SAR¹) apply to this PAT-1 Safety Analysis Report Addendum for the T-Ampoule and its contents. The thermal evaluation of the T-Ampoule contents addressed in this addendum assumes a bounding internal heating scenario where three plutonium metal samples (25 watts total) from a three-nested *Sample Container-1 (SC-1) Assembly* configuration, (Drawing 2A0268, designated SC-1) are collocated along the seal area of the T-Ampoule to present a concentrated heat source. The other configurations described in Section 1 of this addendum, which are the 831 g (1.83 lbm) Pu hollow cylinder, wrapped in tantalum foil or not wrapped based on operational determination, supported with crushed tantalum foil, and the two-nested sample container configuration (*Sample Container-2 [SC-2] Assembly*, Drawing 2A0265, designated SC-2) supported by a titanium *Inner Cradle* (Drawing 2A0385, designated Inner Cradle) present a less concentrated heat source against the seal area. Although the quantity of plutonium metal assumed for the bounding case has a lower decay heat energy (see Section 4 of this addendum) than the 25 watts (85.3 Btu/hr) the PAT-1 package is certified for, the 25-watt decay heat limit is conservatively used for this analysis. The heat absorbed by the components within the T-Ampoule is neglected also for conservatism. Results from thermal analyses presented in this section demonstrate that the thermal performance of the PAT-1 with the proposed metal payload will be acceptable under normal conditions of transport (NCT) as defined in 10 CFR 71.71,² under hypothetical accident conditions (HAC) as defined in 10 CFR 71.73,² and under the accident conditions for air transport of plutonium as defined in 10 CFR 71.74.² The results also demonstrate that the T-Ampoule will provide a eutectic barrier for the proposed metal payload under the accident conditions for air transport of plutonium, as defined in 10 CFR 71.74.² The components of the PAT-1 packaging not modified by this addendum perform as documented in the SAR.¹

3.1 Description of Thermal Design

The thermal design description provided in the SAR¹ remains valid for this addendum, as there are no alterations to the AQ-1 protective overpack (*Overpack AQ*, Drawing 1002, designated AQ-1) or the TB-1 stainless steel containment vessel (*Containment Vessel*, Drawing 1017, designated TB-1). The thermal effects of replacing the PC-1 inner container and aluminum spacer with the T-Ampoule inner container inside the TB-1, with the same 25 watts (85.3 Btu/hr) maximum heat generation, were conservatively bounded in the computer analyses, as explained in the next sections. Changing the content form inside the TB-1 has no negative effects on the thermal performance of the AQ-1 overpack thermal design features or the TB-1 containment vessel. The thermal performance of the PAT-1 package is adequate and will safely contain its

^A The drawing titles are in italics and are used interchangeably with the designated names in this addendum. See Section 1.3.2 in this addendum and Chapter 9 in the SAR¹ for drawing number, title, and revision.

contents as described in ~~the SAR~~ this addendum under the test conditions specified in 10 CFR 71.71, 71.73, and 71.74.²

3.1.1 Design Features

The design features of the PAT-1, TB-1 stainless steel containment vessel, and the AQ-1 protective overpack assembly are unchanged and are described in Chapter 3 of the SAR¹. The *Ring, Filler* (Drawing 2A0262, designated Ring Filler) and the T-Ampoule inner container in the configurations depicted in Figures 1-3 through 1-5 of this addendum replace the PC-1 inner container and aluminum spacer documented in the SAR.¹ The effect of this change was captured in the thermal computer models described later in this section.

There are three basic configurations for plutonium metal contents within the T-Ampoule. One configuration consists of two titanium SC-2 sample containers supported and held in position inside the T-Ampoule by a titanium Inner Cradle (see Figure 1-3 in Section 1 of this addendum). The plutonium metal content within the SC-2 is a solid plutonium (Pu) cylinder of a diameter and length of 1.1 inches (0.0279 m). A second configuration consists of three SC-1 sample containers supported and held in position inside the T-Ampoule by a titanium Inner Cradle (see Figure 1-4). This configuration is similar to the two SC-2 configuration except it consists of three SC-1s and the plutonium metal sample packed in an SC-1 is a solid cylinder 0.88 inches (0.0224 m) in diameter and length. A third configuration consists of a single Pu hollow cylinder weighing from 731 to 831 grams (1.61 to 1.83 lbm) supported by crushed tantalum foil surrounding the cylinder (see Figure 1-5). The T-Ampoule, Ring Filler, SC-1, SC-2, Inner Cradle, and plutonium metal content all have melting temperatures above the 582°C (1080°F) temperature observed in the TB-1 during the plutonium air transport fire test described in SAR,¹ Section 3.6.1.2. Since the maximum total heat generation allowed in the TB-1 is limited to 25 watts (85.3 Btu/hr), a very conservative and bounding case for the application of the internal heating was used in the evaluation discussed in this section.

3.1.2 Decay Heat of the Contents

The PAT-1 package was assessed for a total decay heat load of its radioactive contents of 25 watts (85.3 Btu/hr). Sections 3.3 and 3.4 of this addendum demonstrate that with the 25 watt (85.3 Btu/hr) decay heat, the overall thermal performance of the PAT-1 package with the T-Ampoule and its plutonium metal payload is essentially the same as demonstrated in the SAR.¹ For the purpose of the analysis of the PAT-1 with the T-Ampoule and its plutonium metal content configurations addressed in this evaluation, the decay heat is conservatively assumed to be 25 watts. A bounding internal heating scenario was assumed in the analyses presented in this addendum. All 25 watts (85.3 Btu/hr) were assumed to be concentrated in a small region directly applying heat to the T-Ampoule elastomeric O-ring, as if all the solid plutonium metal cylinders were to group and transfer all their thermal energy to a small seal region. From the three basic configurations of plutonium metal contents discussed in Section 3.1.1 of this addendum, the hypothetical configuration that yields the smallest projected area for heat to flow through and therefore, provides maximum heat flux into the seal region is one where three plutonium metal cylinders are close together and aligned along the seal region as illustrated in Figure 3-1. Assuming the total 25 watts (85.3 Btu/hr) from these three plutonium cylinders are transferred to the seal region through the small projected area illustrated in Figure 3-2, the total concentrated heat flux q'' is:

$$q'' = \frac{25W}{(2.64'')(0.88'')} = \frac{25W}{(0.067056m)(0.022352m)} \cong 16,680 \frac{W}{m^2} \text{ or } 5,288 \frac{Btu}{hr-ft^2}. \quad (3-1)$$

Note that this scenario is extremely unlikely because the Pu cylinders will not come out of the sample containers during NCT or HAC, as documented in Section 2 of this addendum. In addition, if the three Pu cylinders were to align as described, a portion of the assumed 25 watts (85.3 Btu/hr) will be transferred by convection and radiation to other regions (and components) inside the T-Ampoule, and thereby reduce the actual quantity of energy available to be transferred by conduction through the hypothetical localized heating region described herein. Since this highly concentrated heat flux is understood to bound all plutonium metal loading configurations discussed in Section 3.1.1 of this addendum, only this heat flux was used to very conservatively represent the decay heat inside the T-Ampoule during the NCT and HAC evaluations.

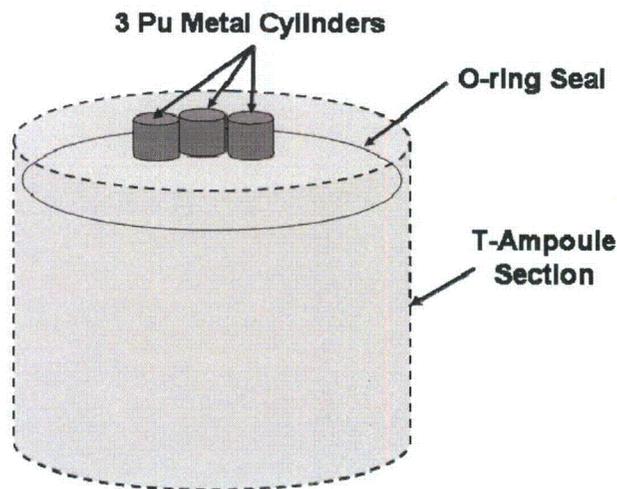


Figure 3-1. Schematic of Assumed Worst-Case Heating-to-the-Seal Scenario

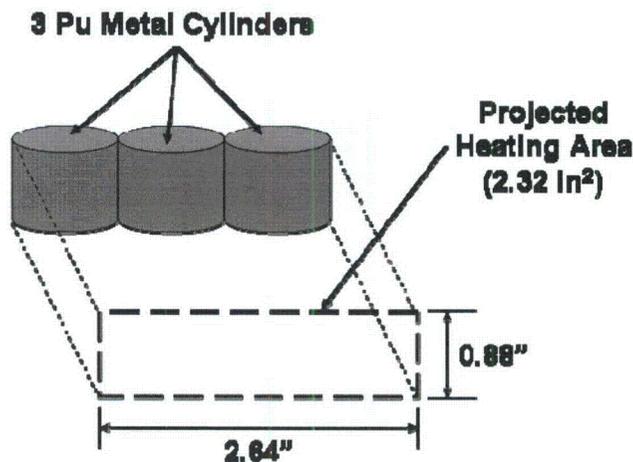


Figure 3-2. Schematic of Approximated Projected Heating Area
 $[m=0.0254 \cdot \text{in.}; m^2=6.45 \times 10^{-4} \cdot \text{in.}^2]$

3.1.3 Summary Tables of Temperatures

The SAR¹ describes how design features in the PAT-1 adequately contain the material inside the TB-1 even after the PAT-1 is exposed to the regulatory conditions specified in 10 CFR 71.71, 71.73, and 71.74.² The results from the thermal evaluation of the AQ-1, TB-1, and the T-Ampoule assuming the bounding concentrated internal heat described in Section 3.1.2 of this addendum are summarized in Table 3-1 of this addendum. These results show that the PAT-1 also protects the new components inside the TB-1 described in this addendum and adequately contains the material inside the TB-1, as the T-Ampoule seal temperatures are within the manufacturer's specifications and the T-Ampoule can withstand the pressure buildup during and after the regulatory specified heating.

Table 3-1. Summary of Temperatures Under NCT and HAC

Component	NCT		HAC
	Maximum	Minimum	Maximum
T-Ampoule (Seal)	122°C (251°F)	-40°C (-40°F)	153°C (308°F) @ 260 minutes after the fire
TB-1 (and TB-1 seal)*	114°C (238°F)	-40°C (-40°F)	147°C (296°F) @ 260 minutes after the 30-minute fire
Center of Redwood Between TB-1 and Load Spreader	99°C (211°F)	-40°C (-40°F)	132°C (270°F) @ 240 minutes after the 30-minute fire
<i>Aluminum Load Spreader</i>	98°C (208°F)	-40°C (-40°F)	131°C (267°F) @ 190 minutes after the 30-minute fire
Center of Redwood Between Load Spreader and Outer Skin	95°C (203°F)	-40°C (-40°F)	164°C (328°F) @ 30 minutes after the 30-minute fire
Stainless Steel Outer Drum	93°C (200°F)	-40°C (-40°F)	1003°C (1837°F) @ end of fire

*Maximum seal temperature was conservatively taken as the TB-1 maximum temperature.

3.1.4 Summary Table of Maximum Pressures

Table 3-2 of this addendum summarizes the maximum pressures inside the T-Ampoule for the NCT, HAC and plutonium air transport accident conditions specified in 10 CFR 71.71,² 71.73,² and 71.74,² respectively. As demonstrated in Sections 2, 3.3.2, 3.4.3, 3.4.5, and 4 of this addendum, the pressures that arise in the container during NCT, HAC, and plutonium air transport accident conditions do not result in a loss of containment.

Table 3-2. Summary of Maximum Pressures inside the T-Ampoule for NCT and HAC

Regulatory Condition	Maximum Pressure
NCT (or MNOP)	132.429 kPa (19.24.2 psig)
HAC	15240 kPa (22.15.8 psig)
Plutonium Air Transport	6.5474.14 MPa (949.5, 600 psig)

3.2 Material Properties and Component Specifications

3.2.1 Material Properties

A summary of the thermophysical properties of the materials used in PAT-1 is provided in the SAR,¹ Section 3.2, Table 3.2. To be consistent with the SAR¹ the same material properties for aluminum, ETC copper, stainless steel, and redwood (up to a certain temperature as described below) were used for the analyses presented in this addendum.

The following was considered for modeling the thermal response of redwood. Slow degradation (slow pyrolysis) of wood occurs in the temperature range of 200°C to 280°C (392°F to 536°F), until active pyrolysis begins in the 280°C to 500°C (536°F to 932°F) range. A temperature of 288°C (550°F) is used to locate the base of the char layer. Reference 3 (*Application of CMA Program to Wood Charring*) and the references cited therein contain additional information about temperature-dependent wood properties and wood charring. The thermal conductivity and specific heat provided in the SAR¹ are given in expressions that are a function of temperature. While these expressions are valid for the temperature range used for ~~the~~ their determination, which was approximately 93°C (200°F) (see Section 3.2 and Appendix 3-A of the SAR¹), the same equations were used to determine properties up to the temperature at which wood starts to decompose (i.e., 200°C [392°F]). Given that the properties of redwood provided in the SAR¹ do not take degradation of wood into account, property values and mathematical expressions from Reference 3 were used at temperatures greater than 200°C (392°F). For thermal conductivity at temperatures above pyrolysis, a fixed value within the range in Reference 3 for charcoal was used. Therefore, the temperature-dependent thermal properties presented in Table 3-3 of this addendum were specified in the P/Thermal model to adequately represent the state and response of the redwood. In cases where wood reached pyrolysis temperatures, it was assumed that the properties would remain those of charred wood throughout the cool-down process. To corroborate the validity of these modeling assumptions, thermal models discussed in Sections 3.3 and 3.4 of this addendum were completed and results compared with tests of the PAT-1 under transient NCT and HAC documented in the SAR.¹ These comparisons showed acceptable agreement as demonstrated by the data presented in those sections. Thus, a computer model that was calibrated with the test and analysis data presented in the SAR¹ was developed and used.

Table 3-3. Thermophysical Properties Used to Represent Redwood

Wood State	Temperature °C [°F]	Density kg/m ³ [lb/ft ³]	Specific Heat J/kg-K [Btu/lb-F]	Thermal Conductivity W/m-K [Btu/hr-ft-°F]	
				Parallel to Grain	Perpendicular to Grain
Before Pyrolysis	16 [60]	352 [22]	1273 [0.30]	0.330 [0.19]	0.117 [0.07]
	38 [100]	352 [22]	1591 [0.38]	0.390 [0.22]	0.136 [0.08]
	93 [200]	352 [22]	2386 [0.57]	0.533 [0.31]	0.190 [0.11]
	199 [390]	352 [22]	3898 [0.93]	0.810 [0.47]	0.290 [0.17]
During Slow and Active Pyrolysis	200 [392]	214 [13]	1151 [0.28]	0.073 [0.04]	0.026 [0.02]
	280 [536]	214 [13]	1314 [0.34]	0.073 [0.04]	0.026 [0.02]
	500 [932]	214 [13]	1657 [0.44]	0.073 [0.04]	0.026 [0.02]
	800 [1472]	214 [13]	1876 [0.45]	0.073 [0.04]	0.026 [0.02]
	1000 [1832]	214 [13]	1861 [0.45]	0.073 [0.04]	0.026 [0.02]

In addition to the material properties listed in the SAR¹ and in Table 3-3 of this addendum, the thermal properties for Ti-6Al-4V used in the computer analysis are presented in Table 3-4 of this addendum. These values were obtained from the MSC PATRAN Thermal (P/Thermal) computer code materials database,⁴ which lists References 5, 6, and 7 as the source. Reference 8 supports the temperature-dependent trend of the data presented in Table 3-4. Materials inside the T-Ampoule were conservatively neglected for the thermal analysis (no credit was taken for heat absorbed by components inside the T-Ampoule); therefore, the thermal properties of those materials are not presented in this section.

Table 3-4. Thermophysical Properties of the Titanium Ampoule (Ti 6Al-4V)

Temperature °C [°F]	Thermal Conductivity W/m-K [Btu/hr-ft-°F]	Specific Heat J/kg-K [Btu/lbm-°F]	Density Kg/m ³ [lbm/ft ³]
-50 [-58]	–	502 [0.120]	4450 [277.8]
0 [32]	6.9 [3.99]	–	
100 [212]	–	561 [0.134]	
200 [392]	9.0 [5.20]	–	
300 [572]	–	615 [0.147]	
400 [752]	11.9 [6.89]	–	

3.2.2 Component Specifications

The service temperature range for package components inside the TB-1 are presented in Table 3-5 of this addendum.

Table 3-5. Service Temperatures of Packaging Components and Content inside the TB-1

Component	Service Temperature Range °C [°F]	Reference
TB-1 and T-Ampoule O-ring	-17-40°C to 204°C [1.4-40°F to 400°F]	Appendix 3.5.2 ⁱ
TB-1 Copper Gasket	-40°C to >582°C [-40°F to >1080°F]	PAT-1 SAR ⁱⁱ
T-Ampoule (as eutectic barrier) ⁱⁱⁱ	-40°C to 625°C [-40°F to 1157°F]	[89]
Titanium Inner Cradle ⁱⁱⁱ	-40°C to 625°C [-40°F to 1157°F]	[89]
Ring, Filler ^{iv}	-40°C to >593°C [-40°F to >1100°F]	[910]
Copper Foam	-40°C to 626°C [-40°F to 1159°F]	[89]
Pu/Be Content ^{vi}	-40°C to 595°C [-40°F to 1103°F]	[89]
Tantalum Foil ^{vii}	-40°C to 640°C [-40°F to 1184°F]	[89]

ⁱ Appendix 3.5.2 of this addendum provides the manufacturer's specifications, ~~compound data sheet, and aging~~ for the O-ring material used in the T-Ampoule and in the SC-1 and SC-2 sample containers.

- ii Based on thermal tests performed and documented in the PAT-1 SAR,¹ the TB-1 maintained containment after experiencing temperatures as high as 582°C (1080°F). Therefore, the copper gasket in the TB-1 can maintain seal at temperatures above these observed maximums.

- iii The melting point of the eutectic that may form when titanium is in contact with gallium is 625°C (1157°F).
- iv. Ti-6Al-4V has a yield strength of about 331 MPa (48 ksi) at 593°C (1100°F), which is approximately 40% of the nominal room temperature value of 827 MPa (120 ksi)⁸⁹ and there are no forces other than gravitational acting on these components during and after the fire accident condition.
- v Copper-Plutonium eutectic melting point.
- vi The plutonium/beryllium eutectic represents the lowest melting point eutectic at 595°C (1103°F) in the system. The Pu/Be is a content, not a component within the TB-1.
- vii Upper temperature assumed to be the Plutonium-Tantalum eutectic melting point. From page 11 of Reference 89, there is insufficient gallium in the entire mass of plutonium metal for Tantalum-Gallium eutectic formation and melting to have a negative effect on the system.

3.3 Thermal Evaluation under NCT

The commercially available MSC Patran Thermal (P/Thermal) finite element (FE) computer code⁴ was used for the thermal evaluation of the PAT-1 package under NCT. P/Thermal is a well-respected FE code widely used to analyze a variety of thermal issues, including those related to nuclear transport packages. P/Thermal can solve one-, two-, and three-dimensional conduction, convection, and radiation heat transfer issues.

A three-dimensional model of the PAT-1 package was built using P/Thermal to demonstrate that containment is maintained by the TB-1 and that the temperature of the O-ring in the T-Ampoule does not exceed the manufacturer's recommended temperature range. The computational mesh of the PAT-1 model built using P/Thermal is shown in Figure 3-3. The model consists of 31,180 hexahedral finite elements and 34,697 nodes. Package features such as the different wood grain orientations and the respective anisotropic thermal properties of the redwood, the aluminum Load Spreader, the copper heat transfer tube, the stainless steel TB-1, and the titanium T-Ampoule were included in the model. The thin-walled outer drum was conservatively neglected. As mentioned in Section 3.1.2 of this addendum, the presence of components inside the T-Ampoule such as the sample containers (SC-1 and SC-2) and the titanium Inner Cradle were also conservatively neglected, and no other mass was assumed to absorb heat inside the T-Ampoule. Additionally, the 25-watt (85.3 Btu/hr) power from the Pu was conservatively applied to a small region on the inner surface of the T-Ampoule to maximize the thermal affect to the T-Ampoule seal, as explained in Section 3.1.2 of this addendum. The regions of the T-Ampoule, internal wall that did not receive this localized heat were conservatively assumed to be perfectly insulated (i.e., no heat transfer was allowed within the T-Ampoule, preventing the localized heated region from losing heat through convection or radiation to cooler T-Ampoule surface regions). Therefore, the small heated region was only allowed to transfer heat to the unheated (solid) regions through conduction.

The simplified temperature- and diameter-dependent correlation for a horizontal cylinder with laminar flow as employed in the TOPAZ heat transfer code⁹¹⁰ was used for the determination of the natural convection coefficient during NCT. That is:

$$h_{\text{natural}} = 1.32 * [(T_{\text{surface}} - T_{\text{ambient}}) / \text{Diameter}_{\text{cylinder}}]^{0.25} \text{ W/m}^2\text{-K} \quad (3-2)$$

Assuming

$T_{\text{surface}} = 176^{\circ}\text{F}$ (80°C) (value obtained from NCT solution in the SAR¹)

$T_{\text{ambient}} = 100^{\circ}\text{F}$ (38°C) (ambient temperature in 10 CFR 71.71²)

$\text{Diameter}_{\text{cylinder}} = 20 \text{ in.}$ (0.5588 m) (PAT-1 approximate external diameter)

$$h_{\text{natural}} = 1.32 * [(80^{\circ}\text{C} - 38^{\circ}\text{C}) / 0.5588 \text{ m}]^{0.25} \text{ W/m}^2\text{-K} \quad (3-3)$$

$$h_{\text{natural}} = 3.9 \text{ W/m}^2\text{-K} \text{ or } 0.69 \text{ Btu/hr-ft}^2\text{-}^{\circ}\text{F} \quad (3-4)$$

This value of h_{natural} is on the low end of typical natural convection heat transfer coefficients for gases⁴⁰¹¹. Ultimately, a more conservative value of $h_{\text{natural}} = 3.5 \text{ W/m}^2\text{-K}$ ($0.62 \text{ Btu/hr-ft}^2\text{-}^{\circ}\text{F}$) was used for the NCT calculation in this addendum.

The PAT-1 package model was subjected to the thermal conditions specified in 10 CFR 71.71² to evaluate if the TB-1 can maintain containment during NCT. It was assumed that the package will be transported horizontally as specified in Section 1 of this addendum. The boundary conditions used in the model to simulate the “heat” conditions specified in 10 CFR 71.71(c)(1)² are summarized in Table 3-6 of this addendum. Note that the temperature of the environment was increased to 54.4°C (130°F) as in the SAR.¹ Also note that the insolation data presented in this table represents a 24-hour average of the values as specified in 10 CFR 71.71,² as is typically assumed when a steady-state simulation is used to evaluate packages under the prescribed environment. For example, for curved surfaces, 10 CFR 71² specifies a 12-hour-period, total insolation energy of 400 g-cal/cm^2 ($16,747 \text{ kJ/m}^2$ or $1,475 \text{ Btu/ft}^2$). In order to more adequately model the NCT in a computer code running in steady-state mode, the total energy per unit area is spread over 24 hours:

$$\text{Insolation}_{\text{Curved_Surfaces}} = \frac{400 \text{ g-cal/cm}^2}{(24 \text{ hr})(3600 \text{ sec/hr})} \cong 4.63 \text{E}^{-3} \frac{\text{g-cal}}{\text{cm}^2\text{-s}} \cong 193.8 \frac{\text{W}}{\text{m}^2} \text{ or } 61.4 \frac{\text{Btu}}{\text{hr-ft}^2} \quad (3-5)$$

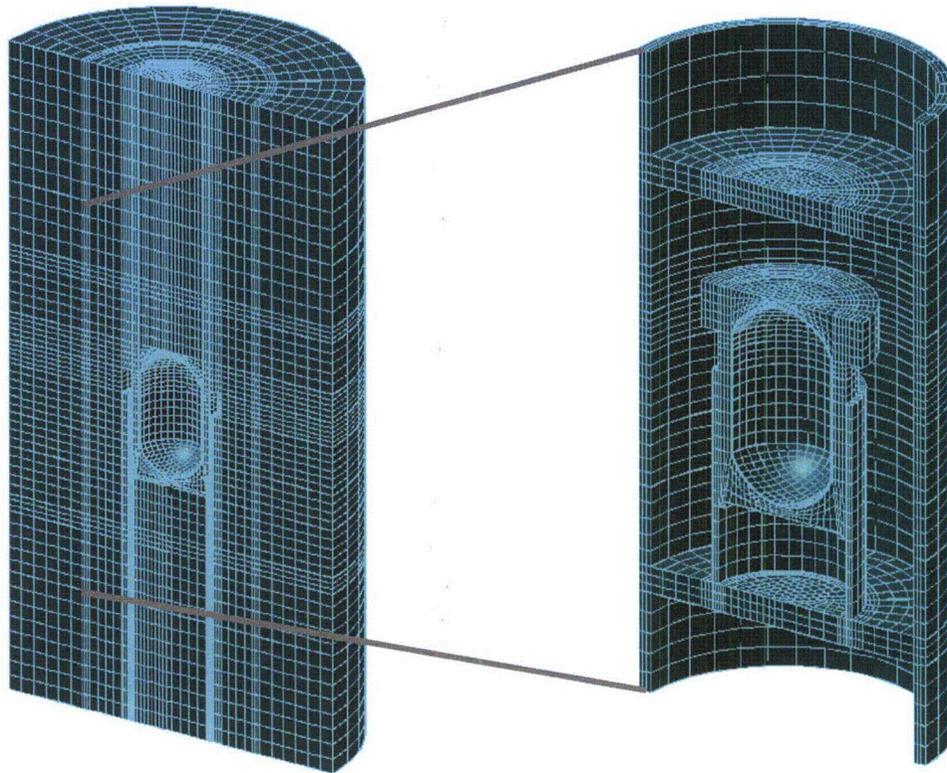


Figure 3-3. Finite Element Mesh of the PAT-1 Half-Symmetry Thermal Model and Enlarged Load Spreader, Copper Cylinder, TB-1, and T-Ampoule

Table 3-6. Boundary Conditions Used for the “Heat” NCT Thermal Evaluation

Boundary Condition	Application Region	Value Used
Environment Temperature	External node representing environment	54.4 °C (130°F)
Convection	Entire outer surface of the package	3.5 W/m ² -K (0.62 Btu/hr-ft ² -°F)
Radiation	Entire outer surface of the package	Package surface emissivity of 0.2,* Environment emissivity of 1
Insolation (Solar Flux averaged over 24 hours)	Curved surfaces	193.83 W/m ² (61.44 Btu/hr-ft ²)
	Flat surfaces transported vertically (package ends)	96.92 W/m ² (30.72 Btu/hr-ft ²)
Internal heat Flux (Decay heat)	Small region described in Section 3.1.2 of this addendum	16,680 W/m ² (5287.5 Btu/hr-ft ²)

* From Table 3.2 in the SAR¹

In addition to the “heat” NCT analysis, the package has to be able to maintain containment when exposed to an ambient temperature of -40°C (-40°F) in still air and shade as specified in 10 CFR 71.71(c)(2).² The results of exposing PAT-1 to these conditions are discussed in Section 3.3.1 of this addendum.

3.3.1 Heat and Cold

The finite element model described above was used for the NCT analysis. First, the model was verified by simulating both the steady-state test and the transient NCT analysis described in the SAR.¹ These models evenly distributed the 25W (85.3 Btu/hr) internal heat load and applied it to the inside wall of the TB-1. The results from this validation exercise are presented in Section 3.3.1.1 of this addendum. Once the model was verified against the results in the SAR,¹ the concentrated internal heat load described in Section 3.1.2 of this addendum was applied to the inner wall of the T-Ampoule. These results are presented in Section 3.3.1.2. of this addendum

3.3.1.1 Model Verification

The FE model described in Section 3.3 of this addendum was verified by simulating both the steady-state test and the transient NCT analysis described in the SAR.¹ The intent of this exercise was to verify the computer model against the data available in the SAR.¹ The validated model was then used to analyze the thermal response of the package with the plutonium metal content. These models evenly distributed the 25W (85.3 Btu/hr) internal heat load and applied it to the inside wall of the TB-1, as was the case for the models in the SAR.¹

First, the computer model was verified against a low-temperature thermal test that was performed and presented in the SAR.¹ This test was performed to empirically determine the effective thermal resistance values for PAT-1 components. While boundary conditions are not well known, it is understood that a PAT-1 package was placed in a temperature-controlled chamber maintained at approximately 93°C (200°F). An internal heater was maintained at 25 watts (85.3 Btu/hr) using a variable resistance power supply. Transient response was measured with thermocouples placed at key locations within and outside the package. These data are documented in Sections 3.4.1.2 and Appendix 3-A of the SAR.¹ The results of the verification analysis are presented in Figure 3-4. Temperature results after 50 hours favorably compare with those reported in Table 3-A.1 of Appendix 3-A in the SAR,¹ as illustrated in Table 3-7 of this addendum. Figure 3-4 also favorably compares with Figure 3.4 in the SAR.¹ The results from this validation exercise demonstrate that the geometry representation, material properties, and finite element representation are adequate to predict the performance of the PAT-1 package when exposed to similar thermal loads.

Second, the computer model was verified against the transient NCT analysis results presented in the SAR.¹ This included variable insolation heating (over time and position) as described in Section 3.4.1.2 in the SAR.¹ All boundary conditions were applied as described in that section of the SAR.¹ In order to model those conditions adequately, the half-symmetry model was mirror-copied to make a full three-dimensional model of the package. The results from this verification exercise, presented in Figures 3-5 and 3-6, compare favorably with the results presented in the SAR.¹ The data documented in Figure 3-6 is in agreement with the data shown in Figure 3.5 of the SAR.¹ This indicates proper three-dimensional modeling of the package. The three-dimensional temperature distribution of the package at the time just before sundown (the most severe case) is shown in Figure 3-7. This temperature distribution shows a peak outer skin temperature of 116°C (241°F), which is approximately 9°C (17°F) hotter than the maximum surface temperature reported in SAR,¹ Section 3.4.1.2.

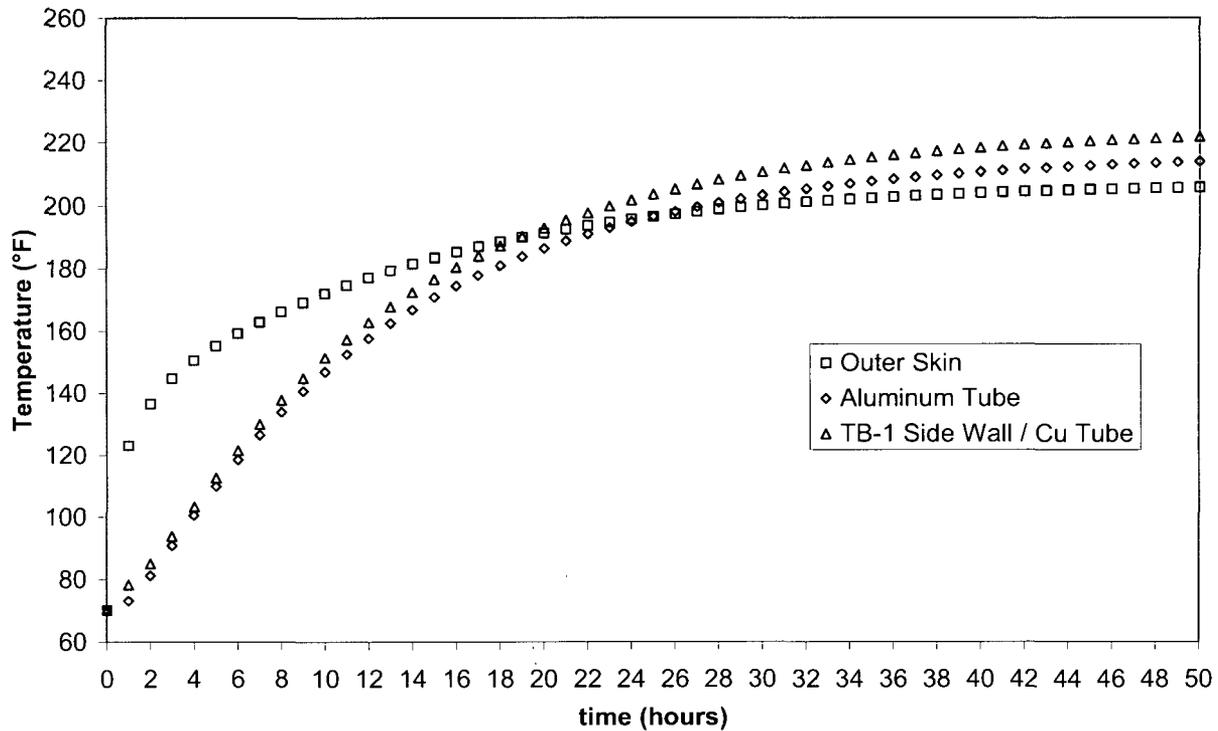


Figure 3-4. Low-Temperature Thermal Test Simulation Results. ($^{\circ}\text{C}=[^{\circ}\text{F}-32]/1.8$)

Table 3-7. Comparison of Test and Analysis Temperatures – Low Temperature Test

Location	Steady-State Temperature – Test Data	Steady-State Temperature – Analysis Data at Package Mid-Height
Cu Tube	105°C (221°F)	105.6°C (222°F)
Al Tube	100°C (212°F)	101°C (214°F)
Outer Skin	93°C (200°F)	96.6°C (206°F)

Third, the boundary conditions in the computer model were changed to reflect those specified in 10 CFR 71.71² in a steady-state simulation and to verify how the package response under these conditions compares to the transient method used in the SAR.¹ The intent of this exercise was to determine if the new analysis for this addendum is still bounding when using the steady-state method. The results from this exercise are presented in Figures 3-7 and 3-8. A comparison of the results in these two figures with those obtained from the transient simulation described above indicate that while the outer temperatures (maximums and distributions) are different, the steady-state analysis thoroughly envelops the transient response of the TB-1 and its surrounding regions. Therefore, it was decided to run a steady-state NCT analysis of the PAT-1 with the new contents configuration. The results from the steady-state analysis for this addendum are presented in Section 3.3.1.2.

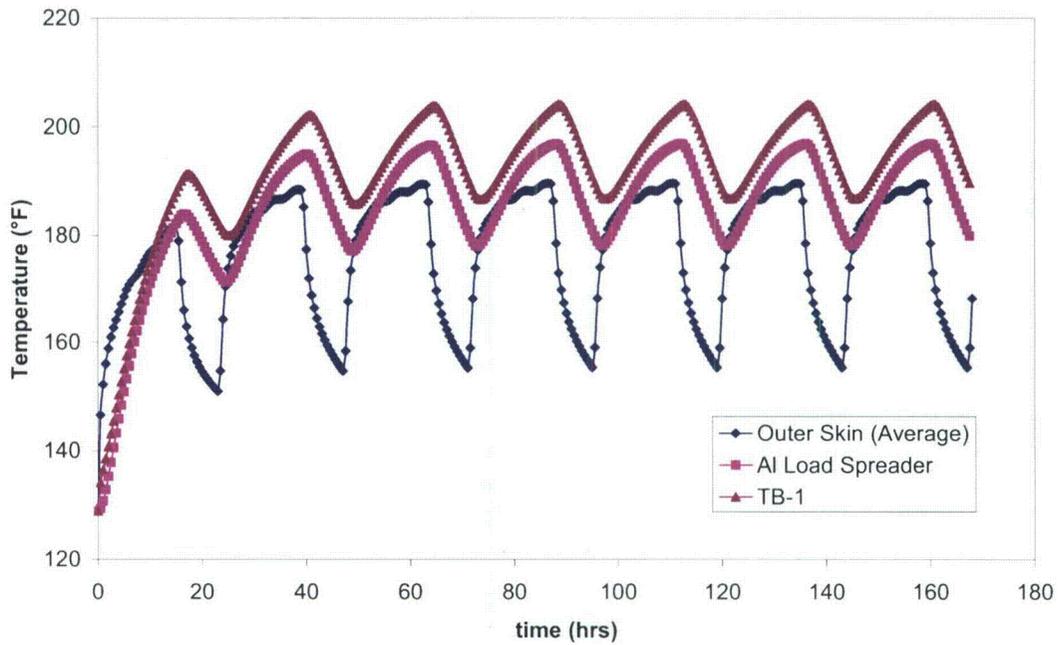


Figure 3-5. Seven-day Thermal Cycling for Quasi-Steady-State Analysis – Package Mid-Height Response ($^{\circ}\text{C}=[^{\circ}\text{F}-32]/1.8$)

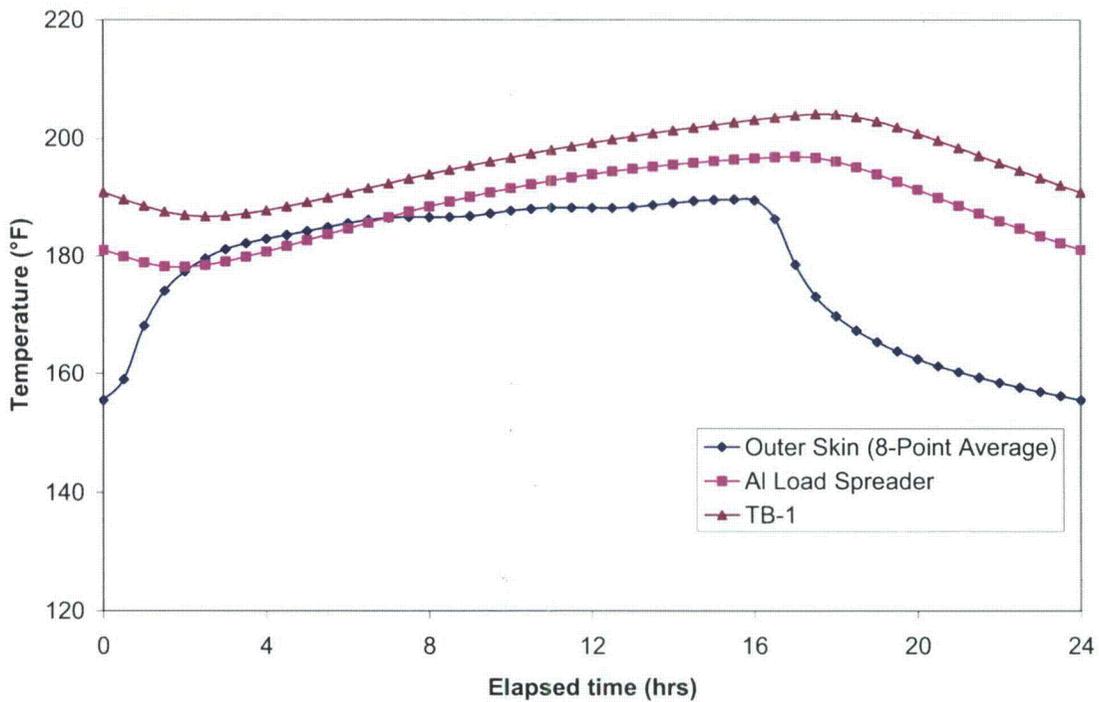


Figure 3-6. NCT Daily Thermal Cycle (Quasi-Steady-State NCT Solution) – Package Mid-Height Response ($^{\circ}\text{C}=[^{\circ}\text{F}-32]/1.8$)

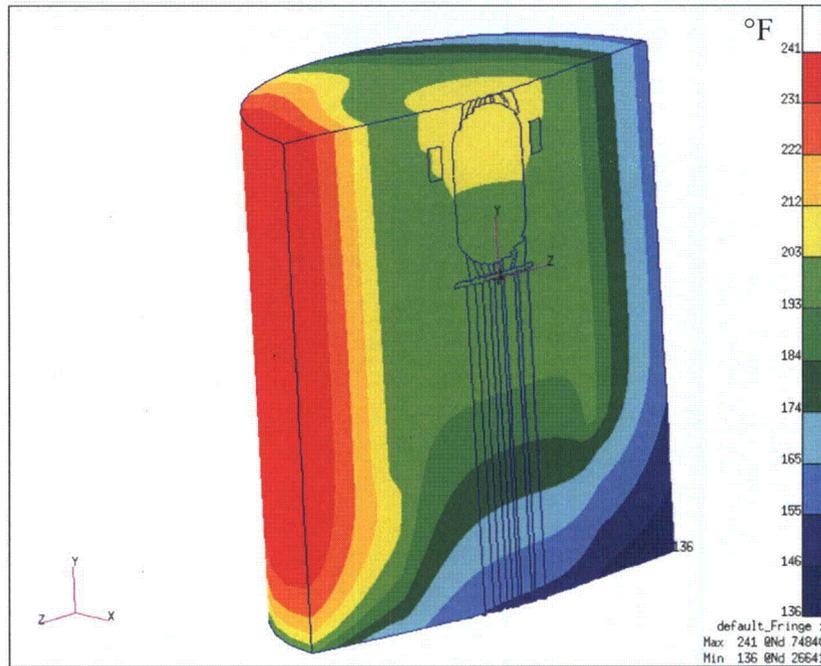


Figure 3-7. Temperature Distribution of PAT-1 Just Before Sundown – Most Severe Case of Transient NCT SAR¹ Analysis (Plot of ¼ of Package, °C=[°F-32]/1.8)

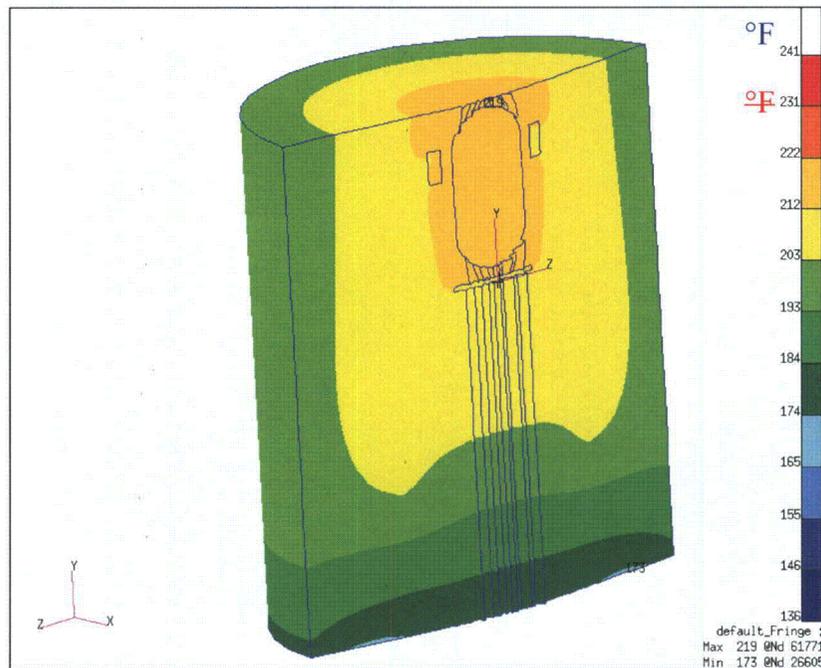


Figure 3-8. Temperature Distribution of PAT-1 – Steady-State NCT SAR¹ Analysis (Plot of ¼ of Package, °C=[°F-32]/1.8)

3.3.1.2 Addendum Analysis

The results from the NCT steady-state analysis of the package with the conservative internal heat load configuration of the new plutonium metal contents are presented in Figure 3-9. Note that the scale of the temperature distribution for this figure (and others in this section) is different from those previously shown. The temperature distribution shown in Figure 3-9 clearly illustrates the effect of the very concentrated heat applied to the seal region as described in Section 3.1.2 of this addendum. The T-Ampoule seal temperature was conservatively assumed to be the inside wall temperature of the T-Ampoule. This is conservative because the T-Ampoule closure was not explicitly modeled; instead the wall thickness of the T-Ampoule was assumed to be constant everywhere and therefore, that seal region had less thermal mass. This allows for more direct heating of the T-Ampoule seal, as energy that would be absorbed by the additional titanium in the vicinity of the seal is neglected and the heat path from the heated surface to the seal is shorter. The maximum T-Ampoule “seal” temperature is approximately 122°C (251°F) even in the very conservative internal heat load scenario. Therefore, the performance of the elastomeric O-ring in the T-Ampoule is not degraded and maintains product quality, as this temperature is within the operating range specified by the manufacturer. The maximum seal region temperature of the TB-1 was 114°C (238°F). This temperature is within the operating temperature range of **both the elastomeric and the metallic seals**. Therefore, the TB-1 is able to maintain containment.

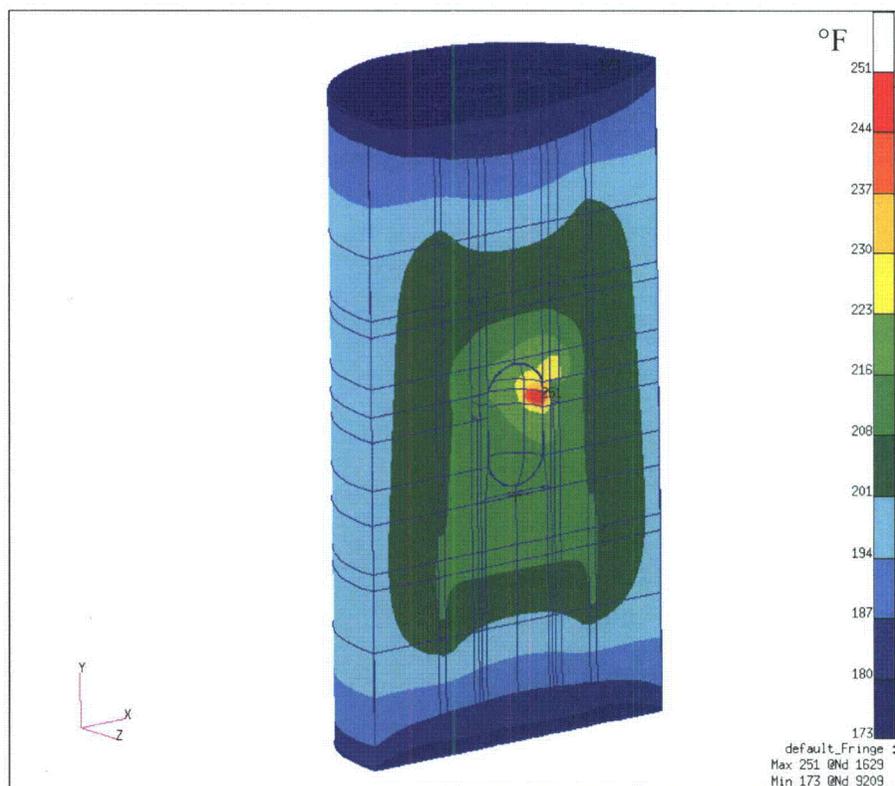
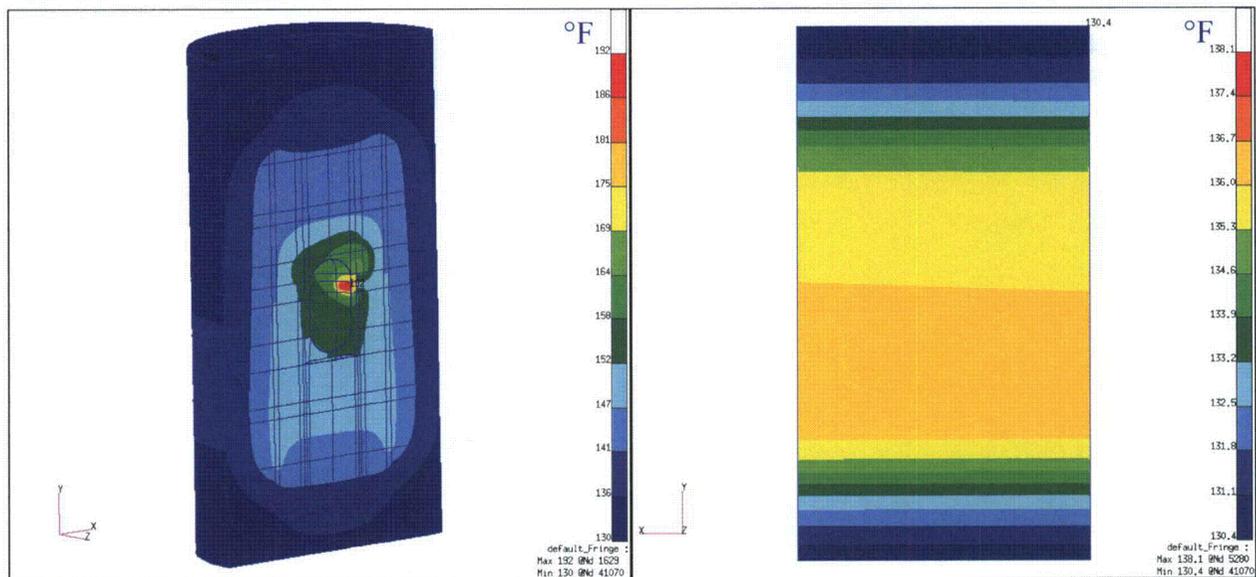


Figure 3-9. NCT Steady-State Temperature Distribution ($^{\circ}\text{C}=[^{\circ}\text{F}-32]/1.8$)

Regulatory requirements in 10 CFR 71.71(c)(2)² specify that the package must be capable of maintaining containment when it is exposed to an ambient temperature of -40°C (-40°F) in still air and shade. If one assumes no internal heating, the minimum temperature any PAT-1 package

component could reach is -40°C (-40°F). As discussed in Section 3.4.6 of the SAR,¹ the copper seal used in the TB-1 is unaffected at this low temperature. ~~The specifications given by the manufacturer of the elastomeric seal of the TB-1 indicate an operating temperature range of -40°C to 204°C (-40°F to 400°F).~~ Therefore, the PAT-1 can maintain containment at this low temperature extreme even without taking credit for any decay heat of the contents, which will definitely heat the seal region of the TB-1 to above -40°C (-40°F).

Since the results in Figure 3-9 show parts of the outer surface at temperatures above 85°C (185°F), an additional analysis was performed assuming the package is in the shade (no insolation), still air, and exposed to the conservative ambient temperature of 55°C (130°F). This was done to demonstrate compliance with 10 CFR 71.43(g),² which specifies that any accessible surface of a package must not exceed 85°C (185°F) in an exclusive use shipment. The results from this analysis are presented in Figure 3-10. Compliance with 10 CFR 71.43(g) is demonstrated, since the maximum outer surface temperature of the package is less than 58°C (137°F). The somewhat “skewed” temperature distribution seen in Figure 3-10(b) is the result of the concentrated internal heating of the package.



(a) Internal Temperatures

(b) Outer Surface Temperatures

Figure 3-10. Steady-State Analysis in the Shade – 10 CFR 71.43(g) ($^{\circ}\text{C}=[^{\circ}\text{F}-32]/1.8$)

3.3.2 Maximum Normal Operating Pressure

The maximum normal operating pressure (MNOP) that may occur within the TB-1 is estimated to be ~~132.429~~ **19.24.2** kPa (~~19.24.2~~ **19.24.2** psig) (see Section 4 of this addendum). This was calculated using the average internal surface temperature of the T-Ampoule as the average temperature of the gas inside the TB-1, which is 103.3°C (218°F) and the contribution to the internal pressure over time due to alpha decay. The MNOP was then estimated as $P_{\text{gauge}} = (P_{\text{initial}} + P_{\text{alpha_decay}}) * (T_2/T_1) - 1 \text{ atm} = [1.801 \text{ atm} (1 \text{ atm} + 0.005 \text{ atm}) * (678^{\circ}\text{R} / 530^{\circ}\text{R}) - 1 \text{ atm}] = 1.3040.286 \text{ atm}$ or ~~132.429~~ **19.24.2** kPa

(~~19.24.2~~ psig), assuming initial fill of the TB-1 is done with gas at a room temperature of 21°C (70°F) and in an environment with an atmospheric pressure of one.

3.4 Thermal Evaluation under HAC

The P/Thermal FE model that was used for the NCT analysis was also used for the HAC analysis. Since the deformations shown in the SAR¹ after the package was dropped from 30 feet are minimal, the computer model used for the HAC thermal evaluation represents an undamaged package. Boundary conditions were modified to meet those specified in 10 CFR 71.73(c)(4).² In addition, the same model was used in a model verification exercise to simulate the 52-minute fire test documented in the SAR.¹

In the SAR,¹ a description of a longer-than-regulatory fire test and results are presented. The PAT-1 package used for the test did not have internal heating. The SAR¹ does not indicate the temperature distribution or overall temperature of the package prior to the test. For the purpose of model verification, an initial uniform temperature of 27°C (80°F) was assumed within the PAT-1 package and no internal heating was applied. The boundary conditions used are summarized in Table 3-8 of this addendum. The estimation for the convection heat transfer coefficients in this table is presented following the table. Note that for the purpose of this model verification exercise, the average temperature of 982°C (1800°F) on the thin-walled AQ-1 drum reported in Table 3.4 in the SAR¹ was used as the effective fire temperature.

Table 3-8. Boundary Conditions Used for the Transient Model Verification Exercise

Boundary Condition	Application Region	Value Used During 52-Minute Fire	Value Used After Fire (Cool-down)
Environment Temperature	External node representing environment	982°C (1800°F)*	27°C (80°F)**
Convection	Entire outer surface of the package	11.5 W/m ² -K (2.03 Btu/hr-ft ² -°F)	3.5 W/m ² -K (0.62 Btu/hr-ft ² -°F)
Radiation	Entire outer surface of the package (exchange with environment node)	Package surface emissivity of 0.8, Fire emissivity of 1	Package surface emissivity of 0.2,*** Environment emissivity of 1
Internal Heat Flux (Decay Heat)	N/A	0	0

*From Table 3.4 in the SAR¹

**Assumed ambient temperature

***From Table 3.2 in the SAR¹

Values for convection heat transfer coefficients were estimated using correlations and verified with typically used values. For the convection heat transfer coefficient applied to the package surface during the fire (h_{fire}), a simplified temperature-only dependent correlation for a horizontal cylinder with turbulent flow as employed in the TOPAZ heat transfer code⁹¹⁰ was used. That is,

$$h_{\text{fire}} = 1.24 \cdot (T_{\text{ambient}} - T_{\text{surface}})^{1/3} \text{ W/m}^2\text{-K}$$

where T_{ambient} is the temperature of the environment around the package and T_{surface} is the outer surface temperature of PAT-1, with both temperatures in °C or Kelvin.

Assuming

$T_{\text{ambient}} = 1475^{\circ}\text{F}$ (800°C) (fire temperature in 10 CFR 71.73)

$T_{\text{surface}} = 176^{\circ}\text{F}$ (80°C) (value obtained from NCT solution in the SAR¹)

$$h_{\text{fire}} = 1.24 \cdot (800^{\circ}\text{C} - 80^{\circ}\text{C})^{1/3} \text{ W/m}^2\text{-K}$$

$$h_{\text{fire}} = 11.11 \text{ W/m}^2\text{-K or } 1.96 \text{ Btu/hr-ft}^2\text{-}^{\circ}\text{F}$$

This value of forced convection coefficient was corroborated using a more complex correlation proposed by Churchill and Bernstein¹² and experimental open-pool fire velocity measurements in Reference 13. In calm wind conditions for open-pool fires, vertical gas velocities are typically in the range of 5-10 m/s (16.4-32.8 ft/s) approximately 2 meters (6.56 ft) above the pool, but decrease to about 1 m/s (3.28 ft/s) near the surface of the pool.¹³ Table 3-9 of this addendum presents typical values of the Grashof number (Gr_D) and the Reynolds number (Re_D) using a 5 m/s (16.4 ft/s) vertical gas velocity. To obtain these values, the temperature of the fire was assumed to be 800°C (1475°F) and air properties were used.

When $Gr_D/(Re_D)^2$ is less than 1, forced convection dominates. Therefore, the correlation suggested by Churchill and Bernstein for forced convection applies and was used to obtain an average convection coefficient:

$$\overline{Nu}_D = 0.3 + \frac{0.62 Re_D^{1/2} Pr^{1/3}}{[1 + (0.4/Pr)^{2/3}]^{1/4}} \left[1 + \left(\frac{Re_D}{282,000} \right)^{5/8} \right]^{4/5} \quad (3-6)$$

where \overline{Nu}_D is the Nusselt number and Pr is the Prandtl number. The convective coefficient, h, is equal to $\overline{Nu}_D k / D$, where k is the thermal conductivity of air and D is the diameter of the package. As demonstrated in Table 3-9 of this addendum the convection heat transfer coefficient is highest at the beginning of the fire when the temperature difference between the flame and the external wall of the cylinder is highest.

Table 3-9. Grashof, Reynolds, Nusselt Numbers for Calm Wind, Open-Pool Fire Conditions

Surface Temperature, T_s	Gr_D	Re_D	Gr_D/Re_D^2	Nu_D (Pr=0.7 for Air)	Convection Coefficient, h $\text{W/m}^2\text{-K}$ [$\text{Btu/hr-ft}^2\text{-}^{\circ}\text{F}$]
80°C [176°F]	2.39E+08	32870	0.22	106.1	10.0 [1.76]
527°C [981°F]	2.39E+07	21166	0.06	81.8	9.5 [1.67]
800°C [1472°F]	0	15102	0	67.4	8.7 [1.53]

Given that the value of h_{fire} using the correlation suggested by Churchill and Bernstein is between 8.7 and 10 and the simplified correlation from Shapiro and Edwards¹⁰ is 11.11, a conservative heat transfer coefficient of $h_{\text{fire}} = 11.5 \text{ W/m}^2\text{-K}$ ($2.03 \text{ Btu/hr-ft}^2\text{-}^{\circ}\text{F}$) was used in the model.

The same simplified temperature- and diameter-dependent correlation for a horizontal cylinder with laminar flow that was used to calculate the natural convection coefficient for NCT in Section 3.3 of this addendum was used to estimate the natural convection coefficient for the modeling of the cool-down process after the fire. That is:

$$h_{\text{natural}} = 1.32 * [(T_{\text{surface}} - T_{\text{ambient}}) / \text{Diameter}_{\text{cylinder}}]^{0.25} \text{ W/m}^2\text{-K} \quad (3-7)$$

Assuming

$T_{\text{surface}} = 1475^{\circ}\text{F}$ (800°C) (assuming outer surface at prescribed regulatory fire temperature for bounding, maximum value calculation)

$T_{\text{ambient}} = 100^{\circ}\text{F}$ (38°C) (ambient temperature in 10 CFR 71.71²)

$\text{Diameter}_{\text{cylinder}} = 20 \text{ in.}$ (0.5588 m) (PAT-1 approximate external diameter)

$$h_{\text{natural}} = 1.32 * [(800^{\circ}\text{C} - 38^{\circ}\text{C}) / 0.5588 \text{ m}]^{0.25} \text{ W/m}^2\text{-K} \quad (3-8)$$

$$h_{\text{natural}} = 8 \text{ W/m}^2\text{-K} \text{ or } 1.4 \text{ Btu/hr-ft}^2\text{-}^{\circ}\text{F} \quad (3-9)$$

This estimated maximum value of h_{natural} is in the mid range of typical natural convection heat transfer coefficients for gases.¹⁰¹¹ However, a more conservative value of $h_{\text{natural}} = 3.5 \text{ W/m}^2\text{-K}$ ($0.62 \text{ Btu/hr-ft}^2\text{-}^{\circ}\text{F}$) (the same value used in the evaluation of NCT) was assumed for the cool-down calculation.

The results from the verification model are presented in Figures 3-11 through 3-15. Figures 3-11 and 3-12 show the temperature distribution of the overall package and the internal components at the end of the 52-minute fire. Figures 3-13 and 3-14 are similar to the previous two, but show the temperature distribution at the time when the internal temperature of the TB-1 peaked (300 minutes after the fire). The plot in Figure 3-15 illustrates the temperature history of the package at selected locations.

When the simulated temperature response was compared to the results of the 52-minute fire test discussed in the SAR,¹ it was found that the computer prediction overestimated the thermal response of the package. The spatial average temperature of the TB-1 at the time the peak temperature occurred was 100°C (212°F). This is 7°C (12°F) hotter than the average TB-1 temperature reported in the SAR.¹ Since the model in this verification exercise overestimated the TB-1 average temperature, the simulation of the package response to the HAC with the concentrated heat is also overestimated. Therefore, it is conservative to use this model to estimate the thermal response of the package configuration for this addendum. The results are presented in the following sections.

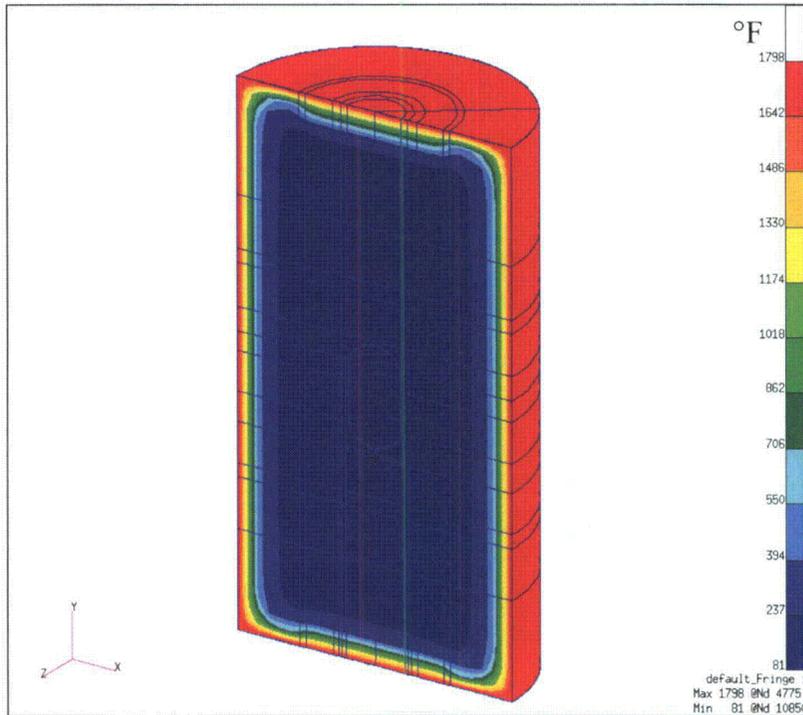


Figure 3-11. Temperature Distribution of the Verification Model at the End of the 52 Minute Fire — Complete Model ($^{\circ}\text{C}=[^{\circ}\text{F}-32]/1.8$)

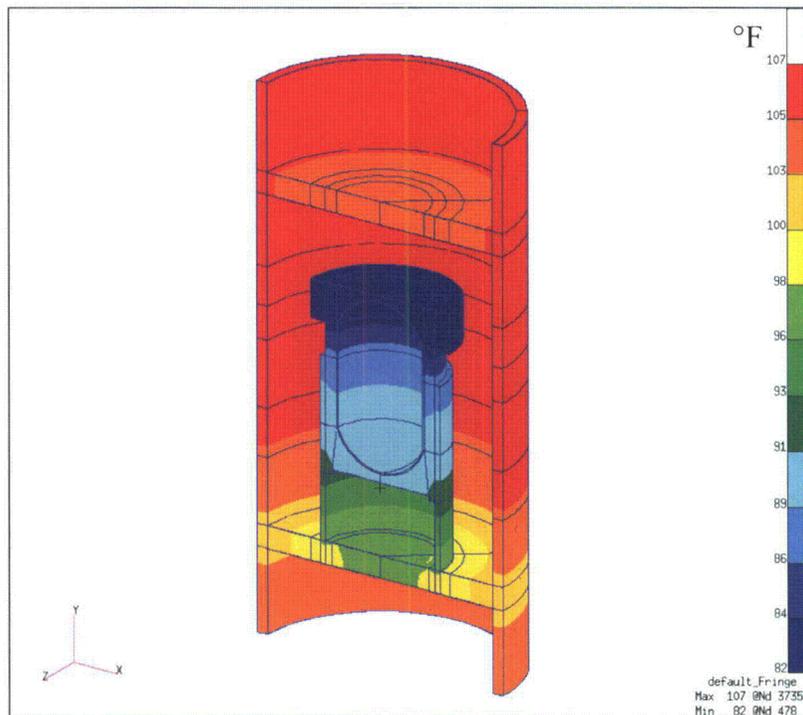


Figure 3-12. Temperature Distribution of the Verification Model at the End of the 52 Minute Fire — T-Ampoule, TB-1, Heat Transfer Cu Cylinder, and Aluminum Load Spreader ($^{\circ}\text{C}=[^{\circ}\text{F}-32]/1.8$)

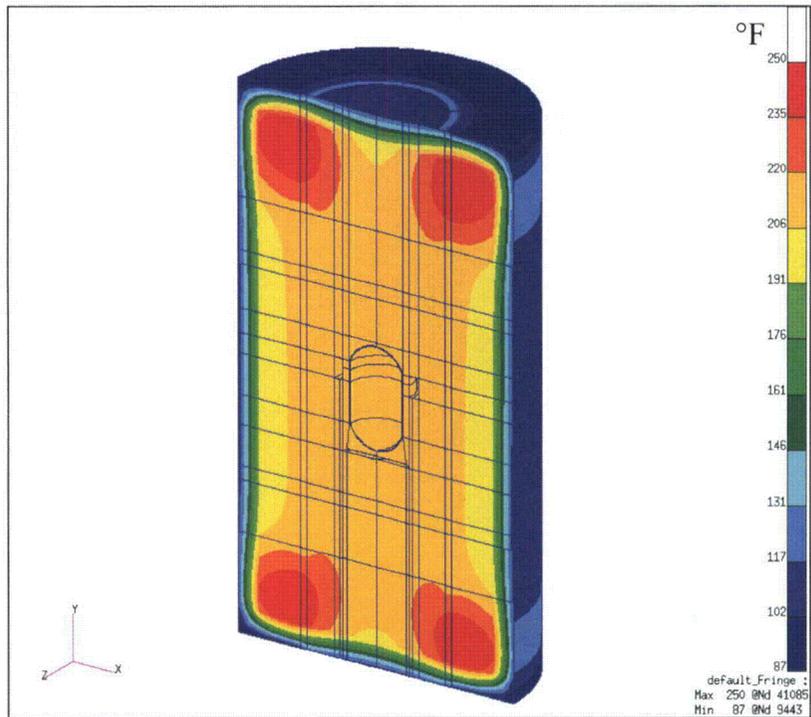


Figure 3-13. Temperature Distribution of the Verification Model at t=352 Minutes (300 Minutes after the 52 Minute Fire) — Complete Model ($^{\circ}\text{C}=[^{\circ}\text{F}-32]/1.8$)

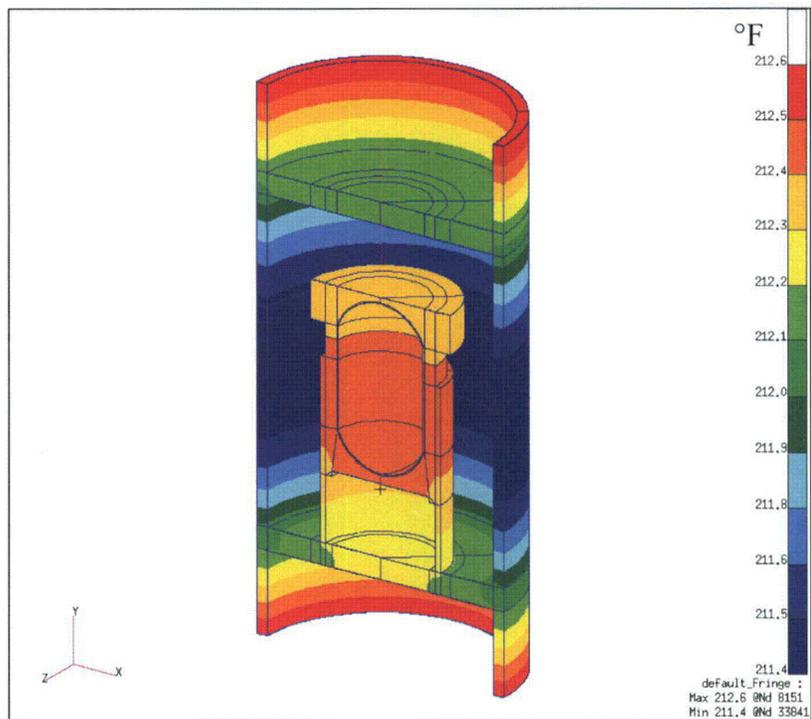


Figure 3-14. Temperature Distribution of the Verification Model at t=352 Minutes (300 Minutes after the 52 Minute Fire) — T-Ampoule, TB-1, Heat Transfer Cu Cylinder, and Aluminum Load Spreader ($^{\circ}\text{C}=[^{\circ}\text{F}-32]/1.8$)

3.4.1 Initial Conditions

The initial condition for the transient thermal analysis described in 10 CFR 71.73² is the temperature distribution calculated for the NCT. This initial temperature distribution is shown in Figure 3-9.

3.4.2 Hypothetical Accident Conditions (HAC)

The PAT-1 package model was subjected to the thermal transient conditions specified in 10 CFR 71.73² to evaluate whether the TB-1 can maintain containment and the T-Ampoule maintain seal (for product quality, not regulatory purpose) during and after a HAC fire event. The boundary conditions that were used in the model are summarized in Table 3-10 of this addendum. Note that only two boundary conditions were changed between this model and the one that was run for the 52-minute fire test verification exercise. That is, the fire duration was set to 30 minutes, and the same concentrated internal heat load applied to the NCT model was also used. As in the SAR,¹ the fire temperature was conservatively assumed to be 1010°C (1850°F) and the environment temperature for the cool-down period was conservatively assumed to be 54.4°C (130°F).

For the simulation of the HAC, the effect of a vertical and a horizontal package orientation in the fire were considered to determine the most damaging configuration. The calculations presented in Section 3.5.4 show that the package would receive more heat during HAC if it is positioned horizontally in the fire. Thus that conservative configuration was assumed for the fire analysis summarized in this section of the Addendum. Section 3.5.4 also shows that the value used for the cool-down is bounding.

The results from the simulation of the 10 CFR 71.73(c)(4)² environment are presented in Figures 3-16 through 3-20. Figures 3-16 and 3-17 show the temperature distribution of the overall package and the internal components at the end of the 30-minute regulatory fire. Figures 3-18 and 3-19 are similar to the previous two but show the temperature distribution at the time when the internal temperature of the TB-1 peaked (260 minutes after the fire). The plot in Figure 3-20 illustrates the temperature history of the package at selected locations.

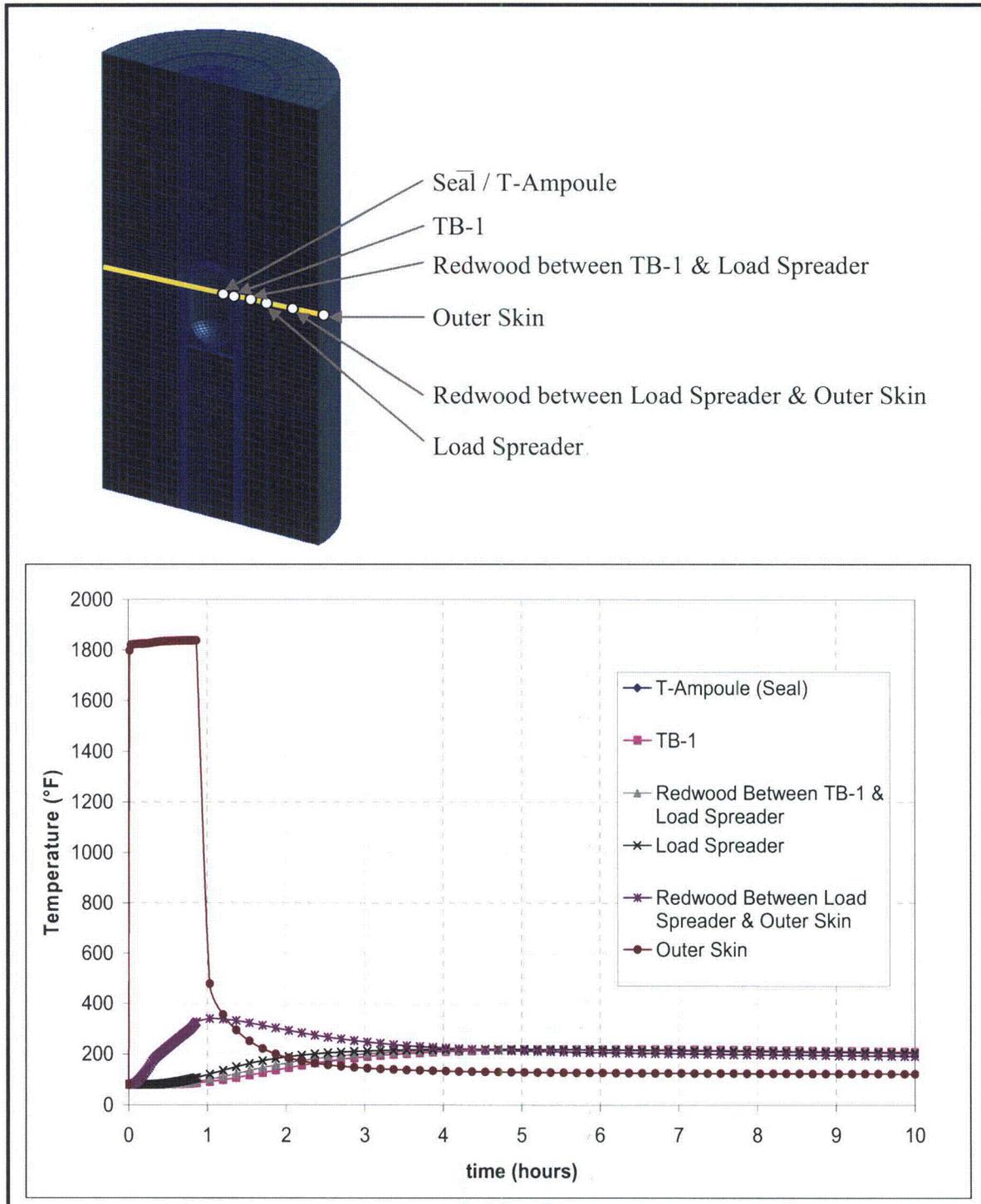


Figure 3-15. Temperature History at T-Ampoule Seal Height for the 52-Minute Fire Model Verification Exercise ($^{\circ}\text{C}=[^{\circ}\text{F}-32]/1.8$). Note: In the schematic above the plot, the reference yellow line crosses the cask at the T-Ampoule-seal height and the white dots are the approximate locations of the temperature history lines in the plot. The “T-Ampoule (Seal)” curve is completely covered by the “TB-1” curve.

Table 3-10. Boundary Conditions Used for the HAC Thermal Evaluation

Boundary Condition	Application Region	Value Used During 30-minute Fire	Value Used After Fire (Cool-down)
Environment Temperature	External node representing environment	1010°C (1850°F)	54°C (130°F)
Convection	Entire outer surface of the package	11.5 W/m ² -K (2.03 Btu/hr-ft ² -°F)	3.5 W/m ² -K (0.62 Btu/hr-ft ² -°F)
Radiation	Entire outer surface of the package	Package surface emissivity of 0.8, Fire emissivity of 1	Package surface emissivity of 0.2,* Environment emissivity of 1
Internal Heat Flux (Decay Heat)	Small region described in Section 3.1.2 of this addendum	16,680 W/m ² (5287.5 Btu/hr-ft ²)	16,680 W/m ² (5287.5 Btu/hr-ft ²)

* From Table 3.2 in the SAR¹

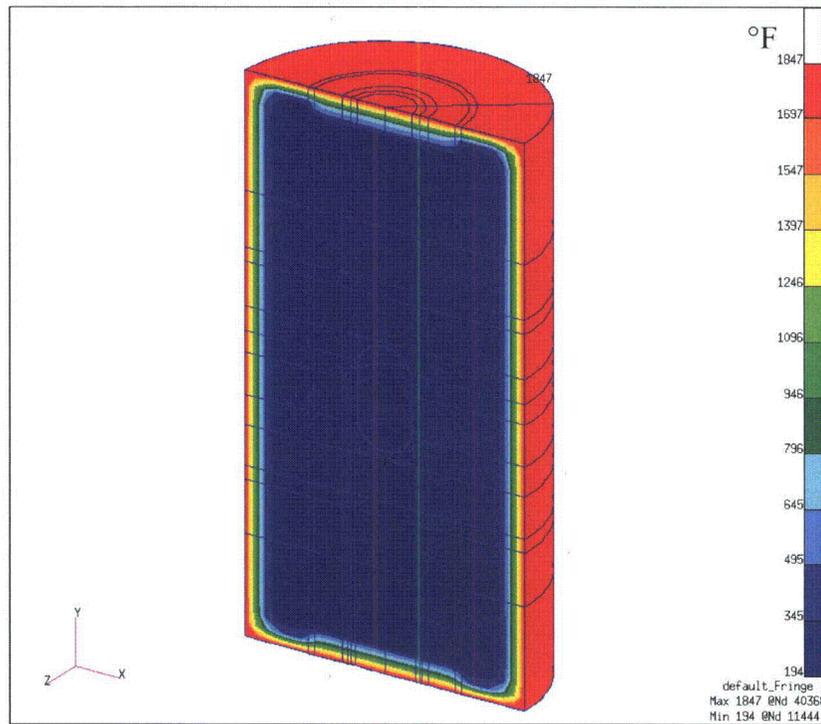


Figure 3-16. Temperature Distribution at the End of the 30-Minute Regulatory Fire — Complete Model (°C=[°F-32]/1.8)

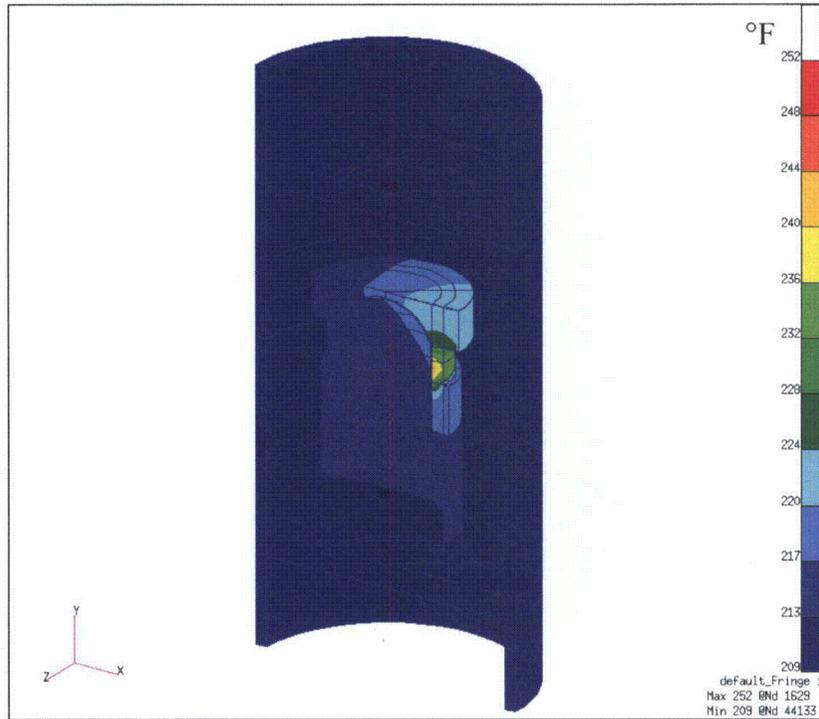


Figure 3-17. Temperature Distribution at the End of the 30-Minute Regulatory Fire — T-Ampoule, TB-1, Heat Transfer Cu Cylinder, and Aluminum Load Spreader ($^{\circ}\text{C}=[^{\circ}\text{F}-32]/1.8$)

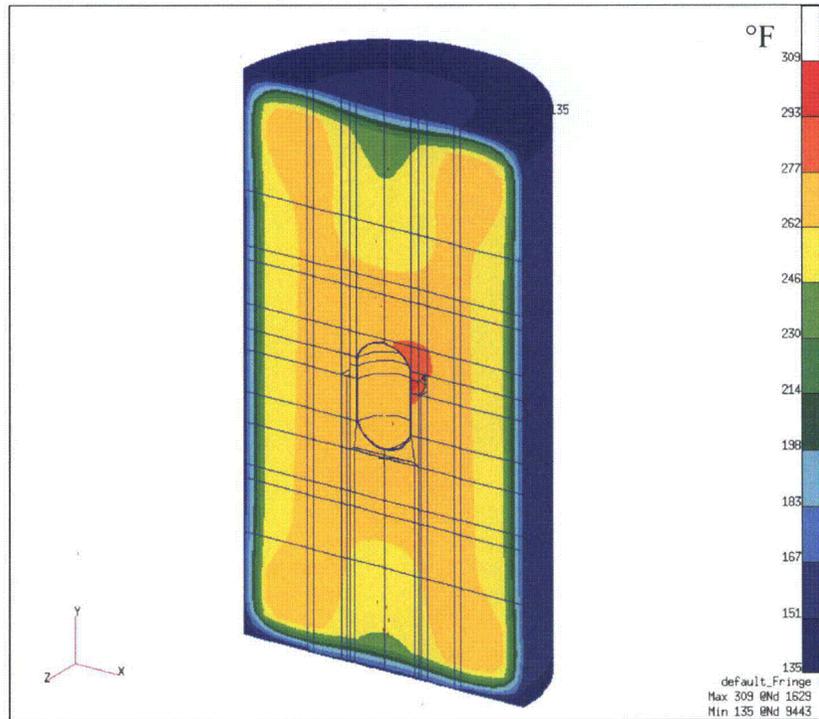


Figure 3-18. Temperature Distribution at t=290 Minutes (260 Minutes after the 30-Minute Fire) — Complete Model ($^{\circ}\text{C}=[^{\circ}\text{F}-32]/1.8$)

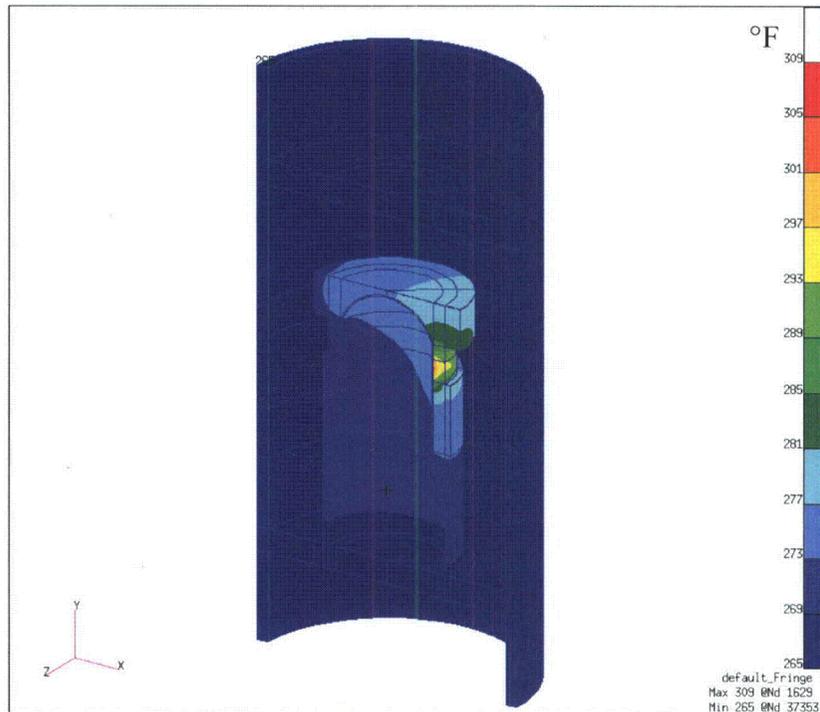


Figure 3-19. Temperature Distribution at t=290 Minutes (260 Minutes after the 30-Minute Fire) — T-Ampoule, TB-1, Heat Transfer Cu Cylinder, and Aluminum Load Spreader ($^{\circ}\text{C}=[^{\circ}\text{F}-32]/1.8$)

3.4.3 Maximum Temperatures and Pressure

Results from the hypothetical accident conditions evaluation of the AQ-1, TB-1, and the T-Ampoule, assuming the bounding concentrated internal heat described in Section 3.1.2 of this addendum and using the conservative transient computer model described in Section 3.4 of this addendum, are summarized in Table 3-11 of this addendum.

The components listed in this table did not reach temperatures of concern. Only the redwood regions closer to the outer skin of the package are expected to degrade ~~as wood chars at temperatures above 288°C (550°F)~~ (see Section 3.2.1 of the Addendum). Nevertheless, PAT-1 protects the package contents during and after the exposure to a severe fire environment, as required by 10 CFR 71.73.

The HAC evaluation indicated a peak T-Ampoule seal temperature of 153°C (308°F) and a peak TB-1 (and seal) temperature of 147°C (296°F). This TB-1 seal temperature is 38°C (69°F) higher than that reported as the TB-1 temperature in Section 3.5.1.1 of the PAT-1 SAR¹ and is, once again, considered to be overestimated (or conservative) due to the concentrated heat loading assumption. Nevertheless, this temperature does not exceed ~~the manufacturer's specification for the elastomeric seal operating range in the TB-1 (-40°C to 204°C [40°F to 400°F])~~ or the limit temperature of the copper seal ~~limit temperature~~. Therefore, the TB-1 is able to maintain containment. In addition, the T-Ampoule is also able to maintain a seal for product quality.

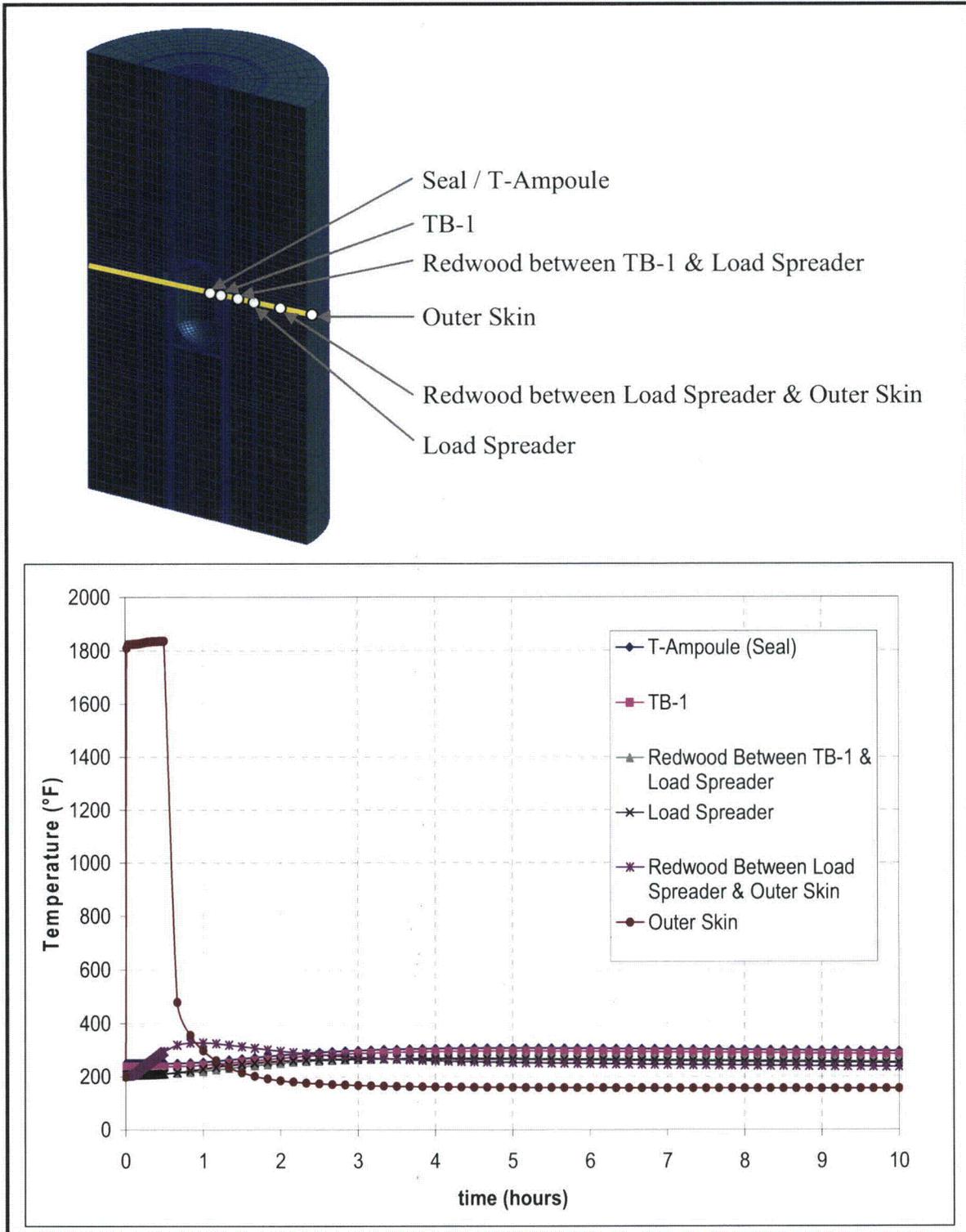


Figure 3-20. Temperature History at T-Ampoule Seal Height for the 30-Minute Regulatory Fire ($^{\circ}\text{C}=[^{\circ}\text{F}-32]/1.8$). Note: In the schematic above the plot, the reference yellow line crosses the cask at T-Ampoule-seal height and the white dots are the approximate locations of the temperature history lines in the plot.

Table 3-11. Summary of Maximum Temperatures and Times for the HAC

Component	HAC Maximum Temperature and Time to Reach Temperature
T-Ampoule (Seal)	153°C (308°F) @ 260 minutes after the fire
TB-1 (and TB-1 seal)*	147°C (296°F) @ 260 minutes after the 30-minute fire
Center of Redwood between TB-1 and Load Spreader	132°C (270°F) @ 240 minutes after the 30-minute fire
Aluminum Load Spreader	131°C (267°F) @ 190 minutes after the 30-minute fire
Center of Redwood between Load Spreader and Outer Skin	164°C (328°F) @ 30 minutes after the 30-minute fire
Stainless Steel Outer Drum	1003°C (1837°F) @ end of fire

*Maximum seal temperature was conservatively taken as the TB-1 maximum temperature.

The average T-Ampoule internal surface temperature was 136°C (276°F). Assuming the gas inside the TB-1 is at this average temperature, the maximum internal pressure that the TB-1 could experience under HAC can be estimated. When calculating this pressure, it was also assumed that the TB-1 was initially loaded at a room temperature of 21°C (70°F) and in a pressure environment of 1 atmosphere. Additionally, pressure generation due to alpha decay as calculated in Section 4 of this addendum was included in the total pressure calculation. Thus:

$$\begin{aligned}
 P_{TB-1@276^{\circ}\text{F-gauge}} &= (P_{\text{initial}} + P_{\text{alpha_decay}}) * (T_2/T_1) - 1\text{atm} = [1.801\text{ atm} * (736^{\circ}\text{R}/530^{\circ}\text{R}) - 1\text{atm}] \\
 &= (1\text{ atm} + 0.005\text{ atm}) * (736^{\circ}\text{R}/530^{\circ}\text{R}) - 1\text{atm} \\
 &= 1.504\text{ atm or } \sim 15240\text{ kPa (22.15.8psig)} \quad (3-10)
 \end{aligned}$$

In summary, these results show that the PAT-1 provides containment for the proposed new payload inside the TB-1 and adequately contains the material inside the T-Ampoule, as maximum seal temperatures are within ~~manufacturer's specifications~~ the service temperature range specified in Table 3-5 and the TB-1 can withstand the pressure that would arise during and after the HAC fire event. Additionally, the eutectic prevention barrier is retained because the T-Ampoule is constructed of titanium 6Al-4V alloy and can withstand the temperatures and pressures observed under the 10 CFR 71² HAC, as documented in Section 2 of this addendum.

3.4.4 Maximum Thermal Stresses

The maximum thermal stresses are determined from results of the differential thermal expansion analysis conducted and documented in Section 2.7.4.2 of this addendum. Since the American Society of Mechanical Engineers (ASME) Boiler and Pressure Vessel (B&PV) code does not provide the coefficient of thermal expansion (α) for Ti-6Al-4V, the value listed in the MIL-HDBK-5E¹⁴ (9.18×10^{-6} m/m/°C [5.1×10^{-6} in/in/°F]) was used in this analysis.

A conservative estimate of the T-Ampoule maximum expansion can be calculated by assuming the T-Ampoule is a 0.2 m (7.418 in.) long cylinder (the actual T-Ampoule is capped) with a diameter of 0.11 m (4.22 in). Assuming a temperature increase of (153°C – 21.1°C) = 132°C

([308°F – 70°F] = 238°F), the expansion produced equals $\alpha\Delta TL$, or 0.23 mm (0.009 in.) in the longitudinal direction and 0.41 mm (0.0161 in.) in circumference (or 0.13 mm [0.0051 in.] in

diameter). Since the gap between the T-Ampoule and the TB-1 is 0.381 mm (0.015 in.) around the entire perimeter, the T-Ampoule will not expand enough to induce any stress on the TB-1, even if thermal expansion of the TB-1 is ignored.

3.4.5 Hypothetical Accident Conditions for Fissile Material Packages for Air Transport

Thermal tests that meet the specifications in 10 CFR 71.64² were conducted on the PAT-1 and are documented in Chapter 3 of the SAR¹. Physical tests were the primary means used to demonstrate that the PAT-1 package met the requirements of the NRC Qualification Criteria (10 CFR 71.74²). The purpose of the assessment documented in Section 3.6 of the SAR¹ was to demonstrate that the maximum TB-1 temperature (reported in Section 3.6.3 of the SAR¹) used in Section 4.4.2 of the SAR¹ was a reasonable upper limit for bounding the results.

The package temperatures cited in Section 3.6.3 of the SAR¹ stated the following: “Based on the analysis and test results in Sections 3.6.1.1 and 3.6.1.2, the TB-1 is estimated to have attained a maximum temperature of approximately 582°C (1080°F) during the thermal test specified in the NRC Qualification Criteria.” This maximum temperature is not affected by any of the packing or content modifications presented in this addendum. That is, the maximum internal heat generation of the content remains the same (25 watts [85.3 Btu/hr]) and the design of the TB-1 and the rest of the packaging outward of the TB-1 is the same as evaluated in the SAR.¹ Therefore, the maximum temperature of the TB-1 used for this addendum, for the calculation of loads due to internal pressure and thermal expansion during the plutonium aircraft fire environment is 582°C (1080°F).

At the maximum temperature of the TB-1 after the plutonium aircraft accident fire, there is a potential for plutonium metal to form eutectics with certain metals such as iron in the TB-1. The materials that were selected for the components within the TB-1 were based on the resistance to eutectic formation with plutonium. The melting temperatures for different material combinations are presented in Section 3.5.3 of this addendum. Given that the melting point of the plutonium-iron eutectic is lower than the maximum TB-1 temperature in the plutonium air transport thermal evaluation, the titanium T-Ampoule is used as a barrier between the plutonium metal and the PH13-8Mo material in the TB-1. The structural analysis documented in Section 2 of this addendum demonstrates that the T-Ampoule wall will not be breached as a result of NCT, HAC, or the accident conditions for air transport of plutonium. Thus, the formation of a Pu-Fe eutectic as a result of the thermal conditions resulting from a 10 CFR 71.74 specified fire is not possible because of the separation between the Pu content and the Fe in the TB-1 provided by the T-Ampoule wall. The service temperatures of all components (T-Ampoule and its packing within the TB-1) shown in Table 3-5 in this addendum, which were derived in part from the eutectic evaluation in Section 3.5.3 in this addendum, are all above 582°C (1080°F).

In addition to the Pu-Fe eutectic potential discussed above, a plutonium-beryllium eutectic may also form. The melting point of this Pu-Be eutectic is 595°C (1103°F) (see Section 3.5.3 in this addendum). This is 13°C (23°F) higher than the highest temperature excursion that occurs in the system.

The maximum internal pressure that may occur within the TB-1 during the air transport thermal evaluation is estimated to be ~~6.547~~ 4.14 MPa (~~949.5~~ 600 psig) (see Section 4 of this addendum). This was

calculated adding the pressure generated from the decomposition of the O-rings in the SC-1 configuration, which includes the elastomeric seal of the ~~TB-1~~, T-Ampoule, and three SC-1s (highest amount of elastomeric material), which yielded a pressure of ~~887.3~~ 302 psi (from Section ~~4.5.4~~ 2.12.8 of this addendum), the pressure generated from the decomposition of the ancillary plastic (270 psi from Table 6a in Section 2.12.8), the pressure generated due to the change in temperature of the initial fill gas [~~($\frac{1540^{\circ}\text{R}}{530^{\circ}\text{R}}$)~~*14.7 psi – 14.7 psi = ~~42.7~~ 28.01 psi], and the pressure from gas generation from alpha decay of plutonium [~~($\frac{1540^{\circ}\text{R}}{530^{\circ}\text{R}}$)~~*11.78 psi = 34.2 psi, based on the largest plutonium content of 1300 grams in Section 4.5.3, Table 3-5 of this addendum for conservatism and corrected for the temperature change][0.110 psi (from Table 6a in 2.12.8)]. This maximum pressure of ~~6.547~~ 4.14 MPa (~~949.5~~ 600 psig) is lower than the maximum TB-1 pressure stipulated in the PAT-1 SAR¹ (1095.3 psig, see Section 4.4.2 of this addendum). Therefore, the TB-1 is capable of sustaining this maximum pressure observed during the plutonium air transport fire accident condition without rupturing. Note that the T-Ampoule will not retain any pressure because its elastomeric O-ring can extrude out of the O-ring groove and no longer maintain a seal at temperatures above its service temperature of 204°C (400°F).

The thermal expansion calculation in Section 2.8.6 of this addendum demonstrates that no stresses will be induced in the TB-1 by differential thermal expansion resulting from the air transport fire accident.

The analysis in this section demonstrates that the replacement of the PC-1 inner container (with its packing and contents) with the T-Ampoule inner container (with its packing and contents) does not alter the thermal performance of the PAT-1. Therefore, the discussion in Section 3.6 of the SAR¹ regarding the ability of the package to meet the requirements in the plutonium air transport regulations due to thermal loads remains valid. That is, the performance of the PAT-1 with the T-Ampoule (with its packing and contents) inside the TB-1 is bounded by the tests presented in the SAR¹ and therefore the TB-1 maintains containment.

3.5 Appendix

3.5.1 References

1. United States. Nuclear Regulatory Commission. NUREG-0361. "Safety Analysis Report for the Plutonium Air Transportable Package, Model PAT-1." Washington, D.C. 1978.
2. United States. Nuclear Regulatory Commission. Code of Federal Regulations, 10 CFR 64, 71, 73, and 74. January 1, 2009.
3. White, R.H., and E.L. Schaffer. "Application of CMA Program to Wood Charring," *Fire Technology*. Volume 14, Number 4 (1978): 279-290.
4. MSC Patran Thermal 2005 r2. MSC Software Corporation. <www.mssoftware.com>
5. Touloukian, Y.S., "Thermophysical Properties of High-Temperature Solid Materials." (1967).
6. Schorsch, R.H., "Engineering Properties of Selected Materials." (1966).
7. Hodge, A.W. and D.J. Maykuth. "Properties of New High-Temperature Titanium Alloys," DMIC Memo 230, Defense Metals Information Center, Battelle Memorial Institute, Columbus Ohio. February 1968.
8. Boivineau, M., C. Cagran, D. Doytier, V. Eyraud, M.-H. Nadal, B. Wilthan, and G. Pottlacher, "Thermophysical Properties of Solid and Liquid Ti-6Al-4V (TA6V) Alloy," *International Journal of Thermophysics*, Vol. 27, No. 2, March 2006.
9. Mason, R.E. and S.P. Willson, "Eutectic Analysis of Ti-6Al-4V with Plutonium and Copper," LA-UR-08-07663. Los Alamos National Laboratory. Los Alamos, NM. 2008. (Presented in Appendix 3.5.3).
10. Shapiro, A.B. and A.L. Edwards. "TOPAZ2D Heat Transfer Code Users Manual and Property Data Base," UCRL-ID--104558. Lawrence Livermore National Laboratory. Livermore, CA. 1990.
11. Incropera, F.P. and D.P. DeWitt. "Fundamentals of Heat and Mass Transfer, 4th ed.," New Jersey: Wiley & Sons, Inc., 1996.
12. Churchill, S.W. and J. M. Bernstein. *Heat Transfer*. 99, 300. (1977).
13. Nakos, J.T., "Uncertainty Analysis of Steady-State Incident Heat Flux Measurements in Hydrocarbon Fuel Fires," SAND2005-7144. Sandia National Laboratories. Albuquerque, NM. December 2004.
14. Department of Defense. *Military Standardization Handbook: Metallic Materials and Elements for Aerospace Vehicle Structures*. MIL-HDBK-5E: May 1988.

3.5.2 Viton® ~~Parker~~ O-Ring ~~Data Sheet~~ Technical Information



Compound Data Sheet
Parker O-Ring Division United States

MATERIAL REPORT

REPORT NUMBER: KJ0835
DATE: 10/10/89

TITLE: Evaluation of Parker Compound V0835-75 to MIL-R-83485
Type 1 Specifications
PURPOSE: To determine if V0835-75 meets the requirements.
CONCLUSION: Compound V0835-75 meets the specification requirements.

Recommended temperature limits: -40°F to 400°F

Recommended For

Low temperature
Petroleum, mineral, and vegetable oils
Silicone fluids
Aromatic hydrocarbons (benzene, toluene)
Chlorinated hydrocarbons
High vacuum
Ozone, weather, and aging resistance

Not Recommended For

Hot water and steam
Auto and aircraft brake fluids
Amines
Ketones
Low molecular weight esters and ethers

Parker O-Ring Division
2360 Palumbo Drive
Lexington, Kentucky 40509
(859) 269-2351



Compound Data Sheet
 Parker O-Ring Division United States

REPORT DATA

Report Number. **KJ0835**

<u>ORIGINAL</u>	<u>MIL-R-83485 TYPE 1, O-RINGS & COMPRESSION SEALS</u>	<u>V0835-75 ACTUAL VALUES</u>
Specific Gravity	As determined	1.75
Hardness points	75 ± 5	78
Tensile Strength, psi min.	1600	1708
Elongation, % min.	120	180
Temperature Retraction, 10% (TR-10), °F, max	-20	-22
<u>AFTER AIR AGING, 70 HRS @ 75° ± 5°F. Compression Set</u>		
% of original deflection, max.	25	- (14)
<u>AFTER AGING, 70 HRS. @ 75°F IN TT-S-735, TYPE III</u>		
Hardness Change, pts.	+5	77 (-1)
Tensile Strength decrease, %, max.	30	1662 (-3)
Elongation decrease, %, max.	20	165 (-8)
Volume change, %, max.	1 to 10	- (+2)
<u>AFTER AIR AGING, 70 HRS. @ 528° ± 5°F</u>		
Hardness change, pts.	+5	78 (0)
Tensile Strength decrease, % max	35	1136 (-33)
Elongation decrease, %, max.	10	235 (+31)
Weight loss, %, max.	12	- (-7)
<u>AFTER AIR AGING, 168 HRS @ 347° ± 5°F. COMPRESSION SET</u>		
% of original deflection, max.	25	- (15)
18 hrs. cooling		- (24)
<u>AFTER AIR AGING, 22 HRS @ 392° ± 5°F. COMPRESSION SET</u>		
% of original deflection, max.	20	- (11)

Parker O-Ring Division
 2360 Palumbo Drive
 Lexington, Kentucky 40509
 (859) 269-2351



Compound Data Sheet
Parker O-Ring Division United States

AFTER AGING, 70 HRS. @ 347° MIL-R-83485 ±5°F in AMS-3021	MIL-R-83485 TYPE 1, O-RINGS \$\$ COMPRESSION SEALS	V0835-75 ACTUAL VALUES
Hardness change, pts	+0, -15	73
Tensile Strength decrease, \$\$, max.	35	1406 (-18)
Elongation decrease, \$\$, max.	20	171 (-5)
Volume change, \$\$	1 to 20	- (+15)
Compression set, \$\$ of original deflection, max. 18 hr. cooling	10	- 7 - 9

Parker O-Ring Division
2360 Palumbo Drive
Lexington, Kentucky 40509
(859) 269-2351

Technical Information

.....
Rev. 6, November 2005



Viton[®]

fluoroelastomer

From DuPont Performance Elastomers

Selection Guide

Introduction

Viton[®] fluoroelastomer was introduced in 1957 to meet the needs of the aerospace industry for a high-performance seal elastomer. Since then, the use of Viton[®] fluoroelastomer has expanded to many other industries, especially in the automotive, fluid power, appliance, and chemical fields. With over 40 years of proven performance, Viton[®] fluoroelastomer has developed a reputation for outstanding performance in high temperature and extremely corrosive environments.

Valuable Properties of Viton[®] Fluoroelastomer

Vulcanizates based on Viton[®] provide an exceptional balance of physical property characteristics, including the following features:

- Resistance to temperature extremes.

Heat—Compared to most other elastomers, Viton[®] is better able to withstand high temperature, while simultaneously retaining its good mechanical properties. Oil and chemical resistance are also essentially unaffected by elevated temperatures. Compounds of Viton[®] remain substantially elastic substantially indefinitely when exposed to laboratory air oven aging up to 204°C or to intermittent exposures up to 316°C. High temperature service limits are generally considered to be:

3,000 hr at 232°C
1,000 hr at 260°C
240 hr at 288°C
48 hr at 316°C

Cold—Viton[®] is generally serviceable in dynamic applications to temperatures of -18 to -23°C. Special formulations permit its use in static applications down to -54°C. Also, Viton[®] has proven to be satisfactory for static seals used under conditions approaching absolute zero. Viton[®] is characterized by its:

- Resistance to degradation by a greater variety of fluids and chemicals than any nonfluorinated elastomer. Excellent resistance to oils, fuels, lubricants, and most mineral acids.
- Extremely low permeability to a broad range of substances, including particularly good performance in oxygenated automotive fuels.
- Resistance to aliphatic, aromatic hydrocarbons that dissolve other rubbers.
- Exceptionally good resistance to compression set, even at high temperatures.
- Exceptionally good resistance to atmospheric oxidation, sun, and weather. Excellent resistance to fungus and mold.
- Good electrical properties in low voltage, low frequency applications.
- Low burning characteristics; inherently more resistant to burning than other, non-fluorinated hydrocarbon rubbers.

Safety and Handling

As with many polymers, minute quantities of potentially irritating or harmful gases may diffuse from uncured Viton® even at room temperature. Therefore, all containers should be opened and used only in well-ventilated areas. In case of eye contact, immediately flush the eyes for at least 15 min with water. Always wash contacted skin with soap and water after handling Viton®.

Potential hazards, including the evolution of toxic vapors, may arise during compounding, processing, and curing of the raw polymers into finished products or under high-temperature service conditions. Therefore, before handling or processing Viton®, make sure that you read and follow the recommendations in the DuPont Performance Elastomers bulletin "Handling Precautions for Viton® and Related Chemicals."

Compounding ingredients and solvents that are used with Viton® to prepare finished products may present hazards in handling and use. Before proceeding with any compounding or processing work, consult and follow label directions and handling precautions from suppliers of all ingredients.

The Various Families and Types of Viton® Fluoroelastomer

Standard types of Viton® fluoroelastomer products are designated as A, B, or F according to their relative resistance to attack by fluids and chemicals. The differences in fluid resistance are the result of different levels of fluorine in the polymer, which is determined by the types and relative amounts of copolymerized monomers that comprise the polymer.

In general, Viton® exhibits outstanding resistance to attack from a wide variety of fluids, including mineral acids and aliphatic and aromatic hydrocarbons. The higher the fluorine content of the polymer, the less will be the effect, as measured by volume increase, for example. The most significant differences between A, B and F types of Viton®, in terms of resistance to volume change or retention of physical properties, are exhibited in low molecular weight, oxygenated solvents (such as methanol and methyl t-butyl ether).

As mentioned above, the fluid resistance of Viton® A, B, and F types improves with increasing fluorine levels. This is shown in Table 1 (note the volume increase after aging in methanol at 23°C). As the fluorine content increases, however, the low temperature flexibility of the polymer decreases, and a compromise must be made between fluid resistance and low temperature flexibility of the final vulcanizate.

For those applications that require the best performance in both fluid resistance and low temperature flexibility a number of specialty types of Viton® were developed that contain a copolymerized fluorinated vinyl ether monomer. Polymers that contain this monomer exhibit significantly improved low temperature flexibility, compared to standard types of fluoroelastomer.

Viton® GLT introduced in 1976, was the first commercial fluoroelastomer to incorporate this fluorinated vinyl ether monomer. This polymer provides the same excellent resistance to heat and fluids that is typical of the A types of Viton® fluoroelastomer. Viton® GFLT, like Viton® GLT, exhibits significantly improved low temperature flex characteristics compared to standard types of fluoroelastomer. In addition, Viton® GFLT provides the same superior resistance to fluids that is typical of the F types of Viton® fluoroelastomer.

Types of Viton® Extreme™

Fluoroelastomers that contain copolymerized vinylidene fluoride (VF2) are subject to attack by high pH materials, including caustics and amines. In addition, standard fluoroelastomers are not resistant to low molecular weight carbonyl compounds, such as methyl ethyl ketone, acetone, or methyl tertiarybutyl ether.

Viton® Extreme™ ETP-600S is a copolymer of ethylene, tetrafluoroethylene (TFE), and perfluoromethylvinyl ether (PMVE). This unique combination of monomers provides outstanding resistance to fluids and is an example of an ETP polymer. The ETP types of Viton® exhibit the same excellent resistance to acids and hydrocarbons typical of A, B and F types of Viton®. Unlike conventional fluoroelastomers, however, ETP types of Viton® also provide excellent resistance to low molecular weight esters, ketones, and aldehydes. In addition, these unique polymers are inherently resistant to attack by base, and thus provide excellent resistance to volume swell and property loss in highly caustic solutions and amines.

Additional information regarding performance differences between the various families and types of Viton® fluoroelastomer is presented in Tables 3-6 to assist in selecting the particular grade of

3

Viton® that is best suited for both a given end-use application and for a specific manufacturing process

Table 1
Polymer Fluorine Content versus Fluid Resistance and Low Temperature Flexibility

	Standard Types			Specialty Types		
	A	B	F	GLT-S	GFLT-S	ETP-S
Nominal Polymer Fluorine Content, wt%	66	68	70	64	67	67
Percent Volume Change in Fuel C, 168 hr at 23°C*	4	3	2	5	2	4
Percent Volume Change in Methylcel, 168 hr at 23°C*	90	40	5	90	5	5
Percent Volume Change in Methyl ethyl Ketone, 168 hr at 23°C*	>200	>200	>200	>200	>200	19
Percent Volume Change in 30% Potassium Hydroxide, 168 hr at 70°C*	(Samples too swollen and degraded to test)					14
Low Temperature Flexibility, TR-10, °C*	-17	-13	-6	-30	-24	-12

*Nominal values, based on results typical of those obtained from testing a standard, 30 phr MT (N620) carbon black-filled, 76 durometer vulcanizate. These are not intended to serve as specifications.

Curing Systems for Viton® Fluoroelastomer

In addition to inherent differences between the various types and families of Viton® fluoroelastomer, a number of compounding variables have major effects on the physical property characteristics of the final vulcanizates. One very important variable is the crosslinking or curing system that is used to vulcanize the elastomer.

Diamine curatives were introduced in 1957 for crosslinking Viton® A. While these diamine curatives are relatively slow curing, and do not provide the best possible resistance to compression set, they do offer unique advantages. For example, compounds cured with diamines exhibit excellent adhesion to metal inserts and high hot tensile strength.

Most fluoroelastomers are crosslinked with Bisphenol AF, a curative introduced in 1970, in the first commercial curative-containing precompound, Viton® E-60C. Compounds of Viton® that use this curative exhibit fast rates of cure and excellent scorch safety and resistance to compression set. In 1987, an improved bisphenol curative was introduced, which was made available in several different precompounds. The modified system provides faster cure rates, improved mold release, and slightly better resistance to compression set, compared to the original bisphenol cure system used in Viton® E-60C and E-430. Additional precompounds of Viton®, incorporating this modified curative, were introduced in 1993, including Viton® A-331C, A-361C, B-601C, and B-651C. A brief description of all these products can be found in Table 6.

In 1976, efficient peroxide curing of fluoroelastomers was made possible for the first time with the introduction of Viton® GLT. The peroxide cure system provides fast cure rates and excellent physical properties in polymers such as GLT and GFLT which cannot be readily cured with either diamine or bisphenol crosslinking systems. In the case of polymers such as Viton® GF, GBL-200, and GBL-900, the peroxide cure provides enhanced resistance to aggressive automotive lubricating oils and steam and acids. Generally, vulcanizates of Viton® fluoroelastomers cured with peroxide do not show any significant difference in resistance to other fluids and chemicals compared to the same polymer cured with bisphenol.

In 2003, a series of peroxide-cure types of Viton® made with Advanced Polymer Architecture was introduced. These polymers, designated as APA polymers by having an "S" suffix on the product name, incorporate a significantly improved cure site. As a result, they provide substantially better processing and physical properties, compared to the original, non-APA peroxide-cure types of Viton®. A comparison of the various processing and physical property characteristics of compounds using the various cure systems is shown in Table 2.

Table 2
A Comparison of Cure Systems Used in Crosslinking Viton®

Property, Processing Characteristic	Type of Cure System		
	Diamine	Bisphenol	Peroxide*
Processing Safety (Scorch)	P-F	E	E
Fast Cure Rate	P-F	E	E
Mold Release/Mold Fouling	P	G-E	G-E
Adhesion to Metal Inserts	E	G	G
Compression Set Resistance	P	E	E
Steam, Water, Acid Resistance	F	G	E
Flex Fatigue Resistance	G	G	G

Rating: E=Excellent G=Good F=Fair P=Poor

*Luperox 101-XL (trademark of Permutit Corporation) and Verac Powder (trademark of R.T. Vanderbilt Co., Inc.) are commonly used.

Selecting a Specific Type of Viton® Fluoroelastomer
Inherent Physical Property Differences Between Types/Families of Viton® Products

The physical properties of vulcanizates based on Viton® fluoroelastomers are determined to a large extent by the type and amount of the filler(s) and curative(s) used in the formulation, and by the temperature and duration of the curing cycle used in their manufacture.

In terms of resistance to compression set, low temperature flexibility, and resistance to certain classes of fluids, however, some inherent differences exist among the various families of Viton® fluoroelastomers. These are the result of differences in the relative amount and type of monomers used in the manufacture of the various types of Viton® fluoroelastomers.

The differences in physical property characteristics which exist between various types and families of Viton® fluoroelastomer products are outlined in general terms in Table 3.

As an example, resistance to compression set is an important property for seals and if this property were considered to be the most important feature for a particular part, then one of the A-types of Viton® might be the best choice for the application. However, if resistance to the widest possible range of fluids is a more important consideration than an F-type Viton® fluoroelastomer might well be a better choice for that particular end-use application. Further, if both fluid resistance and low temperature flexibility are equally important requirements for maximizing the end-use suitability of a given part GFLT-types of Viton® would represent the best overall choice.

Table 3
Physical Property Differences Between Types/Families of Viton® Products

Type of Viton® Fluoroelastomer	Resistance to Compression Set	General Fluids/Chemical Resistance*	Low Temperature Flexibility**
A	1	3	3
B, GBL-S	2	3	3
F, GF-S	3	2	3
GLT-S	2	3	1
GFLT-S	2	2	2
ETP-S	3	1	3

1=Excellent—Best performance capability of all types; 2=Very Good; 3=Good—Sufficient for all typical fluoroelastomer applications

*See Table 4 for a detailed guide to choosing the best type of Viton® fluoroelastomer, relative to specific classes of fluids and chemicals

**Flexibility, as measured by Temperature of Retraction (TR-10), Gehman Torsional Modulus, Glass Transition (Tg), or Clash-Berg Temperature

Crack-Point tests are a measure of impact resistance only and do not correlate at all with the low temperature sealing capability of a vulcanizate

**Selecting a Specific Type of Viton® Fluoroelastomer
Differences in Fluid Resistance Between Types of Viton® Products**

As in the case of physical properties, different polymer compositions will result in inherent differences with regard to fluid resistance.

Table 4 outlines the differences that exist between types of Viton® products, in terms of their resistance to various classes of fluids and chemicals.

Because as certain types of Viton® products may exhibit performance that is superior to other types in one regard, but not quite as good in some other aspect, it is important to consider the requirements of the part to be manufactured, in terms of both physical property requirements and fluid or chemical resistance needs.

Using Tables 3 and 4, the compounder can select the best type of Viton® product for a given end-use application, based on the best combination of physical property and fluid resistance characteristics.

**Table 4
Differences in Fluid Resistance Between Types of Viton® Fluoroelastomer**

	Type of Viton® Fluoroelastomer							
	A	B	F	GBL-S	GF-S	GLT-S	GFLT-S	ETP-S
	Cure System							
	Bisphenol			Peroxide				
Hydrocarbon Automotive, Aviation Fuels	1	1	1	1	1	1	1	1
Oxygenated Automotive Fuels (containing MeOH, EtOH, MTBE, etc.)	NR	2	1	2	1	NR	1	1
Reciprocating Engine Lubricating Oils (SE-SF Grades)	2	1	1	1	1	1	1	1
Reciprocating Engine Lubricating Oils (SG-SH Grades)	3	2	2	1	1	1	1	1
Aliphatic Hydrocarbon Process Fluids, Chemicals	1	1	1	1	1	2	1	1
Aromatic Hydrocarbon Process Fluids, Chemicals	2	2	1	1	1	2	1	1
Aqueous Fluids: Water, Steam, Mineral Acids (H ₂ SO ₄ , HNO ₃ , HCl, etc.)	3	2	2	1	1	1	1	1
Amines, High pH Caustics (KOH, NaOH, etc.)	NR	NR	NR	3	3	3	3	1
Low Molecular Weight Carbonyls (MTBE, MEK, MIBK, etc.)	NR	NR	NR	NR	NR	NR	NR	1

1=Excellent—Best choice of Viton® type(s) for service in this class of fluid/chemical; minimal volume increase, change in physical properties.
 2=Very Good—Good serviceability in this class of fluid/chemical; small amounts of volume increase and/or changes in physical properties.
 3=Good—Suitable for use in this class of fluid/chemical; acceptable amounts of volume increase and/or changes in physical properties.
 NR=Not Recommended—Excessive volume increase or change in physical properties.

Choosing a Viton® Product for Use in a Particular Type of Manufacturing Process

The Viton® product line includes a wide variety of different types of fluoroelastomer products, which exhibit some inherent differences in their end-use capabilities (see Tables 3 and 4). In addition, a broad range of viscosities is offered for most types of Viton®, providing a wide degree of utility in various manufacturing processes.

Having selected a given class of Viton® products for an end use, the compounder must then choose which particular Viton® product is best suited for use in a specific manufacturing process.

The Viton® - Application Guide (Table 5) lists the Viton® products that are recommended for particular end-use applications, according to the various processes that are most commonly used in their manufacture.

The Viton® - Product Listing (Table 6) provides more specific information about the various individual Viton® products. Contact your DuPont Performance Elastomers sales or technical representative to obtain more detailed information or data on specific Viton® products.

How to Use the Viton® Application Guide

The Viton® - Application Guide (Table 5) has been designed to facilitate choice of the type of Viton® that is best suited for meeting both the property requirements of the intended end use and the needs of the production method used to manufacture the finished product.

The guide is divided into five general categories (columns) of end-use products, differentiated primarily by physical form:

- Sheet form goods, such as gaskets, diaphragms, etc.
- Simple shapes, such as O-rings, V-rings, etc., which do not typically require high levels of demolding tear resistance, but which generally require high states of cure to obtain the best compression set possible.
- Complicated molded shapes, such as shaft seals or valve stem seals, which require good hot tear upon demolding due to the undercuts in the molds used to form such parts and good adhesion to metal inserts (obtained during the vulcanization of the parts).
- Complicated molded shapes that do not involve adhesion to metal inserts during vulcanization, but which require good resistance to tear during demolding. Carburetor roll-over cages, boots, and reed valves are examples of such parts.
- Extruded shapes, such as rod, tubing, or hose constructions.

Each general end-use category listed is divided into four columns, each listing Viton® products within a specific family or type of Viton® fluoroelastomer—A, B, F, and specialty types.

The guide is further divided into the five major types of process (rows) by which these general end-use categories might be produced:

- Compression molding
- Transfer molding
- Injection molding
- Extrusion
- Calendering

Within the blocks formed by the "intersection" of a given end-use category (column) and the process type by which the end products will be manufactured (row), we have listed the types of Viton® that we believe are appropriate choices for meeting the physical property requirements of the finished product and that are best suited for the chosen manufacturing process.

The Viton® products we believe will provide the best combination of end-use physical properties, together with the best processing characteristics for given methods of manufacture, are listed in bold type.

Additional details for specific types of Viton® can be found in the Viton® Product Listing and in product-specific data sheets.

**Table 5
Viton® Fluoroelastomer Application Guide**

Manufacturing Process	Reinforced/Unreinforced Sheet Stock (Gaskets, Diaphragms, etc.)				Molded (Non-Bonded), Simple Shapes (O-Rings, V-Rings, etc.)			
	Viton® Types							
	A	B	F	Specialty	A	B	F	Specialty
Compression Molding	A-331C A-361C A-401C A-601C A-500 A-700 AL-600	B-435C B-601C B-651C GBL-600S B-600	F-605C GF-600S	GLT-600S GBLT-600S GFLT-600S ETP-600S	A-401C A-331C A-601C A-500 A-700 AL-600	B-601C B-651C GBL-600S B-600	F-605C GF-600S	GLT-600S GBLT-600S GFLT-600S ETP-600S
Transfer Molding	A-201C A-331C A-361C A-401C A-200 AL-300	B-435C GBL-200S B-202	F-605C GF-200S	GLT-200S GBLT-200S GFLT-200S ETP-600S	A-201C A-331C A-361C A-200 AL-300	B-651C GBL-200S B-202	F-605C GF-200S	GLT-200S GBLT-200S GFLT-200S ETP-600S
Injection Molding	A-201C A-331C A-361C A-200 AL-300	B-435C GBL-200S B-202	GF-200S	GLT-200S GBLT-200S GFLT-200S	A-201C A-331C A-361C A-100 A-200 A-500 AL-300	B-601C B-651C GBL-200S B-202	F-605C GF-200S	GLT-200S GBLT-200S GFLT-200S ETP-600S
Calendering	A-201C A-401C A-331C A-361C AL-300	B-435C B-601C B-651C GBL-200S GBL-600S B-202 B-600	F-605C GF-200S GF-600S	GLT-200S GLT-600S GBLT-200S GBLT-600S GFLT-200S GFLT-600S ETP-600S				
	Molded (Bonded), Complicated Shapes (Valve Stem, Shaft Seals, etc.)				Molded (Non-Bonded), Complicated Shapes (Boots, Valves, etc.)			
Compression Molding	A-361C A-500 A-700 AHV AL-600	B-435C B-651C GBL-600S B-600	F-605C/GF-200S GF-200S GF-600S	GLT-200S GLT-600S GBLT-200S GBLT-600S GFLT-200S GFLT-600S ETP-600S	A-331C A-401C/A-500 A-601C/A-200 A-361C A-700 AHV AL-600	B-435C B-651C GBL-600S B-600	F-605C/GF-600S GF-600S	GLT-600S GBLT-600S GFLT-600S ETP-600S
Transfer Molding	A-361C A-200 A-500 AL-300	B-435C GBL-200S B-202	GF-200S	GLT-200S GBLT-200S GFLT-200S ETP-600S	A-200 A-331C A-361C A-200 A-500 AL-300	B-435C B-651C GBL-200S B-600	F-605C/GF-300 GF-300	GLT-200S GBLT-200S GFLT-200S ETP-600S
Injection Molding	A-361C A-100 A-200 A-500 AL-300	B-435C B-651C GBL-200S B-202	F-605C/GF-200S GF-200S	GLT-200S GBLT-200S GFLT-200S	A-200 A-331C A-361C A-200 A-500 AL-300	B-435C B-651C GBL-200S B-202	F-605C/GF-200S GF-200S	GLT-200S GBLT-200S GFLT-200S

Table 5
Viton® Fluoroelastomer Application Guide (cont'd.)

Manufacturing Process	Extruded Goods (Hose, Tubing, Extruded Profiles, etc.)			
	Viton® Types			
	A	B	F	Specialty
Extrusion	A-201C A-401C A-361C A-200 A-500 AL-300	B-435C B-651C GBL-200S B-202 B-600	F-605C GF-200S	GLT-200S GBLT-200S GFLT-200S ETP-600S

Table 6
Viton® Fluoroelastomer Product Listing

Viton® Product Type	Polymer Properties			Nominal Physical Properties*			Viton® Fluoroelastomer Product Description	Viton® Fluoroelastomer Product Suggested Uses/ Applications
	Nominal Viscosity, ML1 + 10 at 121°C	Specific Gravity	Polymer Fluorine Content, %	Compression Set, % 70 hr/200°C	Temperature of Retraction (TR-10) °C	Volume Increase, After 7 days/ MeOH/23°C		
A-Types: Curative-Containing Precompounds								
A-201C	20	1.81	66.0	15	-17	+75 to 105%	Fast cure rate, excellent injection molding rheology, mold release	FDA-compliant**; injection molding, O-rings, gaskets, extruded shapes
A-331C	30	1.81	66.0	20	-17	+75 to 105%	Excellent mold flow, high elongation/tear resistance	Compression— injection molding of complex shapes, requiring maximum hot tear
A-361C	30	1.81	66.0	20	-17	+75 to 105%	Excellent mold flow, tear resistance, bonding to metal inserts	Compression— injection molding of complex shapes, bonded metal inserts
A-401C	40	1.81	66.0	15	-17	+75 to 105%	Excellent rheology at high shear rates, excellent resistance to compression set	FDA-compliant**; compression, transfer, or injection molding of O-rings
A-601C	60	1.81	66.0	12	-17	+75 to 105%	High viscosity, high state of cure, optimum resistance to compression set	FDA-compliant**; compression molding of O-rings, simple shapes

*Nominal physical properties typical of those that can be expected of vulcanizates based on the specific type of Viton® noted, in a 70A hardness, MT carbon black-filled formulation. These are not intended to serve as specifications.
 **Curative-containing precompounds, and polymers + VC-50 (at levels less than or equal to 2.50 phr rubber) have been determined to be in compliance with FDA 21 CFR-177.2500—Rubber Articles for Repeated Food Contact.

Table 6
Viton® Fluoroelastomer Product Listing (cont'd.)

Viton® Product Type	Polymer Properties			Nominal Physical Properties*			Viton® Fluoroelastomer Product Description	Viton® Fluoroelastomer Product Suggested Uses/ Applications
	Nominal Viscosity, ML1 + 10 at 121°C	Specific Gravity	Polymer Fluorine Content, %	Compression Set, % 70 hr/200°C	Temperature of Retraction (TR-10) °C	Volume Increase, After 7 days/ MeOH/23°C		
A-Types: Gum Polymers								
A-100	10	1.82	66.0	15	-17	+75 to 105%	Ultra-low viscosity; excellent polymer rheology	Coatings, viscosity modifier for higher viscosity types
A-200	20	1.82	66.0	15	-17	+75 to 105%	Low viscosity; excellent polymer rheology	FDA-compliant**, cured w. VC-50; injection molding applications
A-500	50	1.82	66.0	15	-17	+75 to 105%	Intermediate viscosity; excellent polymer rheology	FDA-compliant**, cured w. VC-50; compression, transfer, injection molding
A-700	70	1.82	66.0	15	-17	+75 to 105%	High viscosity; excellent physical properties	FDA-compliant**, cured w. VC-50; compression, transfer, injection molding
A-HV	160	1.82	66.0	15	-17	+75 to 105%	Ultra-high viscosity; excellent physical properties	FDA-compliant**, cured w. VC-50; compression molding, high strength vulcanizates
AL-300	30	1.77	66.0	25	-19	+75 to 105%	Slightly improved low temperature flexibility. Low viscosity	Transfer, or injection molded goods, where A-types are marginal in low-temperature flexibility
AL-600	60	1.77	66.0	20	-19	+75 to 105%	Slightly improved low temperature flexibility. Medium viscosity	General molded goods, where A-types are marginal in low-temperature flexibility

*Nominal physical properties typical of those that can be expected of vulcanizates based on the specific type of Viton® noted, in a 70A hardness, 5MT carbon black-filled formulation. These are not intended to serve as specifications.
 **Various types of Viton® curatives-containing precompounds have been determined to be in compliance with FDA 21 CFR-177.2000—Rubber Articles for Repeated Food Contact

Table 6
Viton® Fluoroelastomer Product Listing (cont'd.)

Viton® Product Type	Polymer Properties			Nominal Physical Properties*			Viton® Fluoroelastomer Product Description	Viton® Fluoroelastomer Product Suggested Uses/ Applications
	Nominal Viscosity, ML1 + 10 at 121°C	Specific Gravity	Polymer Fluorine Content, %	Compression Set, % 70 hr/200°C	Temperature of Retraction (TR-10) °C	Volume Increase, After 7 days/ MeOH/23°C		
B-Types: Curative-Containing Precompounds								
B-435C	40	1.85	68.5	25	-14	+35 to 45%	Improved processing/mold release/bonding vs B-641C, B-651C	Injection—compression molding of metal-bonded parts
B-601C	60	1.85	68.5	20	-14	+35 to 45%	Excellent balance of resistance to compression set/fluids	FDA-compliant**; compression— injection molding of O-rings, sample shapes
B-651C	60	1.85	68.5	30	-14	+35 to 45%	Excellent mold flow, very good tear resistance, bonding to metal inserts	Compression— injection molding of complex shapes, bonded metal inserts
B-Types: Gum Polymers								
GEL-200S	20-30	1.85	67.0	30	-16	+40 to 50%	Excellent resistance to automotive lubricating oils, aqueous fluids	FDA Compliant** Transfer—compression molding auto lubricating oil, coolant system seals
GEL-600S	65	1.85	67.0	30	-16	+40 to 50%	Excellent resistance to automotive lubricating oils, aqueous fluids	FDA Compliant** Compression molding automotive lubricating oil, coolant system seals
B-202	20	1.86	68.5	25	-14	+35 to 45%	Excellent extrudability, lower MeOH permeability than A-types	FDA-compliant**; high shear extrusion applications—fuel hose veneer, coatings
B-600	60	1.86	68.5	20	-14	+35 to 45%	Intermediate viscosity, excellent polymer rheology, superior fluids resistance	FDA-compliant**; compression, transfer, and injection molding

*Nominal physical properties typical of those that can be expected of vulcanizates based on the specific type of Viton® noted, in a 70A hardness, MT carbon black-filled formulation. These are not intended to serve as specifications.

**Various types of Viton® curative-containing precompounds have been determined to be in compliance with FDA 21 CFR-177.2600—Rubber Articles for Repeated Food Contact.

Table 6
Viton® Fluoroelastomer Product Listing (cont'd.)

Viton® Product Type	Polymer Properties			Nominal Physical Properties*			Viton® Fluoroelastomer Product Description	Viton® Fluoroelastomer Product Suggested Uses/ Applications
	Nominal Viscosity, ML1 + 10 at 121°C	Specific Gravity	Polymer Fluorine Content, %	Compression Set, % 70 hr/200°C	Temperature of Retraction (TR-10) °C	Volume Increase, After 7 days/ MeOH/23°C		
F-Types: Curative-Containing Precompounds								
F-605C	60	1.90	69.5	30	-8	+5 to 10%	Improved polymer base vs. F-601C— improved reology, compression set	FDA-compliant**; compression molded goods requiring best fluids resistance
F-Types: Gum Polymers								
GF-200S	25-30	1.91	70.0	35	-6	+3 to 5%	Low viscosity version of GF-600S	FDA-compliant**; Injection transfer, or compression molded goods requiring best fluids resistance
GF-600S	65	1.91	70.0	35	-8	+3 to 5%	Superior resistance to broad range of fluids and chemicals, including MeOH	FDA-compliant**; Compression molded goods requiring best fluids resistance
Low-Temperature Types of Viton® Polymer								
GLT Types								
GLT-200S	25-30	1.78	64.0	30	-30	+75 to 105%	20-30 Mooney GLT: best FKM low-temperature flexibility	FDA Compliant** Injection - transfer molded automotive fuel, chemical, petroleum industry seals
GLT-600s	65	1.78	64.0	35	-30	+75 to 105%	Medium viscosity version of GLT	FDA Compliant** Transfer - compression molded automotive fuel, chemical, petroleum industry seals
GBLT Types								
GBLT-200S	25-30	1.60	65.0	40	-26	+65 to 90%	Low-temperature flexibility/fluid resistance intermediate between GLT/FLT types	Fuel systems parts: resistance to low oxygenates, low-temperature flexibility
GBLT-600S	65	1.60	65.0	35	-26	+65 to 90%	Low-temperature flexibility/fluid resistance intermediate between GLT/FLT types	Fuel systems parts: resistance to low oxygenates, low-temperature flexibility

*Nominal physical properties typical of those that can be expected of vulcanizates based on the specific type of Viton® noted, in a 70A hardness, MT carbon black-filled formulation. These are not intended to serve as specifications.

**Various types of Viton® curative-containing precompounds have been determined to be in compliance with FDA 21 CFR 177.2600—Rubber Articles for Repeated Food Contact.

**Table 6
Viton® Fluoroelastomer Product Listing (cont'd.)**

Viton® Product Type	Polymer Properties			Nominal Physical Properties*			Viton® Fluoroelastomer Product Description	Viton® Fluoroelastomer Product Suggested Uses/Applications
	Nominal Viscosity, ML1 +10 at 121°C	Specific Gravity	Polymer Fluorine Content, %	Compression Set, % 70 hr/200°C	Temperature of Retraction (TR-10) °C	Volume Increase, After 7 days/ MeOH/23°C		
GFLT Types								
GFLT-200S	25-30	1.66	66.5	35	-24	+5 to 10%	30 ML GFLT: best combination of low-temperature flexibility/fluids resistance	Bonded fuel systems parts: resistance to oxygenates, low-temperature flexibility
GFLT-600S	65	1.68	66.5	40	-24	+5 to 10%	65 ML GFLT: best combination of low-temperature flexibility/fluids resistance	Bonded fuel systems parts: resistance to oxygenates, low-temperature flexibility
Viton® Extreme™ Types								
ETP-600S	60	1.82	67.0	40	-12	+10 to 15%	Outstanding resistance to fluids/chemicals, including low molecular weight acids, aldehydes, ketones	FDA-compliant** Transfer – compression molded seals, gaskets

*Nominal physical properties typical of those that can be expected of vulcanizates based on the specific type of Viton® noted, in a 70A hardness, HT carbon black-filled formulation. These are not intended to serve as specifications.

**Various types of Viton® reactive-containing precompounds have been determined to be in compliance with FDA 21 CFR-177.2000—Rubber Articles for Repeated Food Contact.

Applications

Automotive

Parts produced from Viton® fluoroelastomer are widely used in the automotive industry because of their outstanding heat and fluid resistance. They are used in the following areas:

Powertrain Systems

- Crankshaft seals, Valve stem seals, Transmission seals
- Air Intake Manifold gaskets

Fuel Systems

- Veneered fuel hose
- In-tank fuel hose and tubing
- Pump seals, Diaphragms and Injector O-rings
- Accelerator pump cups
- Filter caps and filter seats
- Fuel sender seals, Carburetor needle tips

Appliances

The heat and fluid resistance of Viton® fluoroelastomer, coupled with its good mechanical strength, makes it a natural choice for many appliance parts. The use of seals and gaskets of Viton® has resulted in design of appliances in challenging environments. Here are some typical success stories:

- In one commercial automatic dry cleaning machine, no less than 107 components are made of Viton®: door seals, sleeve-type duct couplings, shaft seals, O-rings, and various static gaskets. They perform in an atmosphere of perchloroethylene fumes at temperatures up to 88°C, conditions that would quickly degrade other elastomers.
- A fluid-activated diaphragm-type thermostat for gas or electric ranges owes its success to the designer's choice of Viton® for the actuator element. Because Viton® adheres well to brass is virtually impermeable to and is not swelled or deteriorated by the fluids used, can withstand operating temperatures of 149 to 204°C, and has the mechanical strength to resist repeated flexing.

Chemical Industry

Viton® fluoroelastomer is essentially a universal seal for chemical process equipment. Its application in the chemical industry is illustrated by the following examples:

- In a pumping station that handles more than 60 different solvents, oils, and chemicals, seals of Viton® are used in the piping's swivel and telescoping joints. When these joints were inspected after two years' service, they were found to be as good as new.
- Valves lined with Viton® reduce heat and corrosion worries in many plants.
- Hose made of Viton® transfers solvents and reactive petrochemicals to and from processing and distribution facilities. There are installations on ocean tankers as well as on highway trailers.
- Processing rolls for hot or corrosive service are covered with Viton®.
- Flange gaskets for glass-bodied valves in a paper bleaching plant are of Viton®.
- Viton® replaced caulking on a process equipment enclosure, previously plagued with hot solvent leaks, and saved \$4,000 per year in maintenance costs.
- Aerosol-propelled solvent solutions of Viton® are sprayed on chemical process equipment as multi-purpose maintenance coatings.

Industrial Use

The good mechanical properties of Viton® fluoroelastomer have permitted it to replace conventional elastomers in a range of applications that cut across industry lines. To cite a few:

- Stable-dimensioned O-rings in the meters of automatic gasoline blending pumps
- High vacuum seals for the world's most powerful proton accelerator
- Heat- and corrosion-resistant expansion joints for a utility company's stack gas exhaust ducts
- Tubing and seals for a variety of top-quality industrial instruments
- Compression pads for heavy-duty vibration mounts used for portable missile ground control apparatus
- Conveyor rolls for a solvent cleaning machine
- Packing rings for hydraulic activators on steel mill ladles
- Clamp cushions for parts dipped in 285°C solder
- Jacketing for steel mill signal cable
- Deflector rolls on high-speed tinplating lines
- Precision-molded balls for check valves in oil or chemical service
- O-ring seals for test equipment in an automotive manufacturer's experimental lab

Aerospace

Reliability of materials under extreme exposure conditions is a prime requisite in this field. Aircraft designers report that O-rings of Viton® fluoroelastomer have a useful thermal range of -54 to 316°C and that Viton® exhibits "long and consistent life," even at the upper end of this range. Higher temperatures can be tolerated for short periods. Viton® also resists the effects of thermal cycling, encountered in rapid ascent to and descent from the stratosphere. Other desirable characteristics of Viton® that are pertinent to aerospace applications are its excellent abrasion resistance and its ability to seal against "hard" vacuum, as low as 10^{-3} mm Hg (133 nPa), absolute.

The high-performance properties of Viton® have been demonstrated in these typical aircraft and missile components:

- O-rings and manifold gaskets
- Coated fabric covers for jet engine exhausts between flights
- Firewall seals
- Abrasion-resistant solution coating over braided-sheathed ignition cable
- Clips for jet engine wiring harnesses
- Tire valve stem seals
- Siphon hose for hot engine lubricants

Fluid Power

Designers and engineers are discovering that seals of Viton® fluoroelastomer work better and last longer than any other rubber in most fluid power applications. Viton® seals effectively up to 204°C and is unaffected by most hydraulic fluids, including the fire-resistant types. Seals of Viton® can also cut maintenance costs under more moderate service conditions (below 121°C) by providing longer, uninterrupted seal reliability.

Some applications in which seals of Viton® can reduce fluid loss and minimize downtime include the following:

- Actuators are the hydraulic components most likely to develop small, steady leaks when rubber seals wear and lose resilience, which can be extremely expensive. In a working year, day-to-day leakage from the average hydraulic system wastes enough fluid to completely fill the system more than four times. Viton® prevents or reduces leakage by maintaining its toughness and resilience longer than other rubber seal materials under normal fluid power conditions.
- In pumps, poor sealing performance increases operating costs by wasting power. When internal seals lose resilience and allow more slippage than the pump design permits, power is wasted. When seals swell and drag, power is wasted. Seals of Viton® keep their resilience and don't swell, thus preventing power waste and helping hold down operating costs.

Test Procedures

Property Measured	Test Procedure
Compression Set	ASTM D3955, Method B (25% deflection)
Compression Set—Low Temperature	ASTM D1299, Method B (25% deflection)
Compression Set, O-Rings	ASTM D1414
Hardness	ASTM D2240, durometer A
Mooney Scorch	ASTM D1646, using the small rotor. Minimum viscosity and time to a 1-, 5-, or a 10-unit rise are reported.
Mooney Viscosity	ASTM D1646, ten pass 100°C and 121°C
ODR (vulcanization characteristics measured with an oscillating disk cure meter)	ASTM D2084
Property Change After Oven Heat-Aging	ASTM D573
Stress/Strain Properties	
100% Modulus	ASTM D412, pulled at 8.5mm/s (20 in/min.)
Tensile Strength	
Elongation at Break	
Stiffness, Torsional, Clash-Berg	ASTM D1043
Temperature Retraction	ASTM D1329
Volume Change in Fluids	ASTM D471

*Note: Test temperature is 24°C, except where specified otherwise.

For further information please contact one of the offices below, or visit our website at www.dupontelastomers.com/vlon

Global Headquarters – Wilmington, DE USA
 Tel. +1-800-853-5515
 +1-302-792-4000
 Fax +1-302-792-4430

European Headquarters - Geneva
 Tel. +41-22-717-4000
 Fax +41-22-717-4001

South & Central America Headquarters - Brazil
 Tel. +55-11-4166-8978
 Fax +55-11-4166-8989

Asia Pacific Headquarters - Singapore
 Tel. +65-6275-8383
 Fax +65-6275-8395

Japan Headquarters – Tokyo
 Tel. +81-3-5521-2990
 Fax +81-3-5521-2991

The information set forth herein is furnished free of charge and is based on technical data that DuPont Performance Elastomers believes to be reliable. It is intended for use by persons having technical skill, at their own discretion and risk. Handling precaution information is given with the understanding that those using it will satisfy themselves that their particular conditions of use present no health or safety hazards. Since conditions of product use and disposal are outside our control, we make no warranties, express or implied, and assume no liability in connection with any use of this information. As with any material, evaluation of any compound under end-use conditions prior to specification is essential. Nothing herein is to be taken as a license to operate or a recommendation to infringe on patents.

Caution: Do not use in medical applications involving permanent implantation in the human body. For other medical applications, discuss with your DuPont Performance Elastomers customer service representative and read Medical Caution Statement H-60237.

DuPont™ is a trademark of DuPont and its affiliates.

Viton® and Viton® Extreme™ are trademarks or registered trademarks of DuPont Performance Elastomers.

Copyright © 1998, 2004, 2005 DuPont Performance Elastomers. All Rights Reserved.

(11/05) Printed in U.S.A.
 Reorder no. VFE-HCB134-00-F1105

DuPont
Performance Elastomers

3.5.3 Eutectic Analysis of Ti-6Al-4V with Plutonium and Copper

LA-UR 08-07663

Plutonium Metal Compatibility with Materials of the Ti-6Al-4V Packaging System

Prepared by:
Richard E. Mason, PMT-1
and
Stephen P. Willson, PMT-1

2 December 2008



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

LA-UR-08-07663

Abstract

This technical basis report considers phase stability of plutonium metal encapsulated in a Ti-6Al-4V ampoule. The maximum temperature that these materials will be exposed to is 582°C. The plutonium metal may also be encapsulated in tantalum foil plus beryllium is potentially in contact with the plutonium. It is concluded by analysis of phase diagrams and composition of materials for all possible binary systems that no liquid phases are expected in this system at 582°C. Furthermore, it is anticipated that the lowest melting point phase that may form within this system is 595°C – the plutonium/beryllium eutectic temperature. This is 13°C higher than the highest temperature excursion considered for the system. This is not a large margin but the 595°C value is a conservative estimate, thus the system in a transient reaching 582°C is still considered safe. Review of the ternary phase diagrams available in the literature involving components of this system supports the conclusions drawn from the binary systems, however, the ternary systems are limited and this is a much more complex system than reviewed in the binary or ternary systems available in the literature.

LA-UR-08-07663

Table of Contents

INTRODUCTION	4
INTERFACIAL REACTION ZONES	6
<i>Aluminum</i>	6
<i>Beryllium</i>	8
<i>Copper</i>	10
<i>Gallium</i>	11
<i>Plutonium</i>	12
<i>Tantalum, Titanium, and Vanadium</i>	13
<i>Binary interaction summary</i>	13
INVESTIGATION OF TERNARY SYSTEMS	14
ADDITIONAL CHEMICAL REACTION	15
CONCLUSIONS	15
REFERENCES	15

LA-UR-08-07663

Introduction

The PAT-1 (Plutonium Air Transport) package was originally designed to transport plutonium oxide across the country and to other countries that process plutonium oxide. The TB-1 containment vessel was designed to contain this material. The TB-1 vessel is stainless steel. Because of the need to air transport alpha and delta-stabilized plutonium metal, the container or ampoule inside the TB-1 containment vessel is newly constructed of the Ti-6Al-4V alloy to protect the TB-1 vessel from attack by plutonium. This analysis focuses on binary eutectic compositions that could form in a hypothetical accident scenario in which the TB-1 vessel attains a maximum temperature of 582°C and is exposed to this temperature for up to four days. Within the liner is a copper foam support structure of $\geq 99.99\%$ copper, and an alpha or delta-stabilized plutonium metal sample. Plutonium metal is loaded into the copper foam and the combined package is loaded into the Ti-6Al-4V liner in an inert atmosphere glove box. The interior void space of the liner is flushed with helium, then sealed and leak-checked.

The melting points of pure metals considered for this analysis are presented in Table 1. [Lide 1991] A summary of the lowest melting points for the possible binary systems has been taken from the binary phase diagrams, and assembled in Table 2.

Table 1. Melting points of pure metals considered in this system.

Element	Melt Temperature (°C)
Aluminum	660
Beryllium	1287
Copper	1085
Gallium	30
Plutonium	640
Tantalum	3017
Titanium	1668
Vanadium	1910

LA-UR-08-07663

Table 2. Lowest melting points and compositions derived from binary phase diagrams.

System	Lowest Melting Point (°C)
Ti6Al4V	1604°C
Aluminum – Beryllium	644°C eutectic
Aluminum – Copper	548°C at compositions between pure aluminum and about 45 atom percent aluminum, 660C for copper alloying with aluminum up to about 3 weight percent Al, greater than 600°C for aluminum alloying with copper up to 25 weight percent Cu
Aluminum – Gallium	26.3°C eutectic
Aluminum – Plutonium	640°C for pure Pu
Aluminum – Tantalum	660C for pure Al
Aluminum – Titanium	660°C for pure Al
Aluminum – Vanadium	660°C for pure Al
Aluminum – Beryllium	644°C eutectic
Beryllium – Copper	The congruent melt temperature of 858°C is the lowest melt temperature in the binary system
Beryllium – Gallium	30°C the gallium melt temperature. The gallium melts and there is minimal solution of the beryllium below 600°C
Beryllium – Plutonium	The additions of small amounts of beryllium may lower the plutonium rich metal to a melt temperature of 595°C
Beryllium – Tantalum	1287°C as there was no binary phase diagram found
Beryllium – Titanium	1287°C of pure Beryllium
Beryllium – Vanadium	1287°C of pure Beryllium
Copper – Gallium	625°C for phases containing greater than 55 atom percent gallium
Copper – Plutonium	626°C for 6 atom% Cu, 1.7 wt% Cu
Copper – Tantalum	1085°C of pure Cu
Copper – Titanium	880°C for 27 atom% Ti, 22 wt% Ti
Copper – Vanadium	1085°C for pure Cu
Titanium – Vanadium	>1600°C for 30 wt% V
Gallium – Aluminum	Compositions above 2 atom% (5 wt%) gallium are liquid at 625°C
Gallium – Copper	Compositions above 55 atom% gallium (57 wt%) are liquid at 625°C
Gallium – Plutonium	Compositions above 75 atom% gallium (47 wt%) are liquid at 625°C
Gallium – Titanium	Compositions above 99 atom% gallium (99 wt%) are liquid at 625°C
Gallium – Vanadium	Compositions above 97 atom% gallium (98 wt%) are liquid at 625°C
Plutonium – Tantalum	640°C of pure Pu
Plutonium – Titanium	640°C of pure Pu
Plutonium – Vanadium	625°C for < 2 wt% V
Tantalum – Titanium	1668°C for pure Ti
Tantalum – Vanadium	1910°C for pure V
Titanium – Vanadium	1668°C for pure Ti

LA-UR-08-07663

Interfacial Reaction Zones

Reactions between metals of the Ti-6Al-4V alloy with the contents it will hold are restricted to contact zones between different metal compositions. Because none of the major individual starting materials reach their melting points during a 582°C temperature excursion, formation of new phases must depend upon solid state transport of material from one of the original phases into another. The original starting materials are not pure materials. Gallium is never in the system as a metal but is dissolved in plutonium and the gallium-plutonium alloy has a melting point well above 582°C. Redistribution of the gallium into a pure metal will not be an issue. Gallium can only influence the performance of the materials in this system if it diffuses to another metal or alloy. Material transport will only occur between phases that are in mechanical contact. Transport will be substantially impeded by the presence of thin surface oxide layers, which will be present on the titanium alloy, the copper, the beryllium and the plutonium. Formation of any new phases in the container, eutectic or otherwise, is explicitly dependent upon sufficient solid state mass transport, which depends on solid state solubility of the components, intimacy of contact between the components, and the time the system is held at the elevated temperature. The kinetic data that would be required to quantitatively address solid state diffusion between the plutonium, the beryllium, the copper, and the titanium ampoule is not available. Qualitative conclusions are drawn based on the available phase diagrams, which capture the thermodynamically stable compositions of binary systems, at a given temperature.

When an alloy is in contact with another metal composition, solid state transport will be different for the different components of the alloy, resulting in preferential reaction with one component, and changing the resultant concentrations of both phases by enriching one and depleting the other with respect to the most mobile component. Contact reaction zones are discussed by reference to binary phase diagrams. At the low temperature of 582°C diffusion will be slow and the integrity of the ampoule alloy will only be compromised if a liquid was to form. As long as all component combinations do not form a liquid, the ampoule will remain intact and contain the material shipped.

Aluminum

Aluminum contact with components of the Ti-6Al-4V packaging system

Aluminum is initially present at only 10 atom percent in the titanium alloy. Although aluminum binaries with the elements of this system are considered, it is improbable that interactions with aluminum alone and the other components would ever occur. The aluminum is alloyed with titanium and vanadium and all three form high temperature alloys with all of the components expected in a shipment of plutonium metal.

Aluminum contact with beryllium

The aluminum-beryllium system forms a eutectic at 644°C, 16°C below the melt temperature of pure aluminum. There are no intermediate phases thus liquid aluminum

LA-UR-08-07663

will exist above this temperature. This temperature is higher than the maximum temperature considered for safe operation of this system..[Landolt-Bornstein 1992]

Aluminum contact with copper

The aluminum-copper system is complex with a eutectic melt temperature of 548°C at 66.8 weight percent aluminum. [Landolt-Bornstein 1992] The 548°C solidus extends from about 5.6 weight percent aluminum to about 45 weight percent aluminum. The solidus temperatures between pure copper and 45 weight percent aluminum are much higher temperatures and with five intermediate phases in the system. Aluminum is an alloying element in copper is solid at 600C up to about 25 weight percent aluminum. This is not an issue because the aluminum is a minor alloy constituent and as titanium content increases the melt temperature of the copper-titanium-aluminum will likely increase. For alloy compositions with aluminum content greater than 45 weight percent aluminum, the melt temperature is much greater than 600°C and more than 5 weight percent aluminum would have to diffuse into the copper for the melt temperature to be lower than 600°C. Significant aluminum would have to diffuse out of the ampoule alloy into the copper or aluminum into the copper. Both are impractical at the maximum temperature that these materials could be exposed to.

Aluminum contact with gallium

Gallium metal melts at 29°C and the aluminum-gallium binary is a eutectic binary system. There are no intermediate phases in this system. This binary system is a simple eutectic system with eutectic temperature at 26.6°. [Landolt-Bornstein 1992] The liquidus is well known but the boundaries of the solid phases are not well known. The solubility of aluminum in gallium metal is very low. The maximum solubility of gallium in aluminum metal is approximately 9 atom percent and the aluminum is solid at 600C up to about 7 atom percent gallium. The formation of a separate gallium-aluminum phase is not credible because both gallium and aluminum are soluble in plutonium at the compositions present and at temperatures below the melting point of plutonium. It is impractical for an alloy composition to form that would be liquid because it would simultaneously require local concentration of the aluminum to 98 atom percent. This phase is highly unlikely.

Aluminum contact with plutonium

Aluminum forms five intermediate phases with plutonium with PuAl_2 being the dominant intermediate phase melting at $1540 \pm 50^\circ\text{C}$. The compound Pu_3Al of the plutonium rich compositions is formed by a very sluggish peritectoid reaction between the plutonium delta phase and PuAl . [Wick 1980]. Aluminum goes into solid solution with plutonium up to 10 atom percent aluminum. As the content of aluminum increases the melt temperature increases up to the PuAl_2 solidus at 801°C . [Wick 1980] In this binary system the combination of the two elements increases the melt temperature.

Aluminum contact with tantalum

Aluminum and tantalum form four intermediate phases. With the addition of a small amount of tantalum to the aluminum the melt temperature of aluminum metal is raised about eight degrees and the solidus exists to 25 atom percent aluminum. At 25 atom percent aluminum Al_3Ta is the solid and it melts at about 1629°C . On the tantalum rich

LA-UR-08-07663

side of Al_3Ta the solidus temperature is a bit lower but remains close to 1629°C until the intermittent phase Al_3Ta_2 is reached where the solidus temperature is a few degrees lower. Thereafter, as the concentration of tantalum increased the solidus temperature increases. [Landolt-Bornstein 1992] Again the melting temperatures of the intermediate phases are much above the maximum temperature this system will be exposed to thus the combination of these two elements will not negatively affect the safe operation of this system but will more likely decrease the likelihood of liquid formation.

Aluminum contact with titanium

At aluminum concentrations between pure and 25 atom percent aluminum the solidus is 665°C . That is, with the addition of a small amount of titanium to the aluminum the melt temperature of aluminum metal is raised about five degrees and remains the solidus to 25 atom percent aluminum. The Al_3Ti melts at about 1387°C . [Landolt-Bornstein 1992] Again the melt temperatures of the intermediate phases are much above the maximum temperature this system will be exposed to thus the combination of these two elements will not affect the safe operation of this system.

Aluminum contact with Vanadium

Aluminum and Vanadium form five intermediate phases. With the addition of a small amount of tantalum to the aluminum the melt temperature of aluminum metal is raised about two degrees and remains the solidus to about 8 atom percent aluminum. As each intermediate phase is reached the solidus temperature is increased as the concentration of Vanadium increases. [Landolt-Bornstein 1992] Again the melting temperatures of the intermediate phases are much above the maximum temperature this system will be exposed to thus the combination of these two elements will not affect the safe operation of this system.

Beryllium

Beryllium and plutonium may contact the Ti-6Al-4V container if they are not wrapped with tantalum foil and either metal penetrates the copper foam. Tantalum may also be wrapped around the beryllium and/or plutonium pieces and in this case these materials would have to penetrate the tantalum wrapping material and then the copper foam before reaching the ampoule alloy.

Beryllium contact with copper

Beryllium and copper alloys are commonly used alloying elements. An alloy of beryllium and copper with 24 atom percent copper melts at 966°C . [Landolt-Bornstein 1992] This is the lowest melting alloy in this binary system with all other compositions and phases melting at higher temperatures. The combination of beryllium and copper will not compromise the safe use of this system.

LA-UR-08-07663

Beryllium contact with gallium

Beryllium and gallium do not form intermediate phases, consequently, at temperatures above gallium's melting point of 30°C and below 600°C there is minimal mixing of the two materials.[Landolt-Bornstein 1992] If the two materials were to interact, then above 30°C the gallium will be liquid at the grain boundaries causing a decrease in mechanical strength of the beryllium. Interaction of these two components of the system is an improbable scenario because the gallium in the plutonium is in solid solution and only at quantities less than 10 atom percent.

Beryllium contact with plutonium

The main feature of the beryllium-plutonium system is one intermediate compound PuBe_{13} which has a higher melt temperature than either pure constituent at $1950 \pm 50^\circ\text{C}$. The eutectic at 96 atom percent plutonium probably lowers the melt temperature only 10°C. [Wick 1980] However, one experimenter reported the eutectic melt temperature lowered by as much as 45°C. Although, Wick et al. report that a melt temperature drop of 10°C is most accurate the worse case would be the 45°C decrease from 640°C of plutonium metal or a melt temperature of 595°C. At 582°C the components are still solid but close to a potential melt temperature.[Wick 1980] This is the lowest melting material or alloy of the systems considered. It is a combination of material that could be present in an accident.

Beryllium contact with tantalum

The phase equilibria are not known.[Landolt-Bornstein 1992] In a sample containing 0.05 atom percent tantalum after solidification from the melt the solidified microstructure indicated a eutectic phase and several intermediate phases with one having a melting temperature of Be_{12}Ta at 1850°C and for $\text{Be}_{17}\text{Ta}_2$ a melting temperature of 1980°C.

Beryllium contact with titanium

There are four or more intermediate compounds in this system with an eutectic at 70 atom percent titanium and at a temperature of 980°C. [Murray 1987 & Ohnuma 2004] Should the beryllium penetrate the copper, the beryllium could be mechanically mixed with the titanium at the surfaces of the pieces. Even mixed the eutectic temperature is not reached and the containment not affected.

Beryllium contact with vanadium

There are three or more intermediate compounds in this system. The solidus temperature is raised more than 230°C when the vanadium content exceeds about 7 atom percent.[Landolt-Bornstein 1992] Vanadium is only 4 atom percent in the ampoule alloy but its contribution to any alloy of these systems would be to increase the melt temperature. Should the beryllium penetrate the copper beryllium could be mechanically mixed with the titanium at the surfaces of the pieces. Even mixed the eutectic temperature is not reached and the containment not affected.

LA-UR-08-07663

Copper

It is not expected that a liquid phase will form at this interface at the highest temperature of any hypothetical accident (582°C). Because the copper surrounds the metal as the structural matrix to hold the plutonium metal in favored positions within the ampoule, it is the first to interact with the plutonium, beryllium or tantalum that the plutonium metal is wrapped in. At 582°C, both copper and the titanium alloy ampoule are solid and 582°C is well below their respective melting points. Aluminum-copper compositions with more than 64 atom percent (43 weight percent) aluminum will melt at 625°C, which is also the melting point of the plutonium-vanadium eutectic, considered later in this report. Aluminum is present in the titanium alloy at a concentration of 10 atom percent. In order to form a melting composition with copper at 625°C, it needs to attain a concentration within the copper of 64 atom percent or greater. Solid state transport on the scale required for formation of a low melting phase (below 625°C) at this boundary in four days is not expected.

Copper contact with gallium

Gallium is in solid solution in copper up to about 19 to 20 atomic percent gallium with the alloying of these two metals lowering the melt temperature to about 900°C at 20 percent gallium.[Landolt-Bornstein 1992] Solid state transport of gallium from a 10 atom percent gallium-plutonium alloy into pure copper sufficient to form a 20 atom percent gallium-copper alloy is improbable. Incorporation of enough gallium into the copper at 582°C to form a liquid phase requires passage through five successive solid state phases. Formation of each of these phases requires a microstructure rearrangement before more gallium atoms can be incorporated, thus reduction of melting temperatures due to the combination of these two metals is very unlikely.

Copper contact with Plutonium

The plutonium rich component of the binary phase has a eutectic at about 6 atom percent copper and a temperature of 625°C. [Wick 1980 & Copper 2000] It is not expected that a liquid phase will form at this interface at a temperature of 582°C. First consider possible reaction of copper with alpha plutonium. Due to the softening of plutonium metal near its melting point, 640°C, and the roughly 5% expansion of alpha plutonium upon conversion to epsilon plutonium it is possible that alpha plutonium samples will tightly contact the copper foam, and reaction will occur at the interface. The progression of the reaction will be limited by the temperature actually reached, and by the time held at that temperature. The plutonium-copper eutectic composition will not melt at 582°C.

Copper contact with Tantalum

The mutual solubility of copper and tantalum is negligibly small and intermediate phases do not exist.[Landolt-Bornstein 1992] Copper and tantalum are immiscible at temperatures lower than 1083°C. Even the solubility of tantalum in liquid copper above the melting point is small. The solubility of Ta in liquid copper amounts to 0.0088 atom percent tantalum at 1200°C. Combining these two materials in this storage system will not lower the melting temperatures of the materials and are of no consequence to the safety of the system but may enhance the safety margin.

LA-UR-08-07663

Copper contact with titanium

The copper-titanium system is also a complex binary system with five intermediate phases and a eutectic at 860°C and 27 atom percent titanium.[Landolt-Bornstein 1992] Combining these two materials in this storage system will not lower the melting temperatures of the materials and are of no consequence to the safety of the system but may enhance the safety margin.

Copper contact with vanadium

The copper vanadium system is a simple eutectic system. The eutectic is on the vanadium rich side at about 15 atom percent copper and a eutectic temperature of 1530°C.[Landolt-Bornstein 1992] Combining these two materials in this storage system will not lower the melting temperatures of the materials and are of no consequence to the safety of the system but may enhance the safety margin.

Gallium

Gallium has an extremely low melting temperature when compared to the other metals in the ampoule material and the material to be shipped. The gallium is soluble in the plutonium and is a component of the plutonium up to 10 atom percent. The only thermodynamic driver of this conversion is the leaching ability of other metals from the plutonium-gallium alloy. Gallium is soluble in the plutonium epsilon phase and will not segregate to the interface and is consequently not easily leachable from the plutonium should one of the other elements have a higher affinity to alloy gallium than plutonium.

Gallium contact with Plutonium

The gallium is soluble in the plutonium up to about 10 atom percent gallium in the plutonium. The delta phase of plutonium is stabilized at room temperature by the addition of less than 10 atom% gallium. [Wick 1980] Because delta plutonium contracts upon conversion to epsilon, it will not experience increased pressure at the interface upon heating. Up to 20 atom percent gallium is soluble in the plutonium epsilon phase, so there will be no segregation of gallium upon transition to epsilon plutonium. A liquid phase will not form in the plutonium rich material until the melt temperature of plutonium is reached. There is also no driver for the gallium to segregate since it is already in solid solution

Gallium in contact with tantalum

There are four intermediate phases in this binary system and with increasing tantalum the solidus increases with each intermediate phase. The liquidus remains at 29°C until the intermediate Ga₃Ta is reached.[Landolt-Bornstein 1992] The phase relations in this system are not sufficient to give additional detail. Given sufficient gallium in the system this combination could compromise the safety of the system but there is simply insufficient gallium in the entire mass of plutonium metal to compromise the container.

Gallium in contact with titanium

LA-UR-08-07663

The gallium-titanium system requires more than 99 atom percent gallium in order to form a phase that melts at 625°C.[Landolt-Bornstein 1992] Because the gallium is soluble and stable at lower concentrations, formation of a phase with such high gallium content, nearly pure gallium is not expected to occur. Formation of a molten phase of either gallium-titanium or gallium-vanadium is unlikely given the available quantity of gallium and the thermodynamic stability of lower concentration solid phases.

Gallium in contact with Vanadium

There are four intermediate phases in this binary system and with increasing vanadium the solidus increases with each intermediate phase. The solidus remains at 29°C until the intermediate Ga_4V_8 is reached where the solidus on the vanadium rich side of this intermediate compound is 500°C. The gallium-vanadium compositions require more than 84 atom percent of gallium in order to form a phase that melts at 625°C.[Landolt-Bornstein 1992] Given sufficient gallium in the system this combination could compromise the safety of the system but there is simply insufficient gallium in the entire mass of plutonium metal to compromise the container.

Plutonium

It is not expected that a liquid phase will form at this interface. In the event that plutonium is sheared from the bulk and contacts the Ti-6Al-4V liner, consideration must be given to the interfacial reaction zone. The possible binary compositions of interest for contact between the liner and alpha plutonium include plutonium-aluminum, plutonium-titanium, and plutonium-vanadium. In the case of both plutonium-aluminum and plutonium-titanium, the melting point is increased relative to that of pure plutonium for all concentrations.

Plutonium contact with tantalum

This combination of materials is very stable and will not negatively impact the safe operation of the system. Tantalum and plutonium form a eutectic very close to pure plutonium. The eutectic reduces the melt temperature by only a degree or two. At temperatures above the 640°C solid tantalum can contain increasing plutonium up to about 25% plutonium near 2550°C.[Boxi 1991] There is also significant solubility of plutonium in the tantalum metal at temperatures above the plutonium melt temperature but limited solubility of plutonium in tantalum at temperatures below 640°C. [Wick 1980] Consequently, pure plutonium stored in pure tantalum foil is compatible at temperatures below plutonium's melting temperature. Above plutonium's melt temperature there is little reaction except that as the temperature rises an increasing amount of plutonium will diffuse into the tantalum metal matrix.

Plutonium contact with titanium

There are no intermediate phases in the binary system. A peritectoid composition at 6.5 atom percent titanium increases the solubility of titanium in the plutonium metal to a maximum of 25 atom percent at 770°C. Above the melting temperature of plutonium the liquid plutonium will combine with the tantalum to form a solid mixture up to 770°C, the highest solidus temperature in the system.[Landolt-Bornstein 1992] This reaction would stabilize the system in a high temperature transient situation.

LA-UR-08-07663

Plutonium contact with vanadium

The plutonium-vanadium eutectic composition forms with less than 2 weight percent vanadium resulting in a solidus temperature of 625°C from 2 to 100 weight percent vanadium. At all concentrations of more than 2 wt% vanadium in plutonium, and at a temperature of 625°C or higher, the plutonium-vanadium system exhibits a liquid phase.[Landolt-Bornstein 1992] At all compositions, at temperatures less than 625°C, only solid phases are present. If mobility into the solid plutonium metal leaves the ampoule alloy depleted in one of its other constituents, the melting point of the liner in the depleted zone will be increased.

Tantalum, Titanium, and Vanadium

Vanadium and aluminum are the minor constituents of the alloy of the ampoule at 10 atom percent or less. Consequently, titanium will probably dominate the interactions of the container with the packaged material. When tantalum is used to wrap the plutonium metal it too will be a major contributor to the performance of the shipping container during the transient. Interaction between or alloying of these four components aluminum, tantalum, titanium and vanadium produce material that will probably not form lower melt temperature

Tantalum contact with titanium

The Ti-Ta binary phase diagram is characterized by an isomorphous body centered cubic phase field extending from pure titanium at elevated temperatures to pure tantalum with limited mutual solubilities.[Landolt-Bornstein 1992] Since there are no intermediate phases and the solidus is essentially linear between the melt temperature of titanium (1670°C) and tantalum (3017°C), a combination of these metals with other compound will probably increase the melt temperature of the system.

Tantalum contact with Vanadium

There are no intermediate phases and the solidus and liquidus increase from the 1910°C melt temperature to the 3017°C melt temperature of tantalum. Addition of any of these two metals will likely increase the melt temperature of the resulting mixture.

Titanium contact with Vanadium

There are three intermediate phases and the solidus and liquidus increase from the 1668°C titanium melt temperature to the 1910°C melt temperature of vanadium.[Landolt-Bornstein 1992] Addition of any of these two metals will likely increase the melt temperature of the resulting mixture of container and package materials.

Binary interaction summary

The lowest melt temperature is 595°C between the plutonium and beryllium with the next lowest between the plutonium-vanadium eutectic at 625°C. The 595°C temperature may be a low estimate because of impurities in the material tested with the melt temperature of the beryllium-plutonium probably closer to 630°C. However, for safety evaluations this is the worst case temperature.

LA-UR-08-07663

The lowest melting phase with plutonium/vanadium liner contact is 625°C, and is unlikely to form based on the absence of a clean contact surface under pressure between the plutonium and the liner. The melting temperature of this eutectic is 43°C higher than that of the proposed high temperature excursion.

Addition of the beryllium to the system brings the melt temperature close to the maximum temperature that the ampoule may be exposed to. If all the components internal to the titanium ampoule are combined and intimately mixed, that is, plutonium, beryllium, gallium, tantalum, and copper are completely alloyed, the melt temperature could be lower than 582°C. There is no data to show otherwise and 595°C is close to this temperature. However, it is unlikely and impractical to intimately mix these components together by mechanical impact and then expose them to temperatures above the binary melting points. Significant work on this complex metal alloy system would be required if a mechanism could be hypothesized to form such an alloy by impact of separate alloys and metals but it is not considered plausible.

Investigation of Ternary Systems

Published information was available for eleven of the possible ternary systems considered. [Petzow 1992 & Villars 1995] The Ti-6Al-4V alloy was designed to be solid to 1604°C. The tantalum-titanium-aluminum system is solid above 1100°C. [Weaver 1995] It is generally true that for the ternary phase diagrams reviewed, there was little new information with respect to melting temperatures that was not captured by the binary diagrams. Expected compositions are those that do not require achieving large concentrations of a particular element in a phase against a strong concentration gradient. For example, given that aluminum begins at 10 atom percent in the titanium alloy used, it is considered unlikely that it would achieve concentrations of 20 atom percent or more in another phase. The same rule is applied with respect to the vanadium and gallium components, both of which begin at low concentrations in their respective thermodynamically stable alloys.

Reviewed binary and ternary systems that possess a liquid component at temperatures below 625°C are those with high concentrations of aluminum and gallium (greater than 50 atom percent combined aluminum and gallium content). It is considered improbable that with less than 9 atom percent gallium in the plutonium and 10 atom percent aluminum in the titanium alloy, any phases will form containing more than 50 atom percent combined gallium and aluminum.

In both titanium and plutonium, aluminum and gallium may substitute for each other, partially or completely, without altering the observed phase. Several of the ternary systems reviewed show no ternary phases, only mixtures of binary phases, all of which have already been captured by the preceding review of binary phase diagrams. The only ternary diagram available that contained plutonium was the aluminum-gallium-plutonium diagram.

LA-UR-08-07663

Conclusions drawn by reference to the binary phase diagrams are consistent with the information present in the ten available ternary phase diagrams.

Additional Chemical Reaction

Finely divided metals tend to oxidize rapidly in air due to the high surface area relative to mass of metal present. The oxidation reaction for a metal is generally exothermic, and in the event of finely divided powders in air, can often result in pyrophoricity. During the proposed accident scenario for this analysis, the system containment is not mechanically breached, and an inert environment is maintained. The small amount of oxygen in the system will exist as oxide on the various system components, rather than as gaseous oxygen. In the event that small particles are generated within the titanium alloy ampoule, they will not ignite due to an absence of oxygen necessary for the reaction. The initial system components are bulk metal materials. These are not pyrophoric.

Conclusions

All of the expected phases formed from the original materials at a temperature of 582°C are solid. The lowest probable binary phase melting point is 595°C (plutonium-Beryllium). The second lowest probable binary phase melting point is 625°C (plutonium-vanadium) and the third lowest melting point is 626°C (plutonium-copper). The lowest is possible if other impurities not considered in this technical basis were present. It is anticipated that the second and third lowest compositions will not form due to the presence of surface oxide layers on the initial components of the system. A review of available ternary phase diagrams supports the conclusions drawn from the binary phase diagrams. However, the many combinations of the product materials and the container materials make it impossible to absolutely rule out a lowering of the melting point due to mechanical mixing that could occur in a severe impact and post impact fire until some testing verification on the materials are conducted.

References

- Boxi, H.C., Massalski, T.B., and Rizzo, H.F., 1991, *The Pu-Ta (Plutonium-Tantalum) System*, Journal of Phase Equilibria, 12 No. 5 pp 593
- Brandes, E. A., ed. 1983. *Smithells Metals Reference Book*, Sixth Edition. Ch. 11.
- Kaufmann, A.R., Gordon, P., Lillie, D.W. 1950, *ASM Trans. Q.* 42 p 801.
- Cooper, N. G., ed. 2000. *Challenges in Plutonium Science, Volume II. Plutonium and Its Alloys*, pp. 291-335.
- Landolt-Bornstein – Group IV Physical Chemistry Volumes 5b and 5j (1992)
- Lide, D. R., ed. 1991. *CRC Handbook of Chemistry and Physics*, pp. 4-122, 4-123.

LA-UR-08-07663

Murray, J.L., 1987, The Be-Ti (Beryllium-Titanium) System, *Phase Diagrams of Binary Titanium Alloys*, J.L. Murray, Ed., ASM International, p 40-43

Ohnuma, I.; Kainuma, R.; Uda, M.; Iwadachi, T.; Uchida, M., Kawamura, H., and Ishida, K., 2003 "Phase Equilibria in the Be-V and Be-Ti Binary Systems," *Proc. Sixth International Workshop on Beryllium Technology for Fusion, 2003*, Japan. Atom. Energy Res. Inst.,

Petzow, G., Effenberg, G., ed., 1992, *Ternary Alloys*. VCH Publishers, NY, NY: ASM International.

Villars, P.; Prince, A.; Okamoto, H., 1995. *Handbook of Ternary Alloy Phase Diagrams*. Materials Park, OH: ASM International.

Weaver, M.L. and Kaufman, M.J., 1995 "Phase Relationships and Transformations in the Ternary Aluminum-Titanium-Tantalum system," *Acta metall, mater.* Vol. 43, No. 7, pp. 2625-2640.

Wick, O. J., ed. 1980. *Plutonium Handbook*. Chaps. 7 and 12-3. La Grange Park, IL: American Nuclear Society

3.5.4 Determination of Most Damaging Package Orientation for HAC Analysis

This section of the Appendix contains a summary of the calculations used to determine which package orientation is the most thermally damaging configuration for the HAC analysis. The PAT-1 package was considered as a cylinder exposed to a fully-engulfing, uniform temperature, fire and to an open (cool) environment in both the vertical and the horizontal orientations. In both orientations, the maximum heat flux exchange between the package and the environment occurs soon after the fire starts or soon after the fire is extinguished. Assuming a fire environment temperature of 800°C (1472°F), an ambient temperature of 38°C (100°F), and equal view factor and emissivity for both orientations, the difference in absorbed or released heat flux between a vertically- and a horizontally-oriented package would be a function of the convective heat flux exchange only. Whether the package is heating or cooling, or in the vertical or horizontal positions, the model assumes the following dimensions, thermal conditions, and gas properties:

Parameters	Values
Hot temperature	$T_h := 1073K$
Cold temperature	$T_c := 311K$
Flow velocity during fire	$V = 5 \frac{m}{s}$
Diameter of package	$D := 0.5715m$
Length of package	$L := 1.08585m$
Conductivity of the fluid (Air)	$k_f := 52 \cdot 10^{-3} \frac{W}{m \cdot K}$
Kinematic viscosity of fluid (Air)	$\nu := 68 \times 10^{-6} \frac{m^2}{s}$
Thermal diffusivity (Air)	$\alpha := 98 \times 10^{-6} \frac{m^2}{s}$
Prandtl Number	$Pr := \frac{\nu}{\alpha} = 0.694$
Area of cylindrical sides	$A_{cyl} := \pi \cdot D \cdot L = 1.95 m^2$
Area of circular ends	$A_{ends} := \frac{\pi \cdot D^2}{4} = 0.257 m^2$

During the fire, convection is predominately considered to be forced convection as suggested by the ratio of Gr/Re^2 given in Table 3-9 of the Addendum. This ratio is much less than one; hence, only force convection is considered. On the other hand, during the cool-down process, convection is predominately free convection since the buoyancy forces are weak with no imposed flow. Therefore, there are four cases that need to be considered to determine which package orientation is the most thermally damaging configuration for the PAT-1:

1. Horizontal orientation with force convection during the fire
2. Vertical orientation with force convection during the fire
3. Horizontal orientation with free convection during the cool down period
4. Vertical orientation with free convection during the cool down period

In Case 1, the package is in the horizontal position and gas flows around the perimeter of the cylinder and across the vertical flat ends with an imposed velocity of 5 m/s (16.4 ft/s). In Case 2, the package is in the vertical position and gas “impinges” on the bottom (flat end) of the cylinder and flows across the vertical cylinder walls at an imposed velocity of 5 m/s (16 ft/s). In both cases, the maximum convection heat transfer will occur initially during the fire when the temperature of the fire is much greater than that of the package. For both of these cases, the following Nusselt (Nu_{avg}) number correlation is used to determine the effective convective heat transfer coefficient:

$$Nu_{avg}(C, m, Re, Pr) := C \cdot Re^m \cdot Pr^{\frac{1}{3}}$$

where C and m are experimentally determined coefficients; Re is the Reynolds number; and Pr is the Prandtl number. The coefficients C and m vary with the relative orientation between the flow and the object and with the geometry of the object. Values for C and m are given in Incropera and Dewitt (1996) and in Kobus and Shumway (2006).

The equations below show the calculations performed to obtain the effective convection heat transfer coefficient for Case 1. The effective convective heat transfer coefficient was obtained by assuming the same temperature difference for all surfaces (i.e., $T_h - T_s$).

$Re := \frac{V \cdot D}{\nu} = 4.202 \times 10^4$	
$Nu_{cyl} := Nu_{avg}(0.027, 0.805, Re, Pr) = 125.996$	$Nu_{ends} := Nu_{avg}(0.68, 0.5, Re, Pr) = 123.408$
$h_{cyl} := \frac{k_f \cdot Nu_{cyl}}{D} = 11.464 \frac{W}{m^2 \cdot K}$	$h_{ends} := \frac{k_f \cdot Nu_{ends}}{D} = 11.229 \frac{W}{m^2 \cdot K}$
$h_{hor_eff} := \frac{h_{cyl} \cdot A_{cyl} + 2 \cdot h_{ends} \cdot A_{ends}}{A_{cyl} + 2 \cdot A_{ends}} = 11.415 \frac{W}{m^2 \cdot K}$	

The following equations show the calculations performed to obtain the effective convection heat transfer coefficient for Case 2. Note that the top (flat) end of the vertical cylinder is conservatively assumed to have the same convective heat transfer coefficient as the bottom (“impinged”) flat end.

$Re_{cyl} := \frac{V \cdot L}{\nu} = 7.984 \times 10^4$	$Re_{end_btm} := \frac{V \cdot D}{\nu} = 4.202 \times 10^4$
$Nu_{cyl} := Nu_{avg}(0.68, 0.5, Re_{cyl}, Pr) = 170.106$	$Nu_{end_btm} := Nu_{avg}(0.966, 0.46, Re_{end_btm}, Pr) = 114.517$
$h_{cyl} := \frac{k_f \cdot Nu_{cyl}}{L} = 8.146 \cdot \frac{W}{m^2 \cdot K}$	$h_{end_btm} := \frac{k_f \cdot Nu_{end_btm}}{D} = 10.42 \cdot \frac{W}{m^2 \cdot K}$
$h_{ver_eff} := \frac{h_{cyl} \cdot A_{cyl} + 2 \cdot h_{end_btm} \cdot A_{ends}}{A_{cyl} + 2A_{ends}} = 8.62 \cdot \frac{W}{m^2 \cdot K}$	

In Case 3 and Case 4, free convection dominates since the package is allowed to cool naturally. In both cases, the maximum free convection heat transfer will occur immediately after the fire which is when the temperature of the package is much higher than that of the environment. The following Nu_{avg} correlations are used to determine the effective convective heat transfer coefficient for both of these cases:

Nusselt number for free flow across a cylinder

$$Nu_{cyl}(Ra, Pr) := \left[0.60 + \frac{0.387 \cdot Ra^{\frac{1}{6}}}{\left[1 + \left(\frac{0.559}{Pr} \right)^{\frac{9}{16}} \right]^{\frac{8}{27}}} \right]^2,$$

Nusselt number for free flow across a plate

$$Nu_{plate}(Ra, Pr) := \left[0.825 + \frac{0.387 \cdot Ra^{\frac{1}{6}}}{\left[1 + \left(\frac{0.492}{Pr} \right)^{\frac{9}{16}} \right]^{\frac{8}{27}}} \right]^2,$$

Nusselt number for free flow perpendicular to a circular plate

$$Nu_{cyl_ends}(C, m, Ra) := C \cdot Ra^m,$$

where Ra is the Raleigh number, and C and m are empirical constants determined from experiments. The constants C and m vary with the relative orientation between the flow and the object. Values for C and m are given in Incropera and Dewitt (1996).

The equations below show the calculations performed to obtain the effective convection heat transfer coefficient for Case 3.

$Gr := \frac{g \cdot (T_h - T_c) \cdot D^3}{\frac{(T_c + T_h)}{2} \cdot \nu^2} = 4.4 \times 10^8$	$Ra := Gr \cdot Pr = 3 \times 10^8$
$Nu_{hcyl} := Nu_{cyl}(Ra, Pr) = 79.354$	$Nu_{ends} := Nu_{plate}(Ra, Pr) = 84.915$
$h_{hcyl} := \frac{Nu_{hcyl} \cdot k_f}{D} = 7.22 \cdot \frac{W}{m^2 \cdot K}$	$h_{ends} := \frac{Nu_{ends} \cdot k_f}{D} = 7.726 \cdot \frac{W}{m^2 \cdot K}$
$h_{hor_eff} := \frac{h_{hcyl} \cdot A_{cyl} + 2 \cdot h_{ends} \cdot A_{ends}}{A_{cyl} + 2A_{ends}} = 7.326 \cdot \frac{W}{m^2 \cdot K}$	

The following equations show the calculations performed to obtain the effective convection heat transfer coefficient for Case 4. Note that the Nusselt number for flow over a plate was used for the cylindrical sides of the package. This assumption is valid as long as the ratio of D/L is greater or equal to the ratio of $35/Gr^{0.25}$.

$Gr_{vcyl} := \frac{g \cdot (T_h - T_c) \cdot L^3}{\frac{(T_h + T_c)}{2} \cdot \nu^2} = 3 \times 10^9$	$Gr_{ends} := \frac{g \cdot (T_h - T_c) \cdot D^3}{\frac{(T_h + T_c)}{2} \cdot \nu^2} = 4.4 \times 10^8$
$Ra_{vcyl} := Gr_{vcyl} \cdot Pr = 2.1 \times 10^9$	$Ra_{ends} := Gr_{ends} \cdot Pr = 3 \times 10^8$
$\frac{D}{L} \geq \frac{35}{\frac{1}{Gr_{vcyl}^{0.25}}}$	Since D/L is greater than the ratio of $35/Gr^{0.25}$, the vertical plate correlation can be used for the vertical walls of the cylinder.
$Nu_{vcyl} := Nu_{plate}(Ra_{vcyl}, Pr) = 153.5$	$h_{vcyl} := \frac{Nu_{vcyl} \cdot k_f}{L} = 7.4 \cdot \frac{W}{m^2 \cdot K}$
$Nu_{btm_end} := Nu_{cyl_ends}(0.27, 0.25, Ra_{ends}) = 35.6$	$h_{btm_end} := \frac{Nu_{btm_end} \cdot k_f}{D} = 3.2 \cdot \frac{W}{m^2 \cdot K}$
$Nu_{top_end} := Nu_{cyl_ends}(0.54, 0.25, Ra_{ends}) = 71.2$	$h_{top_end} := \frac{Nu_{top_end} \cdot k_f}{D} = 6.5 \cdot \frac{kg}{K \cdot s^3}$
$h_{ver_eff} := \frac{h_{vcyl} \cdot A_{cyl} + h_{btm_end} \cdot A_{ends} + h_{top_end} \cdot A_{ends}}{A_{cyl} + 2 \cdot A_{ends}} = 6.8 \cdot \frac{W}{m^2 \cdot K}$	

In all cases, the difference between the vertical and the horizontal orientation was minimal, with the horizontal orientation being slightly more severe for the package. That is, the horizontal configuration provides the highest convection during the fire and the lowest convection during the cool-down.

For the HAC analysis in the Addendum, a value of $11.5 \text{ W/m}^2\text{-K}$ ($2.03 \text{ Btu/hr-ft}^2\text{-}^\circ\text{F}$) was used during the regulatory fire analysis and a value of $3.5 \text{ W/m}^2\text{-K}$ ($0.62 \text{ Btu/hr-ft}^2\text{-}^\circ\text{F}$) was used during the cool-down period. The values used in the analyses described in the Addendum are conservative, as they bound all values that are presented in this section. That is, a higher convection heat transfer coefficient than those calculated in this section was used for the fire analysis and a lower convection heat transfer coefficient than those calculated in this section was used for the cool-down process.

References:

1. Incropera, F.P. and D.P. DeWitt. "Fundamentals of Heat and Mass Transfer, 4th ed.," New Jersey: Wiley & Sons, Inc., 1996.
2. Kobus, C.J. and G. Shumway. "An experimental investigation into impinging forced convection heat transfer from stationary isothermal circular disks," International J. of Heat and Mass Transfer 49 (2006), pp. 411–414.

This page intentionally left blank

4. CONTAINMENT

The Plutonium Air Transportable Package, Model PAT-1, is certified under Title 10 Code of Federal Regulations, Part 71,¹ by the U.S. Nuclear Regulatory Commission (NRC) per Certificate of Compliance (CoC) USA/0361/B(U)F-96 (current Revision 9).² The current authorized contents are plutonium oxide (PuO₂) and its daughter products, or a mixture of PuO₂ and uranium oxide (UO₂) and its daughter products. The (-96) in the certificate of compliance number indicates that the NRC has evaluated the PAT-1 against the current regulations (including 10 CFR 71.63) and determined that the package satisfies the current regulations.

The purpose of this addendum is to incorporate plutonium metal as a new payload for the PAT-1 package and to demonstrate that the package with the new *T-Ampoule Assembly*^A (Drawing 2A0261, designated the T-Ampoule) and packing within the TB-1 *Containment Vessel* (Drawing 1017, designated TB-1) meet the current containment requirements in 10 CFR 71.³ The 71.63 requirement is satisfied for the PAT-1 with the T-Ampoule and its packing material configuration because the plutonium metal payload contents are solid, pure or alloyed plutonium metal contents or Pu/Be composite samples.

The CoC² describes the TB-1 as a stainless steel containment vessel surrounded by a stainless steel and redwood overpack (*Overpack, AQ*, Drawing 1002, designated AQ-1). The plutonium oxide contents are sealed within a stainless steel product can (designated PC-1). The CoC does not identify the PC-1 as a “containment vessel,” but as a “sealed ... product can.” For the plutonium metal content packaging configuration described in this addendum, the PC-1, aluminum honeycomb top spacer and packing material is replaced with a T-Ampoule, *Ring, Filler* (Drawing 2A0262, designated Ring Filler) and packing material which provides a eutectic prevention barrier between the TB-1 and the plutonium metal content. The T-Ampoule provides the following:

- A eutectic prevention barrier between the stainless steel TB-1 and the plutonium metal payload for NCT, HAC, and air transport accident conditions.
- A T-Ampoule seal area that is not significantly deformed (see Sections 2 and 3 of this addendum) nor a seal temperature that exceeds the allowable temperature of the gasket material during NCT or HAC. The T-Ampoule is expected to remain sealed during NCT and HAC, like the PC-1.
- A retained eutectic prevention barrier function following the air transport accident condition drops and fire. Although the O-ring in the T-Ampoule would be expected to fail in the 10 CFR 71.74 air transport of plutonium fire test, the T-Ampoule is shown in Sections 2 and 3 of this addendum to remain intact (no significant deformation in the seal area and no breaches). The T-Ampoule is more robust than the PC-1.

The documentation and analysis in this section and other sections of this addendum demonstrate that the replacing the PC-1 with oxide content and associated packing material with

^A The drawing titles are in italics and are used interchangeably with the designated names in this addendum. See Section 1.3.2 in this addendum and Chapter 9 in the SAR⁴ for drawing number, title, and revision.

the T-Ampoule with plutonium metal content and associated packing material satisfies the requirements specified in 10 CFR 71.19(d). That is, the modifications of the PAT-1 described in this addendum are not significant with respect to the design, operating characteristics, safe performance of the containment system, or prevention of criticality when the package is subjected to the tests specified in 10 CFR 71.71, 71.73, and 71.74.

4.1 Description of the Containment System

The CoC USA/0361/B(U)F-96² defines the TB-1 as the containment vessel for the PAT-1 for the current PuO₂ and its daughter products and UO₂ and its daughter products as authorized contents. The description of the TB-1 containment vessel is provided in Sections 1 and 9 of the SAR.⁴ For this plutonium metals addendum, the TB-1 containment vessel (see Figure 4-1) provides the containment boundary for the proposed metal contents as it did for the oxide contents. The T-Ampoule replaces the PC-1. The TB-1 O-ring is not used for the plutonium metal shipments.

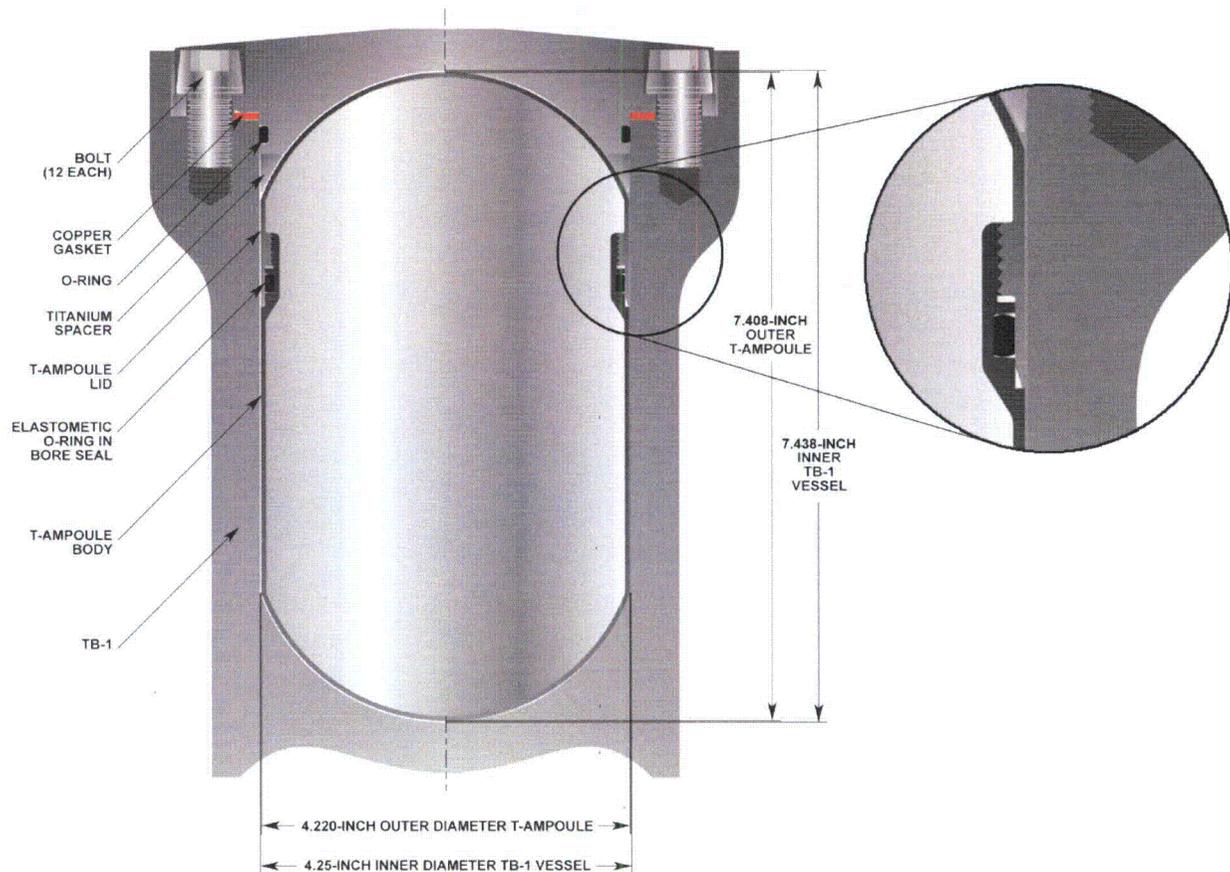


Figure 4-1. TB-1 Containment Vessel and T-Ampoule Contents Container

Table 4-1 of the SAR⁴ summarizes the results of the post-test assessment of PAT-1 containment of its surrogate PuO₂ powder contents during the three transport tests (10 CFR 71.71, 10 CFR 71.73, and 10 CFR 71.74) and demonstrates that the containment criteria are met.

Table 4-1. PAT-1 Package Post-Test Containment

Component	Test Condition	Regulatory Acceptance Standard	Post Test Results	
			Helium Leak-Rate (atm-cc/sec)	Maximum Mass of Powder Release ^b (mg)
TB-1	NCT (71.71)	10^{-6} A ₂ /hr	Less than 1×10^{-10}	0
	HAC (71.73)	A ₂ /week	Less than 1×10^{-10}	0
	Plutonium Air Transport (71.74)	A ₂ /week ^a	Less than 4.5×10^{-5}	0.17

^a For a typical mixture of plutonium oxide (PuO₂) powder, an A₂ quantity is approximately 2.55 mg.

^b Depleted uranium oxide powder was used as the surrogate for plutonium oxide powder during PAT-1 testing. From the SAR, the bounding magnitude of potential PuO₂ powder leakage from the TB-1 vessel would be less than 0.17 mg in one week.

Section 4.5.5 provides a determination of A₂ for the PAT-1 package with plutonium metal in its most dispersible form as contents and Section 4.5.6 provides calculations of the PAT-1 containment vessel's regulatory reference air leakage rates.

The containment criteria for radioactive, fissile material packages are given in 10 CFR 71.51(a)(1) for NCT ($\leq 10^{-6}$ A₂/h), in 71.51(a)(2) for HAC ($\leq A_2$ in a week), and 71.64(a)(1)(i) for accident conditions for air transport of plutonium ($\leq A_2$ in a week). In Section 4.5.5, the A₂ value for the mixture of isotopes was determined to establish the content containment criteria and to determine the maximum release quantity that is allowed by the regulations. The A₂ values of the plutonium content to be shipped were evaluated based on the mass and weight percents of materials shown in Section 1.2.2. The analysis in Section 4.5.5 was conducted to establish an upper limit for the total activity and the maximum number of A₂s proposed for transport in the PAT-1 package. The values were determined using a maximum of 1300 g of plutonium as a bounding condition.

The PAT-1 leak-testing requirements of the containment boundary are based on the smallest maximum allowable leakage rate generated from the maximum plutonium content defined in Table 4.5.5.1 given the allowable leak rates defined in ANSI N14.5-1997, which defines the maximum allowable leakage rate based on the maximum allowable release rate. L_N, L_A, and L_{PA} are the maximum allowable seal leakage rates for NCT, HAC, and accident conditions for air transport of plutonium (ACATP). The worst case maximum allowable leakage rates are used to calculate an equivalent leakage hole diameter following ANSI N14.5-1997, Appendix B, for each condition of transport. This leakage hole diameter is used to calculate a reference air and helium leakage rate for leak testing. The bounding mass for the plutonium content of 1300 g was used in this calculation; note that a 831 g weight limit for the plutonium hollow cylinder was used in the structural analysis and is the maximum plutonium metal content for certification. The use of 1300 g was conservative; the maximum allowable leak rates are calculated using this maximum content mass in a much more dispersive form (oxide powder) for additional conservatism at the highest calculated pressures (assuming the maximum amount of material for decomposition) and temperatures as analyzed in Section 2.12.8.

The regulatory leakage criteria for 1300 g plutonium (bounding case for containment analysis assuming oxide) is shown in Table 4-1a.

In accordance with Table 4.2 of the SAR, the highest measured air leakage rate following the accident conditions for air transport of plutonium was 4.5×10^{-5} cc/s at atmosphere conditions (atm cc/s). This leakage rate is less than the calculated maximum allowable regulatory leakage rate requirement of 2.3570×10^{-3} ref cc/s (air) shown above for ACATP at 613 psia as reported in Section 2.12.8. As a very conservative bounding condition, if the maximum pressure for the TB-1 is used, the calculated maximum allowable regulatory leakage rate requirement is 1.3152×10^{-3} ref cc/s (air) as shown above. It can be concluded that the TB-1 containment vessel inside of the PAT-1 package maintains containment for NCT, HAC, and Accident conditions for air transport of plutonium.

The mass release during the Accident conditions for air transport of plutonium was calculated in Section 4.5.6. For the 1300 g bounding case, the allowable mass release for no decay of Pu-241 is 2.7634×10^{-1} g and for complete decay of Pu-241 to Am-241 is 2.3336×10^{-1} g. The maximum amount of powder released shown in Table 4-1 above after the Accident conditions for air transport of plutonium test was less than 0.17 mg.

Table 4-1a. Regulatory Leakage Criteria for 1300 g Plutonium (Bounding Case)

Isotopic Distribution	NCT @ 218°F – 18.872 psia		HAC @ 276°F – 20.486 psia		ACATP @ 1080°F - 613 psia (P _{PA1})		ACATP @ 1080°F - 1125 psia (P _{PA2})	
	L _{R,N-air} (ref-cm ³ /s)	L _{R,N-He} (cm ³ /s)	L _{R,PA-air} (ref-cm ³ /s)	L _{R,PA-He} (cm ³ /s)	L _{R,A-air} (ref-cm ³ /s)	L _{R,A-He} (cm ³ /s)	L _{R,PA-air} (ref-cm ³ /s)	L _{R,PA-He} (cm ³ /s)
No Pu-241 decay	5.1244 E-06	8.8373 E-06	9.4686 E-02	9.8072 E-02	2.7762 E-03	3.2341 E-03	1.5478 E-03	1.8527 E-03
Complete Pu-241 decay to Am-241	4.2787 E-06	7.4737 E-06	7.9817 E-02	8.3008 E-02	2.3570 E-03	2.7661 E-03	1.3152 E-03	1.5870 E-03

4.1.1 Special Requirements for Plutonium

The proposed plutonium metal contents meet the current requirements set forth in 10 CFR 71.³ In 10 CFR 71.63, “Shipments containing plutonium must be made with contents in solid form, if the contents contain greater than 0.74 TBq (20 Ci) of plutonium.” This requirement is satisfied for the PAT-1 with the T-Ampoule and its packing because the proposed plutonium metal payload contents are solid, pure or alloyed plutonium metal or Pu/Be composite samples.

The PAT-1 Certificate of Compliance² (CoC) (USA/0361/B(U)F-96) (current Revision 9) in Item 5. (a) Packaging, (2) includes the description of the PAT-1,

“A stainless steel containment vessel (designated TB-1) surrounded by a stainless steel and redwood overpack (designated AQ-1). The contents are sealed within a stainless steel product can (designated PC-1) inside the containment vessel.”

The “-96” in the certificate of compliance number indicates that the NRC has evaluated the PAT-1 against the current regulations (including 10 CFR 71.63) and determined that the package satisfies the current regulations. The CoC² identifies the TB-1 as the containment vessel.

For this addendum, the PAT-1 is unchanged from the inside surface of the TB-1 containment vessel to the outside surface of the AQ-1 overpack. The only change to the PAT-1 package is replacement of the PC-1 and its contents, top spacer and packing material with the T-Ampoule and its contents, Ring Filler and packing material. The T-Ampoule, a titanium container, provides eutectic prevention for the metal payload.

The proposed contents include plutonium metal in the form of hollow cylinders, disks, plates, solid cylinders and test samples. The plutonium metal contents are typically loaded into the T-Ampoule in a glove box* containing a limited quantity of oxygen and moisture (≤ 100 ppm ~~0.5%~~). Prior to loading, the contents are brushed clean to remove any oxide present on the surface. The quantity of oxide

* Standard glove box line atmosphere: Nitrogen/Argon/Helium (N/Ar/He) with an oxygen (O) content not exceeding 0.5% and a water content not exceeding 20 ppm.

that could form in the T-Ampoule during transport is limited by ~~the 0.5%~~ less than 100 ppm concentration of oxygen and moisture in the glove box atmosphere. The estimate of oxide formation due to this atmosphere is provided in Section 4.1.1 and is approximately 0.08 g (0.00018 lb). If the atmosphere is assumed to be air and because this is an oxygen-limited system, the estimated quantity of oxide formed on the metal contents is 3.46 g, the activity of PuO₂ formed is 3.74 Ci if no decay is assumed (100% Pu-241), and 0.397 Ci if 100% decay is assumed (100% Am-241). If the metal contents are not cleaned sufficiently, conservative estimates that double the quantity of oxide could be present on the metal, 6.92 g, which is less than 8 Ci.

The function of the T-Ampoule is to provide a safety barrier that prevents the formation of a eutectic between the plutonium metal contents and the iron in the TB-1 containment vessel. The structural analyses in Section 2 of this addendum demonstrate that the bore seal area (see Figure 4-1) of the T-Ampoule is not significantly deformed and is expected to remain intact for all accident conditions analyzed. It can be concluded from these analyses that the T-Ampoule is more robust than the PC-1.

The PC-1 Product Can used for the oxide shipment must not be used for the metal shipment since the iron in the can could possibly form a eutectic with the plutonium metal contents. The titanium material for the T-Ampoule was selected to provide a eutectic prevention barrier between the metallic Pu contents and the TB-1 containment vessel. The *Body, T-Ampoule* (Drawing 2A0259, designated T-Ampoule Body) and *Lid, T-Ampoule* (Drawing 2A0260, designated T-Ampoule Lid) are fabricated from a solid block of Ti-6Al-4V Grade 5 alloy. There are no welds, penetrations, valves, or pressure relief devices in the T-Ampoule. Once placed within the TB-1, the T-Ampoule cannot be opened unintentionally. The clearance between the T-Ampoule and the TB-1 is 0.038 cm (0.015 in.) all around; thus, both walls have immediate contact to resist the impact forces created by the deceleration of the internal Pu contents during the impact accident environment. The sample containers (*Sample Container-1 [SC-1] Assembly*, Drawing 2A0268, designated SC-1, and *Sample Container-2 [SC-2] Assembly*, Drawing 2A0265, designated SC-2) and structure (*Inner Cradle*, Drawing 2A0385, designated Inner Cradle) are also constructed of Ti-6Al-4V Grade 5 alloy that is resistant to the formation of eutectics with the plutonium metal content. Tantalum foil, which may be used to wrap and protect the samples from contamination, ~~and the copper foam, which may be used as packing material, were~~ was selected for ~~their~~ its resistance to eutectic formation.

The shielding evaluation in Section 5 of this addendum demonstrates that the package with plutonium metal contents complies with the dose rate limits of 10 CFR 71.47(a) (non-exclusive use) for the normal conditions of transport (NCT) and 10 CFR 71.51(a)(2) for hypothetical accident conditions (HAC). The criticality evaluation in Section 6 of this addendum demonstrates that the package with plutonium metal contents remains subcritical under NCT and HAC and has a CSI value of 0.1 per 10 CFR 71.59.

The modifications to the PAT-1 package are not significant with respect to design, operating characteristics, or safe operation of the PAT-1 package when subjected to the tests specified in 10 CFR 71.71 and 10 CFR 71.73:

- The PAT-1 package is unchanged from the inside surface of the TB-1 containment vessel to the outside surface of the AQ-1 overpack.

- The T-Ampoule and its contents, Ring Filler and packing material replace the PC-1 and its contents, top spacer and packing material and provide protection for its metal contents.
- The T-Ampoule is a eutectic prevention barrier between the plutonium metal contents and the stainless steel TB-1 containment vessel. The structural analysis in Section 2 of this addendum demonstrates that the T-Ampoule does not breach during the 10 CFR 71.71, 10 CFR 71.73, and 10 CFR 71.74 structural evaluations, thus maintaining its eutectic function.
- The structural analyses in Section 2 demonstrated that the TB-1 met containment requirements. The TB-1's containment capability will be unaffected by the addition of metals contents through the plutonium air transport tests.
- The packing materials within the T-Ampoule are also not susceptible to eutectic formation with plutonium metal.
- The structural analysis in Section 2, the thermal analysis in Section 3, the shielding analysis in Section 5, and the criticality analysis in Section 6 of this addendum show that the requirements of 10 CFR 71.19(d) are met because the modifications to PAT-1 package are not significant with respect to the design, operating characteristics, or safe performance of the package design when subjected to the tests specified in 10 CFR 71.71 and 10 CFR 71.73.

4.1.2 Plutonium Metal Contents

The proposed plutonium metal contents (~~see Section 4.1.1 for estimate of oxides formed within the T-Ampoule~~) include:

- Electro-Refined (ER) Pu (Purity $\geq 99.8\%$ Pu 239) ~~with up to 0.08 g (0.00018 lb) of surface oxide (0.5% oxygen in a limited inert atmosphere).~~
- Pu of various ages containing stabilization alloys such as gallium (Ga) ~~with up to 0.08 g (0.00018 lb) of surface oxide (0.5% oxygen in a limited inert atmosphere).~~
- Composite samples consisting of Pu ~~with up to 0.08 g (0.00018 lb) of surface oxide (0.5% oxygen in a limited inert atmosphere)~~ and beryllium (Be) separated by an alpha barrier (Ti) to preclude neutron generation.
- The forms of the metal include hollow cylinders, cylinders, discs, strips, etc.
- The container configurations within the TB-1 containment vessel are:
- T-Ampoule for bulk metal hollow cylinders and sample containers; and
- Sample containers (SC-1 and SC-2) carried within the Inner Cradle of the T-Ampoule for smaller metal samples.

The isotopic compositions, masses, A_2 values, decay heat, activities, and impurities for ER plutonium metal, alloyed plutonium metal, and bonded plutonium metal are presented below.

4.1.2.1 ER Plutonium Metal⁵

The maximum ER content is 831 g (1.83 lb) for an isotopic composition that ~~excludes~~ assumes no Pu-241 decay (see Table 4-2). The ER metal mass estimates for 3000 A₂ range from 831 g (1.83 lb)

assuming no Pu-241 decay (Table 4-2), and 707 g (1.56 lb) assuming 100% Pu-241 decay (see Table 4-3). Table 4-3 assumes that all of the Pu-241 has decayed to Am-241 which results in the 707 g quantity for 3000 A₂. Note that Table 4-3 is used for comparative purposes only to determine the effect of assuming 100% Pu-241 decay to Am-241. The ER metal will be manufactured and shipped prior to significant Pu-241 decay. The minimum ER cylinder weight as documented in Table 1-1 of Section 1 is 731 g.

Table 4-2. 831 g (1.83 lb): 3,000 A₂ Quantity of ER Plutonium Metal Assuming No Pu-241 Decay to Am-241

831 grams: 3,000 A ₂ quantity of ER Pu metal assuming no Pu241 decay									
Meta-Mass (g) (max)	Mass % (max)	Grams (max)	Isotope	Pu Isotope % (max)	Pu Isotope mass (g)	Decay Heat (W)	Activity (Ci)	A ²	
831.00	Plutonium 93.04%	Plutonium 029.67	Isotope Pu-239	Pu-239	0.05%	0.41	2.35E-01	7.05E+00	2.61E+02
				Pu-237	92.35%	765.20	1.40E+00	4.75E+01	1.75E+03
				Pu-240	6.50%	53.93	3.63E-01	1.24E+01	4.55E+02
				Pu-241	1.00%	8.33	1.04E-01	0.30E+02	5.15E+02
				Pu-242	0.10%	0.83	0.30E-05	3.24E-03	1.30E-01
				Am-241	0.00%	0.00	0.00E+00	0.00E+00	0.00E+00
	Impurities	Impurities		Impurities N/A					
* stated as % balance			Total			2.10E+00	0.97E+02	3.00E+03	

831 grams: 3,000 A ₂ quantity of ER Pu metal assuming no Pu-241 decay to Am-241									
Meta-Mass (g) (max)	Mass % (max)	Grams (max)	Isotope	Pu Isotope % (max)	Pu Isotope mass (g)	Decay Heat (W)	Activity (Ci)	A ²	
831.00	Plutonium 93.04%	Plutonium 029.67	Isotope Pu-239	Pu-239	0.05%	0.41	2.35E-01	7.05E+00	2.61E+02
				Pu-237	92.35%	765.20	1.40E+00	4.75E+01	1.75E+03
				Pu-240	6.50%	53.93	3.63E-01	1.24E+01	4.55E+02
				Pu-241	1.00%	8.33	1.04E-01	0.30E+02	5.15E+02
				Pu-242	0.10%	0.83	0.30E-05	3.24E-03	1.30E-01
				Am-241	0.00%	0.00	0.00E+00	0.00E+00	0.00E+00
	Impurities	Impurities		Impurities N/A					
* stated as % balance			Total			2.10E+00	0.97E+02	3.00E+03	

Table 4-3. 707 g (1.56 lb): 3,000 A₂ Quantity of ER Plutonium Metal Assuming 100% Pu-241 Decay to Am-241

707 grams: 3,000 A ₂ quantity of ER Pu metal assuming 100% Pu241 decay										
Metal Mass (g) (max)	Mass % (max)	Grams (max)	Isotope	Pu Isotopic % (max)	Pu Isotopic mass (g)	Decay Heat (W)	Activity (Ci)	A ²		
707 00	Plutonium 99.84%	Plutonium 705 87	LAFG Special on 551-000720	Pu239	0.05%	0.35	2.00E-01	6.00E+00	2.22E+02	
				Pu239*	92.35%	651.87	1.24E+00	4.04E+01	1.50E+03	
				Pu240	6.50%	45.88	3.26E-01	1.06E+01	3.91E+02	
				Pu241	0.00%	0.00	0.00E+00	0.00E+00	0.00E+00	
				Pu242	0.10%	0.71	7.06E-05	2.75E-03	1.02E-01	
				Am241	1.00%	7.05	8.10E-01	2.40E+01	8.89E+02	
	Impurities	Impurities		Impurities N/A						
0.16%	1.13									
* stated as % balance						Total	2.57E+00	8.10E+01	3.00E+03	
Note: Table shown for comparative purposes only. ER metal will be manufactured and shipped prior to significant Pu241 decay										

707 grams: 3,000 A ₂ quantity of ER Pu metal assuming 100% Pu-241 decay to Am-241										
Metal Mass (g) (max)	Mass % (max)	Grams (max)	Isotope	Pu Isotopic % (max)	Pu Isotopic mass (g)	Decay Heat (W)	Activity (Ci)	A ₂		
707 00	Plutonium 99.84%	Plutonium 705 87	LAFG Special on 551-000720	Pu239	0.05%	0.35	2.00E-01	6.00E+00	2.22E+02	
				Pu239*	92.35%	651.87	1.24E+00	4.04E+01	1.50E+03	
				Pu240	6.50%	45.88	3.26E-01	1.06E+01	3.91E+02	
				Pu241	0.00%	0.00	0.00E+00	0.00E+00	0.00E+00	
				Pu242	0.10%	0.71	7.06E-05	2.75E-03	1.02E-01	
				Am241	1.00%	7.05	8.10E-01	2.40E+01	8.89E+02	
	Impurities	Impurities		Impurities N/A						
0.16%	1.13									
* stated as % balance						Total	2.57E+00	8.10E+01	3.00E+03	
Note: Table shown for comparative purposes only. ER metal will be manufactured and shipped prior to significant Pu-241 decay										

4.1.2.2 Alloyed Plutonium Metal⁵

The maximum contents in two SC-2 sample containers within the T-Ampoule is 676 g (1.49 lb). A₂ calculations were performed assuming no Pu-241 decay (2410 A₂) (see Table 4-4) and Pu-241 decay (2840 A₂) (see Table 4-5). Alloyed plutonium metal may be shipped in a hollow log form in the T-Ampoule if the requirements in Table 1-1 of this addendum and the shipper are met.

Table 4-4. 676 g (1.49 lb): Alloyed Plutonium Metal Assuming 100% Pu-241 Decay to Am-241

676 grams: Alloyed Pu metal assuming 100% Pu241 decay										
Metal Mass (g) (max)	Mass % (max)	Grams (max)	Isotope	Pu Isotopic % (max)	Pu Isotopic mass (g)	Decay Heat (W)	Activity (Ci)	A ²		
676.00	Plutonium 99.84%	Plutonium 666.16	U.S. Specification 59-453723	Pu238	0.05%	0.33	1.89E-01	5.66E+00	2.10E+02	
				Pu239*	92.35%	617.04	1.17E+00	3.83E+01	1.42E+03	
				Pu240	6.50%	43.43	3.06E-01	9.99E+00	3.70E+02	
				Pu241	0.00%	0.00	0.00E+00	0.00E+00	0.00E+00	
				Pu242	0.10%	0.67	6.68E-05	2.61E-03	9.65E-02	
				Am241	1.00%	6.69	7.67E-01	2.27E+01	8.41E+02	
	Impurities	Impurities 0.16%		Impurities 1.09	Impurities: N/A					
Gadolinium	Gadolinium 1.00%	Gadolinium 6.76	Gadolinium: N/A							
* stated as % balance						Total	2.44E+00	7.66E+01	2.84E+03	

676 grams: Alloyed Pu metal assuming 100% Pu-241 decay to Am-241										
Metal Mass (g) (max)	Mass % (max)	Grams (max)	Isotope	Pu Isotopic % (max)	Pu Isotopic mass (g)	Decay Heat (W)	Activity (Ci)	A ²		
676.00	Plutonium 99.84%	Plutonium 666.16	U.S. Specification 59-453723	Pu238	0.05%	0.33	1.89E-01	5.66E+00	2.10E+02	
				Pu239*	92.35%	617.04	1.17E+00	3.83E+01	1.42E+03	
				Pu240	6.50%	43.43	3.06E-01	9.99E+00	3.70E+02	
				Pu241	0.00%	0.00	0.00E+00	0.00E+00	0.00E+00	
				Pu242	0.10%	0.67	6.68E-05	2.61E-03	9.65E-02	
				Am-241	1.00%	6.69	7.67E-01	2.27E+01	8.41E+02	
	Impurities	Impurities 0.16%		Impurities 1.09	Impurities: N/A					
Gadolinium	Gadolinium 1.00%	Gadolinium 6.76	Gadolinium: N/A							
* stated as % balance						Total	2.44E+00	7.66E+01	2.84E+03	

Table 4-5. 676 g (1.49 lb): Alloyed Plutonium Metal Assuming No Pu-241 Decay to Am-241

676 grams: Alloyed Pu metal assuming no Pu241 decay									
Metal Mass (g) (max)	Mass % (max)	Grams (max)	Isotope	Pu Isotope % (max)	Pu Isotope mass (g)	Decay Heat (W)	Activity (Ci)	A ²	
676.00	Plutonium 93.04%	Plutonium 669.16	Pu238	0.05%	0.33	1.63E-01	5.66E+00	2.16E+02	
			Pu239	92.35%	617.04	1.17E+00	3.83E+01	1.42E+03	
			Pu240	6.50%	43.43	3.03E-01	9.99E+00	3.76E+02	
			Pu241	1.00%	6.69	8.35E-02	6.66E+02	4.16E+02	
			Pu242	0.10%	0.67	6.66E-05	2.61E+03	9.65E-02	
			Am241	0.00%	0.00	0.00E+00	0.00E+00	0.00E+00	
	Impurities	Impurities	Impurities: N/A						
0.16%	1.03								
Gadolinium	Gadolinium	Gadolinium: N/A							
1.00%	6.76								
* stated as % balance						Total	1.75E+00	7.22E+02	2.41E+03

676 grams: Alloyed Pu metal assuming no Pu-241 decay to Am-241									
Metal Mass (g) (max)	Mass % (max)	Grams (max)	Isotope	Pu Isotope % (max)	Pu Isotope mass (g)	Decay Heat (W)	Activity (Ci)	A ²	
676.00	Plutonium 93.04%	Plutonium 669.16	Pu238	0.05%	0.33	1.63E-01	5.66E+00	2.16E+02	
			Pu239	92.35%	617.04	1.17E+00	3.83E+01	1.42E+03	
			Pu240	6.50%	43.43	3.03E-01	9.99E+00	3.76E+02	
			Pu241	1.00%	6.69	8.35E-02	6.66E+02	4.16E+02	
			Pu242	0.10%	0.67	6.66E-05	2.61E+03	9.65E-02	
			Am241	0.00%	0.00	0.00E+00	0.00E+00	0.00E+00	
	Impurities	Impurities	Impurities: N/A						
0.16%	1.03								
Gadolinium	Gadolinium	Gadolinium: N/A							
1.00%	6.76								
* stated as % balance						Total	1.75E+00	7.22E+02	2.41E+03

4.1.2.3 Bonded Plutonium Metal⁵

A 60 g (0.13 lb) bonded 16.85 mm diameter × 16.85 mm height Pu/Be metal cylinder (or a number of smaller cylinders [up to 25 5.1 mm diameter × 5.1 mm height cylinders] as described in Table 1.1, Section 1 of this addendum) may each be shipped in the SC-1 sample container for a total payload weight of 180 g (0.39 lb) (657 A₂) or in the SC-2 sample container for a total payload weight of 120 g (0.26 lb) within the T-Ampoule. The composite payload weight is limited to 60 grams or less in each sample container. See Table 4-6 for estimate of curies, number of A₂, decay heat, weight, and isotopic composition of the Pu/Be material based upon a disk configuration.

Table 4-6. 60 g (0.13 lb): Bonded Pu/Be Metal Disk Assuming 100% Pu-241 Decay to Am-241

60 grams: Bonded Pu/Be metal disc assuming 100% Pu241 decay									
Component %	Metal Mass (g) (max)	Mass % (max)	Grams (max)	Isotope	Pu Isotopic % (max)	Pu Isotopic mass (g)	Decay Heat (W)	Activity (Ci)	A ²
Pu metal 87.00%	52.20	MT52 Plutonium 93.04%	MT52 Plutonium 51.59	Pu238	0.05%	0.03	1.46E-02	4.39E-01	1.62E+01
				Pu239	92.35%	47.65	9.65E-02	2.95E+00	1.05E+02
				Pu240	6.50%	3.35	2.32E-02	7.71E-01	2.66E+01
				Pu241	0.00%	0.00	0.00E+00	0.00E+00	0.00E+00
				Pu242	0.10%	0.05	5.16E-06	2.01E-04	7.45E-03
				Am241	1.00%	0.52	5.92E-02	1.75E+00	6.50E+01
		Impurities	Impurities	0.16%	0.03	Impurities N/A			
		Gadolinium	Gadolinium	1.00%	0.52	Gadolinium N/A			
Beryllium 13.00%	7.80	Beryllium 13.00%	Beryllium 7.80	Beryllium N/A					
Alpha Barrier 0.00%	0.00	Alpha Barrier 0.00%	Alpha Barrier 0.00	Assumes no alpha barrier to yield maximum dose					
100.00%	60.00					←←← Totals →→→	1.62E-01	5.92E+00	2.19E+02
* stated as % balance									

60 grams: Bonded Pu/Be metal disc assuming 100% Pu-241 decay to Am-241									
Component %	Metal Mass (g) (max)	Mass % (max)	Grams (max)	Isotope	Pu Isotopic % (max)	Pu Isotopic mass (g)	Decay Heat (W)	Activity (Ci)	A ²
Pu metal 87.00%	52.20	MT52 Plutonium 93.04%	MT52 Plutonium 51.59	Pu238	0.05%	0.03	1.46E-02	4.39E-01	1.62E+01
				Pu239	92.35%	47.65	9.65E-02	2.95E+00	1.05E+02
				Pu240	6.50%	3.35	2.32E-02	7.71E-01	2.66E+01
				Pu241	0.00%	0.00	0.00E+00	0.00E+00	0.00E+00
				Pu242	0.10%	0.05	5.16E-06	2.01E-04	7.45E-03
				Am241	1.00%	0.52	5.92E-02	1.75E+00	6.50E+01
		Impurities	Impurities	0.16%	0.03	Impurities N/A			
		Gadolinium	Gadolinium	1.00%	0.52	Gadolinium N/A			
Beryllium 13.00%	7.80	Beryllium 13.00%	Beryllium 7.80	Beryllium N/A					
Alpha Barrier 0.00%	0.00	Alpha Barrier 0.00%	Alpha Barrier 0.00	Assumes no alpha barrier to yield maximum dose					
100.00%	60.00					←←← Totals →→→	1.62E-01	5.92E+00	2.19E+02
* stated as % balance									

4.2 Containment under Normal Conditions of Transport (NCT)

The TB-1 containment vessel meets the regulatory acceptance standard for NCT of 10⁻⁶ A₂/hr as demonstrated in Table 4-1. The T-Ampoule is not a containment vessel under NCT.

The thermal analysis in Section 3.3 of this addendum, which analyzed a localized 25-watt (85.3 Btu/hr) thermal source against the O-ring seal of the T-Ampoule, indicated an average temperature of 103.3°C (218°F).

The internal pressure within the TB-1 during NCT with an internal heat generation of 25 watts (85.3 Btu/hr) from the plutonium metal contents indicated a maximum pressure of 18.8 psia, due to the temperature difference. The calculation assumes an initial room temperature of 20°C (70°F), then:

$$P_2 = 1\text{atm} * (678/530R) = 1.28\text{ atm or } \sim 18.8\text{ psia}$$

To determine the pressure generated from the alpha decay of plutonium, the TB-1 was assumed to be filled at ambient temperature and to reach the NCT temperature quickly (see Section 0). The helium pressure, shown below, is thus:

$$P_{\text{He}} = n_{\text{He}} * (RT/V)$$

where $n_{\text{He}} = \text{gm}_{\text{He}}/4$

T = the NCT average temperature in Kelvin (absolute)

V = 1.252 liters

R = 0.082 l-atm/mole-K, the gas constant

Pressure in psi = 14.7 * Pressure in atmospheres

The pressure from helium (He) generation for 1300 g Pu (for conservatism) at NCT temperature via alpha decay is ~~15.1~~0.067 psia.

The total pressure as the result of internal heat generation and alpha decay is ~~33.9~~18.9 psia, or ~~19.2~~4.2 psig, which defines the maximum normal operating pressure (MNOP) for the TB-1.

The MNOP of ~~19.2~~4.2 psig (~~33.9~~18.9 psia) calculated above is slightly less than that calculated for the PuO₂ contents in the SAR (34.3 psia) since a small quantity of moisture was assumed to be present in the PuO₂ within the TB-1.

4.3 Containment under Hypothetical Accident Conditions (HAC)

The TB-1 meets the regulatory acceptance standard for HAC of A₂ in a week as documented in Table 4-1. The T-Ampoule is not a containment vessel under HAC.

The thermal analysis in Section 3.4 of this addendum includes localized heating produced by the plutonium metal contents, and the HAC evaluation indicated that the average temperature is 136°C (276°F) in the T-Ampoule. The temperature of the T-Ampoule seal does not exceed the manufacturer's specification for the operating range of the seal material (204°C [400°F]).

The pressure calculated within the TB-1 as the result of internal heat generation of 25 watts from the plutonium metal contents and the HAC indicated that the maximum pressure is 20.4 psi. The calculation assumes an initial room temperature of 21°C (70°F), then:

$$P_2 = 1\text{atm} \cdot (736\text{R}/530\text{R}) = 1.39\text{ atm or } \sim 20.4\text{ psia}$$

Pressure from He generation for 1300 g of Pu metal (for conservatism) via alpha decay is ~~16.4~~0.073 psia from Section 4.5.3 of this addendum.

The total pressure as a result of internal heat generation and alpha decay is ~~36.8~~20.5 psia. The pressure of ~~36.8~~20.5 psia is less than the HAC pressure reported in the SAR⁴ (38.7 psia [Section 3.5.4 of the SAR⁴]).

4.3.1 Containment under Plutonium Air Transport Fire Test

The TB-1 meets the regulatory acceptance standard for the plutonium air transport tests of A₂ in a week as documented in Table 4-1. The T-Ampoule is not a containment vessel under the plutonium air transport conditions.

In Section 2.12.8, ~~LA-UR-08-07810, Thermal Decomposition of Viton® O-rings for PAT-1 Accident Scenario,~~⁶ the calculation (~~see Section 0~~) was performed to examine the rise in pressure from decomposition of the elastomeric O-rings within the ~~TB-1, T-Ampoule,~~ and two SC-2 or three SC-1 sample containers and a range of weights for ancillary plastics. The three SC-1 configuration and the selected 70 gram quantity of HDPE yielded the highest pressure rise of 572 psia. ~~The pressure rise assuming that the O-rings char was 443.17 psi, and with no char (complete decomposition which is very conservative) was 887.28 psi.~~

Including the rise in pressure from ambient temperature to 582°C (1080°F) of 42.7 psia and the helium pressure generation from 1300 g of plutonium (for conservatism) from alpha decay of ~~34.20.11~~ psia, the total pressure within the TB-1 is ~~964.2615~~ psia. The PAT-1 SAR,⁴ Section 4.4.2 stipulates that the maximum allowable TB-1 pressure during the post-fire plutonium air transport accident condition was 1,110 psia.

The results of the highly conservative calculation of the thermal degradation of *Viton A*® *O*-rings and ancillary plastic (HDPE) in ~~LA-UR-08-07810~~ Section 2.12.8 show that this maximum internal pressure is not exceeded.

In summary, the TB-1 structure is unaffected by the impact and thermal environments and maintains its containment integrity for HAC.

4.4 Leakage Rate Tests for Type B Packages

The leakage rate tests for the TB-1, which is the primary containment vessel, ~~remain unchanged from the SAR.~~⁴ is described in Sections 7 and 8.

4.5 Appendix

4.5.1 References

1. United States. Nuclear Regulatory Commission. Code of Federal Regulations. 10 CFR 71. "Packaging and Transportation of Radioactive Material." January 1, 2009.
2. United States. Nuclear Regulatory Commission. "Certificate of Compliance for Radioactive Material Packages." Certificate Number 0361, Revision Number 9, Docket Number 71-0361, Package Identification Number USA/0361/B(U)F-96. March 4, 2009.
3. United States. Nuclear Regulatory Commission. Code of Federal Regulations. 10 CFR 71.63. "Special requirements for plutonium shipments," as published in 69 FR 3795. January 26, 2004.
4. United States. Nuclear Regulatory Commission. NUREG-0361, "Safety Analysis Report for the Plutonium Air Transportable Package, Model PAT-1." Washington, D.C. 1978.
5. Caviness, M. L., and J.B. Rubin. "Authorized Contents Proposed for the Plutonium Air Transporter (PAT-1) Packaging (U)," LA-UR-08-05154. Los Alamos National Laboratory. Los Alamos, NM: August 7, 2008.
6. Rubin, J. B. "Thermal Decomposition of Viton® O-rings for the PAT-1 Packaging Accident Scenario," LA-UR-~~09-05112~~-10-05846. Los Alamos National Laboratory. Los Alamos, NM: ~~December 10, 2008~~ August 31, 2010.

4.5.2 PAT-1 Contents

LA-UR-08-05154

Approved for public release;
distribution is unlimited.

Title: Authorized Contents Proposed for the Plutonium Air
Transporter (PAT-1) Packaging (U)

Author(s): Michael L. Caviness, PMT-3
Jim B. Rubin, PMT-2

Intended for: Development of an application to the US Nuclear Regulatory
Commission for the transport of plutonium metal by air in the
Plutonium Air Transporter (PAT-1) packaging



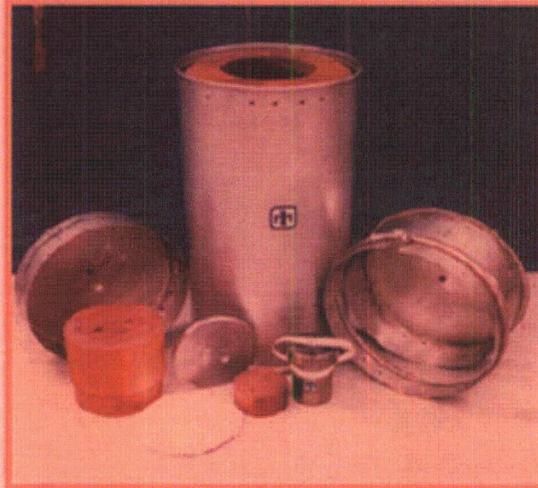
Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-05NA25396. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Form 836 (7/05)

Authorized Contents Proposed for the Plutonium Air Transporter (PAT-1) Packaging

Authors: Michael Caviness, PMT-3, Nuclear Materials Management

Jim Rubin, PMT-2, Actinide Process Chemistry

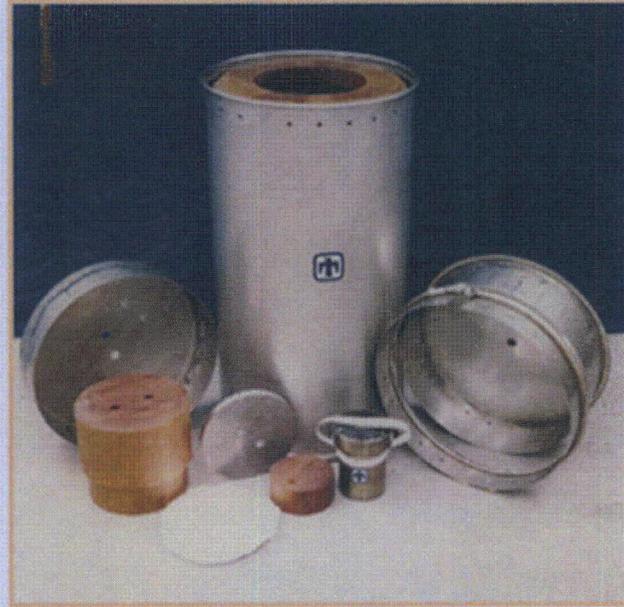


PAT-1 Packaging Assembly

Authorized Contents Proposed for the Plutonium Air Transporter (PAT-1) Packaging

Authors: Michael Caviness, PMT-3, Nuclear Materials Management

Jim Rubin, PMT-2, Actinide Process Chemistry



PAT-1 Packaging Assembly

Page 1 of 5

ELECTRO-REFINED PLUTONIUM METAL

1,300 grams: Maximum quantity of Electro-refined (ER) Pu metal excluding Pu241 decay

Metal Mass (g) (max)	Mass % (max)	Grams (max)	Isotope	Pu Isotopic % (max)	Pu Isotopic mass (g)	Decay Heat (W)	Activity (Ci)	A ²	
1,300.00	99.9%	1297.92	Pu238	0.05%	0.65	3.89E+01	1.10E+01	4.09E+02	
			Pu239P	92.35%	1198.63	2.29E+00	7.40E+01	2.75E+03	
			Pu240	6.50%	84.36	5.86E+01	1.94E+01	7.19E+02	
			Pu241	1.00%	12.96	1.62E+01	1.30E+03	8.11E+02	
			Pu242	0.10%	1.30	1.30E+04	5.09E+03	1.87E+01	
			Am241	0.00%	0.00	0.00E+00	0.00E+00	0.00E+00	
Impurities: N/A									
* stated as % balance						Total	3.41E+00	1.40E+03	4.66E+03

Reference Values	
Decay Heat	
Isotope	Watt/gram
Pu238	5.87E+01
Pu239	1.90E+03
Pu240	7.19E+02
Pu241	1.28E+02
Pu242	1.90E+04
Am241	1.19E+01

DOE-ER-07-018, Table 9.6

831 grams: 3,000 A² quantity of ER Pu metal assuming no Pu241 decay

Metal Mass (g) (max)	Mass % (max)	Grams (max)	Isotope	Pu Isotopic % (max)	Pu Isotopic mass (g)	Decay Heat (W)	Activity (Ci)	A ²	
831.00	99.9%	829.67	Pu238	0.05%	0.41	2.39E+01	7.28E+00	2.81E+02	
			Pu239P	92.35%	768.20	1.49E+00	4.79E+01	1.78E+03	
			Pu240	6.50%	53.93	3.81E+01	1.24E+01	4.58E+02	
			Pu241	1.00%	8.30	1.04E+01	8.30E+02	5.19E+02	
			Pu242	0.10%	0.83	8.30E+04	3.24E+03	1.30E+01	
			Am241	0.00%	0.00	0.00E+00	0.00E+00	0.00E+00	
Impurities: N/A									
* stated as % balance						Total	2.19E+00	8.87E+02	3.00E+03

Reference Values		
A ² values of radioisotopes		
Isotope	A ² (Ci)	Ci/g
Pu238	2.70E+02	1.70E+01
Pu239	3.70E+03	6.30E+03
Pu240	2.70E+02	2.30E+01
Pu241	1.80E+00	1.00E+02
Pu242	2.70E+03	3.80E+03
Am241	2.70E+02	3.40E+00

46 CFR 173.405, Table of A1 and A2 values for Radioisotopes

707 grams: 3,000 A² quantity of ER Pu metal assuming 100% Pu241 decay

Metal Mass (g) (max)	Mass % (max)	Grams (max)	Isotope	Pu Isotopic % (max)	Pu Isotopic mass (g)	Decay Heat (W)	Activity (Ci)	A ²	
707.00	99.9%	705.07	Pu238	0.05%	0.35	2.00E+01	6.00E+00	2.20E+02	
			Pu239P	92.35%	651.87	1.24E+00	4.94E+01	1.80E+03	
			Pu240	6.50%	45.96	3.29E+01	1.06E+01	3.81E+02	
			Pu241	0.00%	0.00	0.00E+00	0.00E+00	0.00E+00	
			Pu242	0.10%	0.71	7.07E+04	2.79E+03	1.02E+01	
			Am241	1.00%	7.06	5.10E+01	2.40E+01	8.80E+02	
Impurities: N/A									
* stated as % balance						Total	2.87E+00	8.10E+01	3.00E+03

Impurity Limits (max)		
Values in parts per million (ppm)		
Al: 100	Pu: 200	Ta: 100
Am: 200	Ca: 300	Th: 100
B: 50	Hg: 500	Tl: 100
Be: 3	Mn: 100	U: 100
C: 200	Ni: 100	W: 200
Co: 500	Nb: 100	Zn: 100
Cr: 10	Pb: 100	
Cr: 100	Si: 100	
Cu: 100	Sr: 100	

LANS Specification 97-008728

Note: Table shown for comparative purposes only. ER metal will be manufactured and shipped prior to significant Pu241 decay.

ALLOYED PLUTONIUM METAL

676 grams Alloyed Pu metal assuming 0% Pu-241 decay

Isotope	Pu Isotope % (Mass)	Pu Isotope mass (g)	Decay Heat (W)	Activity (Ci)	A ²
Pu-238	0.2%	0.30	1.62E+01	6.82E+00	2.12E+03
Pu-239	89.2%	602.04	1.17E+00	3.22E+01	1.42E+03
Pu-240	0.5%	43.43	3.77E+01	9.28E+00	3.72E+03
Pu-241	1.0%	6.76	9.28E+00	6.82E+00	4.12E+03
Pu-242	0.1%	0.67	6.69E+01	2.71E+01	8.49E+03
Am-241	0.0%	0.00	0.00E+00	0.00E+00	0.00E+00
Cerium N/A					
Gadolinium N/A					
Total			1.72E+00	7.22E+01	2.47E+03

Isotope	Weighting
Pu-238	0.27E+01
Pu-239	1.60E+01
Pu-240	2.17E+01
Pu-241	1.22E+01
Pu-242	0.69E+01
Am-241	0.12E+01

Reference Values		
A ² values of isotopes		
Isotope	A ² (Ci)	Q ₂₃₅
Pu-238	2.12E+03	1.72E+01
Pu-239	3.22E+01	0.22E+01
Pu-240	3.72E+03	2.32E+01
Pu-241	4.12E+03	1.02E+01
Pu-242	8.49E+03	3.92E+01
Am-241	0.00E+00	0.00E+00

676 grams Alloyed Pu metal assuming 100% Pu-241 decay

Isotope	Pu Isotope % (Mass)	Pu Isotope mass (g)	Decay Heat (W)	Activity (Ci)	A ²
Pu-238	0.2%	0.30	1.62E+01	6.77E+00	2.12E+03
Pu-239	89.2%	602.04	1.17E+00	3.22E+01	1.42E+03
Pu-240	0.5%	43.43	3.77E+01	9.28E+00	3.72E+03
Pu-241	0.0%	0.00	0.00E+00	0.00E+00	0.00E+00
Pu-242	0.1%	0.67	6.69E+01	2.71E+01	8.49E+03
Am-241	1.0%	6.76	2.77E+01	2.77E+01	0.41E+03
Cerium N/A					
Gadolinium N/A					
Total			2.46E+00	7.62E+01	2.64E+03

Reference Values		
Values by decay heat (W)		
Isotope	Decay Heat (W)	Decay Heat (W)
Am-241	0.00E+00	0.00E+00
Ce N/A	0.00E+00	0.00E+00
Gd N/A	0.00E+00	0.00E+00
Pu-238	1.62E+01	0.27E+01
Pu-239	1.17E+00	0.22E+01
Pu-240	3.77E+01	2.32E+01
Pu-241	9.28E+00	1.02E+01
Pu-242	6.69E+01	3.92E+01
Am-241	2.77E+01	0.41E+03

ALLOYED PLUTONIUM METAL

676 grams: Alloyed Pu metal assuming no Pu-241 decay to Am-241

Material (g)	Mass % (wt)	Grams (wt)	Isotope	Pu Isotope % (wt)	Pu Isotope mass (g)	Decay Heat (MW)	Activity (Ci)	A
676.00	Plutonium 99.04%	Plutonium 670.15	Pu-238	0.05%	0.33	1.05E-01	5.67E-02	2.10E-02
			Pu-239	92.35%	617.61	1.17E-02	3.03E-01	1.42E-03
			Pu-240	5.52%	3.73	2.05E-01	9.22E-02	3.20E-02
			Pu-241	1.02%	0.69	0.25E-02	6.69E-02	4.17E-02
			Pu-242	0.17%	0.12	6.67E-05	2.81E-03	9.16E-02
			Am-241	0.00%	0.00	0.00E-00	0.00E-00	0.00E-00
	Impurities	Impurities 0.15%	Impurities 1.00	Impurities: N/A				
Gadolinium	Gadolinium 1.00%	Gadolinium 6.76	Gadolinium: N/A					
Classed as % balance			Total			2.25E-02	2.20E-01	2.41E-03

Reference Values
Decay Heat

Isotope	Wt % (wt)
Pu-238	5.67E-01
Pu-239	1.05E-02
Pu-240	2.17E-02
Pu-241	1.27E-02
Pu-242	1.00E-04
Am-241	1.41E-01

676 grams: Alloyed Pu metal assuming 100% Pu-241 decay to Am-241

Material (g)	Mass % (wt)	Grams (wt)	Isotope	Pu Isotope % (wt)	Pu Isotope mass (g)	Decay Heat (MW)	Activity (Ci)	A
676.00	Plutonium 99.04%	Plutonium 670.15	Pu-238	0.05%	0.33	1.05E-01	5.67E-02	2.10E-02
			Pu-239	92.35%	617.61	1.17E-02	3.03E-01	1.42E-03
			Pu-240	5.52%	3.73	2.05E-01	9.22E-02	3.20E-02
			Pu-241	0.00%	0.00	0.00E-00	0.00E-00	0.00E-00
			Pu-242	0.17%	0.12	6.67E-05	2.81E-03	9.16E-02
			Am-241	1.00%	0.67	2.82E-01	2.20E-01	8.41E-02
	Impurities	Impurities 0.15%	Impurities 1.00	Impurities: N/A				
Gadolinium	Gadolinium 1.00%	Gadolinium 6.76	Gadolinium: N/A					
Classed as % balance			Total			2.41E-02	2.05E-01	2.25E-03

Reference Values
Activity (Ci)

Isotope	A (Ci)	Wt % (wt)
Pu-238	2.10E-02	5.67E-01
Pu-239	2.82E-02	6.70E-03
Pu-240	2.20E-02	2.20E-02
Pu-241	1.00E-02	1.00E-02
Pu-242	2.20E-02	3.03E-01
Am-241	2.20E-02	2.82E-01

Reference Values
Decay Heat (MW)

Isotope	Decay Heat (MW)	Wt % (wt)
Pu-238	1.05E-01	5.67E-01
Pu-239	3.03E-01	6.70E-03
Pu-240	9.22E-02	2.20E-02
Pu-241	6.69E-02	1.00E-02
Pu-242	2.81E-03	3.03E-01
Am-241	2.20E-01	2.82E-01

BONDED PLUTONIUM METAL

60 grams: Bonded Pu/Be metal disc assuming 100% Pu241 decay

Compound %	Metal Mass (g) (max)	Mass % (max)	Grams (max)	Isotope	Pu Isotope % (max)	Pu Isotope mass (g)	Decay Heat (W)	Activity (Ci)	A*
Pu metal 87.0%	52.30	Wt% Plutonium 95.54%	Wt% Plutonium 51.58	Pu238	0.05%	0.03	1.48E-02	4.36E-01	1.62E+01
				Pu239	40.35%	47.66	9.05E-02	2.66E+00	1.06E+02
				Pu240	6.50%	3.35	2.38E-02	7.71E-01	2.86E+01
				Pu241	0.30%	0.30	0.00E+00	0.00E+00	0.00E+00
				Pu242	0.12%	0.07	8.16E-06	2.24E-04	7.49E-03
				Am241	1.20%	0.52	5.82E-02	1.79E+00	6.80E+01
		Impurities	Impurities	Impurities: N/A					
		0.10%	0.06	Gallium: N/A					
		1.00%	0.52	Beryllium: N/A					
Beryllium 13.00%	7.80	Beryllium 13.00%	Beryllium 7.80	Beryllium: N/A					
Alpha Barrier 0.00%	0.00	Alpha Barrier 0.00%	Alpha Barrier 0.00	Assumes no alpha barrier to yield maximum dose					
100.00%	60.00			4 4 4 Table 9-3-3			1.88E+01	8.40E+00	3.18E+02

Reference Values		
Decay Heat		
Isotope	Wt%/gsm	
Pu238	8.67E-01	
Pu239	1.90E-03	
Pu240	7.10E-03	
Pu241	1.26E-02	
Pu242	1.00E-04	
Am241	1.05E+01	

50E-010-3(12-01), Table 9-3

Reference values		
A* value of microcuries		
Isotope	A* (Ci)	Dij
Pu238	2.70E+02	1.70E+01
Pu239	2.70E+02	6.20E+02
Pu240	2.70E+02	2.30E+01
Pu241	1.80E+00	1.00E+02
Pu242	2.70E+02	3.90E+03
Am241	2.70E+02	3.40E+00

49-CFR 173.405, Table 9.3(1) and (2) Values for Radioisotopes

Dose rate calculations:

Total (max) dose (Sv)	Surface	0.3m (1ft)	1.0m (3.3ft)
	9.72E+03	2.69E+01	2.48E+01

The maximum dose rates stated above assumes the following: 1) three bonded Pu/Be discs are assumed to preferentially ablate during HAC conditions (see figure at right); 2) the alpha barrier between the 3 bonded Pu/Be discs are conservative; 3) the 3 bonded Pu/Be discs without alpha barriers yield 5 times dose of Pu/Be contact surfaces; and 4) the dose rate is calculated for SX at given Pu/Be surface area of an undefined disc diameter (max)***

*** The bonded Pu/Be disc diameter is not stated due to a security classification determination. The information (disc diameter) is available through classified consultation.

Unit dose (transfuran) provided in LANL Memorandum, SF-3-06-02, Crawford to Carless, Subject: WTSO-Be Interface Disc Dose Calculations

Configuration Layout:

The following configuration shows 3 bonded Pu/Be discs preferentially ablated with the alpha barriers conservatively removed to yield 5 times dose of Pu/Be contact surfaces.

Surface contact 1F	Pu	Disc 1
Surface contact 2F	Be	
Surface contact 3F	Pu	Disc 2
Surface contact 4F	Be	
Surface contact 5F	Pu	Disc 3
Surface contact 6F	Be	

Impurity Limits (max)		
Values in parts per million (ppm)		
Al: 100	Pu: 200	Ta: 100
Am: 200	Ce: N/A	Ti: 100
B: 50	Mg: 500	Th: N/A
Be: N/A	Mn: 100	U: 100
C: 200	Na: 100	W: 200
Ca: 500	Sp: 100	Zn: 100
Ce: 10	Pb: 100	
Cr: 100	Sr: 100	
Cu: 100	Sn: 100	

LANL Specification 337-4307-05

Page 4 of 5

Maximum Pu Oxide and Oxides (O₂) formed in the TB-1 with a 21% Oxygen

Oxide and Oxide Values

AD energy (10 ¹⁸ Btu/yr)			150% energy (10 ¹⁸ Btu/yr)		
Isotope	AD energy (10 ¹⁸ Btu/yr)	Pu mass	Isotope	AD energy (10 ¹⁸ Btu/yr)	Pu mass
Pu-238	1.72E+00	3.84E+00	Pu-238	1.72E+00	3.84E+00
Pu-239	7.27E+00	1.89E+01	Pu-239	7.27E+00	1.89E+01
Pu-240	3.22E+01	5.17E+01	Pu-240	3.22E+01	5.17E+01
Pu-241	7.47E+02	1.49E+03	Pu-241	7.47E+02	1.49E+03
Pu-242	3.46E+03	1.39E+04	Pu-242	3.46E+03	1.39E+04
AMU-11	0.00E+00	0.00E+00	AMU-11	3.46E+03	1.39E+04
Total	3.46E+03	3.74E+04	Total	3.46E+03	3.74E+04

Weight % Pu	
Pu-238	0.05%
Pu-239	63.25%
Pu-240	4.10%
Pu-241	0.00%
Pu-242	0.07%
AMU-11	0.00%
Total	100.000000000000%

Reference Values		
Isotope	A ^o (g)	G ₀
Pu-238	2.72E+02	1.22E+01
Pu-239	3.27E+02	6.25E+01
Pu-240	3.72E+02	2.92E+01
Pu-241	1.80E+00	1.00E+00
Pu-242	2.72E+02	3.46E+00
AMU-11	2.72E+02	3.46E+00

G₀(1) = G₀, Total of A^o and G₀ shown for AMU-11

Basis of Calculated Values			
Variable	Variable Unit	Value	Description of value
pressure inside of TD-1 P	atmosphere (atm)	0.20	1 atmosphere pressure at 21% O ₂ in TD-1
internal volume of TD-1 V	cubic centimeters (cm ³)	1.40E+00	internal volume of TD-1 without contents as noted in the PAT-1 CAS
oxygen gas constant R	constant	0.20	gas constant value based on pressure and volume units
temperature, T	kelvin (K)	298.15	assumes room temperature of 20C
O ₂ in TD-1 internal volume, n	mole	0.013	n = PV/RT. Ideal gas law is suitable since the compressibility factor (Z) for air at 1.01 bar and (298.15K) is 0.9999
Pu ₂ O ₃ formed from O ₂ in the TD-1 m	mole	0.013	Pu ₂ O ₃ + O ₂ = Pu ₂ O ₄
molar mass Pu ₂ O ₃ , M	constant	370	grams per mole assuming molar mass of Pu = 240
Pu ₂ O ₃ formed, g	grams (g)	3.45	grams of Pu ₂ O ₃ formed when all O ₂ reacts completely in the sealed TD-1

Maximum PU Oxide and Curies (Ci) formed in the TB-1 with a 21% Oxygen

Oxide and Curie Values						Isotopic % (max)		Reference Values		
No Pu-241 decay (100% Pu-241)			100% Pu-241 decay (100% Am-241)			Pu-238	0.05%	radionuclides ¹		
Isotope	Oxide (g)	Curies	Isotope	Oxide (g)	Curies	Pu-239	92.35%	Isotope	A ₂ (Ci)	Ci/g
Pu-238	173E-03	2.94E-02	Pu-238	173E-03	2.94E-02	Pu-240	6.50%	Pu-238	2.70E-02	170E+01
Pu-239	3.20E+00	198E-01	Pu-239	3.20E+00	198E-01	Pu-241	100%	Pu-239	2.70E-02	6.20E-02
Pu-240	2.25E-01	5.17E-02	Pu-240	2.25E-01	5.17E-02	Pu-242	0.10%	Pu-240	2.70E-02	2.30E-01
Pu-241	3.46E-02	3.46E+00	Pu-241	0.00E+00	0.00E+00	Am-241	0.00%	Pu-241	160E+00	100E+02
Pu-242	3.46E-03	1.35E-05	Pu-242	3.50E-03	1.37E-05	LANL Specification 55Y-638728		Pu-242	2.70E-02	3.90E-03
Am-241	0.00E+00	0.00E+00	Am-241	3.46E-02	1.8E-01	49 CFR 173.435, Table of A ₁ and A ₂ Values for Radionuclides				
Total:	3.46E+00	3.74E+00	Total:	3.46E+00	3.97E-01					

Basis of Calculated Values			
Variable:	Variable Unit:	Value	Definition of value
pressure inside of TB-1 P	atmosphere (atm)	0.21	1atmosphere pressure at 21% O ₂ in TB-1
Internal volume of TB-1 V	cubic centimeters (cm ³)	1460.00	internal volume of TB-1 without contents as stated in the PAT-1SAR
universal gas constant, R	constant	82.06	gas constant values based on pressure and volume units
temperature, T	kelvin (K)	298.00	assumes room temperature of 25°C
O ₂ in TB-1 internal volume, n	moles	0.03	n = PV/RT (ideal gas law is suitable since the compressibility factor (Z) for air at 101bar and 15°C(59°F) is 0.9992)
PuO ₂ formed from O ₂ in the TB-1, m	moles	0.03	Pu(s) + O ₂ (g) -> PuO ₂ (s)
Molar mass PuO ₂ , M	constant	276	grams per mole (assuming molar mass of Pu = 244)
PuO ₂ formed, g	grams (g)	3.46	grams of PuO ₂ formed when all O ₂ reacts completely in the sealed TB-1

Basis of Calculated Values			
Variable:	Variable Unit:	Value	Definition of value
pressure inside of TB-1 P	atmosphere (atm)	0.00010	1atmosphere pressure at 100ppm O ₂ in TB-1
Internal volume of TB-1 V	cubic centimeters (cm ³)	1460.00	internal volume of TB-1 without contents as stated in the PAT-1SAR
universal gas constant, R	constant	82.06	gas constant values based on pressure and volume units
temperature, T	kelvin (K)	298.00	assumes room temperature of 25°C
O ₂ in TB-1 internal volume, n	moles	5.97E-06	n = PV/RT (ideal gas law is suitable since the compressibility factor (Z) for air at 101bar and 15°C (59°F) is 0.9992)
PuO ₂ formed from O ₂ in the TB-1, m	moles	5.97E-06	Pu(s) + O ₂ (g) -> PuO ₂ (s)
Molar mass PuO ₂ , M	constant	276.06	grams per mole (assuming molar mass of Pu = 244)
PuO ₂ formed, g	grams (g)	165E-03	grams of PuO ₂ formed when all O ₂ reacts completely in the sealed TB-1

4.5.2.1 Summary of Maximum Pu Oxide and Curies (Ci) Formed in the TB-1 with 21% and 100 ppm Oxygen:

An analysis¹ was performed to determine the maximum quantity of PuO₂ that would form on the plutonium metal content contained within the TB-1 containment vessel. The table on Page 5 of 5 in LA-UR-08-05154 in this appendix presents the analysis methodology for calculating the quantities of oxides formed. The TB-1, which is normally filled with glove box atmosphere, was assumed to contain 1 atmosphere of air at 21% O₂. Using a TB-1 conservative internal empty volume of 1460 cm³ (89.19 in³) and the Ideal Gas Law, there are 0.013 moles of O₂ in the internal volume and 0.013 moles of PuO₂ in the TB-1. The molar mass of PuO₂ is 276 g/mole assuming a molar mass of Pu = 244. The quantity of PuO₂ formed is 3.46 g when all of the O₂ reacts completely inside of a sealed TB-1. Because this is an oxygen-limited system, no more than 3.46 g (0.0076 lb) of PuO₂ are formed when all of the O₂ completely reacts inside of a sealed TB-1 containment vessel.

If a glove box atmosphere (assume all 100 ppm oxygen in an inert atmosphere) is assumed within the TB-1, the quantity of PuO₂ formed on the surface of the plutonium metal content is 1.64 mg (3.62 E-6 lb).

To determine the isotopic composition of the PuO₂ that was formed, Los Alamos National Laboratory (LANL) Specification 55Y-638728⁴ on Page 5 of 5 in LA-UR-08-0515 in this appendix presents the maximum isotopic composition for the Pu contents. Included in the table are oxide and curie values assuming no decay (100% Pu-241) and 100% Pu-241 decay to ~~(100% Am-241)~~.

The above calculations provide estimates of the amount of oxides formed due to the oxygen present in the T-Ampoule from the glovebox atmosphere and assumption of air. The oxide formation does not affect the safety of the package since the containment analysis assumed that all of the plutonium material was in its most dispersible form.

4.5.2.2 Reference

1. Caviness, M. L., and J.B. Rubin. "Authorized Contents Proposed for the Plutonium Air Transporter (PAT-1) Packaging (U)," LA-UR-08-05154. Los Alamos National Laboratory. Los Alamos, NM: August 7, 2008.

~~For 3.46 g of oxide, the activity of PuO₂ is 3.74 Ci if no decay is assumed (100% Pu-241), and 0.397 Ci if 100% decay is assumed (100% Am-241). 3.46 g of oxide would be the maximum quantity, since the process of packing the plutonium metal includes brushing the plutonium metal with a stiff bristle brush just before transfer into an inert glove box. The brushing removes the majority of the surface oxide and any remaining oxide would be of minimal mass. For conservatism, in addition to the process knowledge provided, even if the quantity of oxide evaluated in the TB-1 volume calculation (3.46 g) was doubled, the total yield would be 6.92 g with an activity of 7.76 Ci.~~

~~If a glove box atmosphere (0.5% oxygen in a limited inert atmosphere) is assumed within the TB-1, the quantity of PuO₂ formed on the surface of the plutonium metal content is 0.08 g (0.00018 lb).~~

4.5.3 Helium Generation

PAT-1 Analyses for Helium Generation

Ruth F. Weiner

Sandia National Laboratories

Calculation of Helium Production

A helium is produced when an alpha particle, which is a helium nucleus, picks up an electron. The production rate of helium is thus directly proportional to the production rate of alpha particles. The production rate of alpha particles is equal to the rate of decay of alpha emitters: each decay results in an alpha particle. The basic equation for radioactive decay is

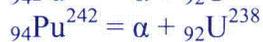
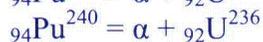
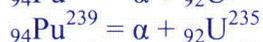
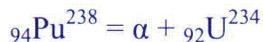
$$N = N_0 \exp(-\lambda t) \tag{1}$$

Where N = the number of atoms of the radionuclide at time t

N_0 = the number of atoms of the radionuclide at time t=0

$\lambda = \ln 2 / t_{1/2}$; $t_{1/2}$ is the half life of the radionuclide

When a radionuclide emits an alpha particle, the atomic number decreases by 2 and the mass number decreases by 4, because an alpha particle is a helium nucleus: ${}^2_2\text{He}^4$. The radionuclides in delta plutonium emit alpha particles by the following equations:



However, ${}_{94}\text{Pu}^{241}$ is a beta emitter and decays by the equation ${}_{94}\text{Pu}^{241} = \beta^- + {}_{95}\text{Am}^{241}$ since a beta particle is the same as an electron. ${}_{95}\text{Am}^{241}$ decays by emitting an alpha particle by the equation

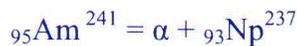


Table 1a gives the radioactive composition of delta plutonium and the half-lives of each radioactive component:

Table 1a. Radioactive Composition of Delta and Half-Lives of Each Radioactive Component

Element	Atomic mass	gm/gm delta ¹	t _{1/2} (yr)	t _{1/2} sec	λ	Bq/gm delta	Ci/gm delta
Pu	238	0.0001	87.7	2.77E+09	2.51E-10	6.34E+07	1.71E-03
Pu	239	0.9378	24100	7.60E+11	9.12E-13	2.15E+09	5.82E-02
Pu	240	0.06	6560	2.07E+11	3.35E-12	5.04E+08	1.36E-02
Pu	241	0.002	14.4	4.54E+08	1.53E-09	7.62E+09	2.06E-01
Pu	242	0.0002	3.75E+05	1.18E+13	5.86E-14	2.92E+04	7.88E-07
Am	241	0	432	1.36E+10	5.09E-11	0	0
U	234	0	2.46E+05	7.76E+12	8.93E-14	0	0

One becquerel (Bq) is = sec^{-1} . The numbers in the last column were obtained by the equation that converts mass to radioactivity:

$$Bq = \frac{(\ln 2)(6.02 \times 10^{23}) \left(\frac{\text{gm}}{\text{gm atoms/gwt}} \right)}{t_{1/2}} \quad (2)$$

Where Bq = the radioactivity in sec^{-1} ; one curie (Ci) = 3.7×10^{10} Bq.

6.02×10^{23} is Avogadro's number, the number of atoms in one gram atomic weight

$t_{1/2}$ = half life of the radionuclide in seconds.

$$\ln(2)/t_{1/2} = \lambda$$

So that, e.g.

$$6.34 \times 10^{-7} = \lambda (6.02 \times 10^{23})(0.0001/238) = (2.51 \times 10^{-10}) (6.02 \times 10^{23})(0.0001/238)$$

The last column in Table 1 thus gives the initial activity—the N_0 —of each radionuclide.

${}_{95}\text{Am}^{241}$ builds up as ${}_{94}\text{Pu}^{241}$ decays, by the first Bateman equation

$$N_{Am}(t) = N_{Pu}(t) * \left(\frac{\lambda_{Pu}}{\lambda_{Am} - \lambda_{Pu}} \right) * \{ \exp(-\lambda_{Pu}t) - \exp(-\lambda_{Am}t) \}$$

Where $N_{Am}(t)$ = the number of ${}_{95}\text{Am}^{241}$ atoms at time t

$N_{Pu}(t)$ = the number of ${}_{94}\text{Pu}^{241}$ atoms at time t

Am refers to ${}_{95}\text{Am}^{241}$

Pu refers to ${}_{94}\text{Pu}^{241}$

${}_{92}\text{U}^{234}$ builds up by a similar equation. Because of its long half-life, however, its alpha decay does not contribute significantly to helium production.

Conversion from radioactivity to weight can be done in two ways—by using Equation (2) or by calculating Bq/gm delta or Ci/gm delta from Table a (which is based on Equation (2)). The latter was used, resulting in Table 1b. The values for ${}_{95}\text{Am}^{241}$ and ${}_{92}\text{U}^{234}$ were calculated using Equation (2).

Table 1b. Weight Conversions

Element	gm/gm delta	Ci/gm delta	Ci/gm
Pu-238	0.0001	1.71E-03	1.71E-03
Pu-239	0.9378	5.82E-02	6.21E-02
Pu-240	0.06	1.36E-02	2.27E-01
Pu-241	0.002	2.06E-01	1.03E+02
Pu-242	0.0002	7.88E-07	3.94E-03
Am-241	0	0	3.43
U-234	0	0	6.21E-03

Every decay produces an alpha particle and every alpha particle becomes a helium atom. Equation (1) allows calculation of decay of each radionuclide, and Equation (2) relates that decay to loss of mass of that radionuclide. Because of conservation of mass, the mass of He produced is equal to the total loss of mass of the decaying radionuclides, or

$$\text{gm}(\text{He}_t) = \text{gm}(\text{delta}_{t=0}) - \{ \text{gm}(\text{Pu-238}_t) + \text{gm}(\text{Pu-239}_t) + \text{gm}(\text{Pu-240}_t) + \text{gm}(\text{Pu-241}_t) + \text{gm}(\text{Pu-242}_t) + \text{gm}(\text{Am-241}_t) + \text{gm}(\text{U-234}_t) \} \quad (3)$$

where the subscript t is time.

Calculation of Gas Pressure

The basic equation is the Ideal Gas Law:

$$\begin{aligned} pV &= nRT \\ p &= nRT/V \end{aligned} \quad (4)$$

where p = total pressure in the volume V

V = void volume

T = absolute temperature (K)

N = number of moles of gas

R = the gas constant, 0.082 liter-atm/mole-K

Calculations were done using liters, atmospheres, etc., and converted to psia at the end.

Conversions used were:

1 mole He = 4 grams

$n(\text{He}_t) = \text{gm}(\text{He}_t)/4$

$\text{gm}(\text{He}_t)$: from Equation (3).

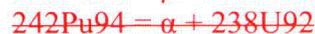
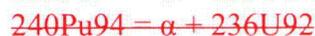
$K = ^\circ\text{C} + 273$

1 atm = 14.7 psia

Since the container was initially filled at atmospheric pressure, the total pressure in atmospheres at any time t, at a particular volume and temperature, is

$$p_t = 1 + p(\text{He}_t) = 1 + n(\text{He}_t)*RT/V \quad (5)$$

Alpha particles are helium nuclei and, when emitted during alpha decay, pick up two electrons to form helium, a chemically inert gas that exists as helium atoms. In the present case, the relevant nuclear reactions are:



Helium is an ideal gas and at the temperatures considered behaves in accordance with the ideal gas law

$$PV = nRT \quad (1)$$

where P = pressure

V = volume

n = moles of gas

R = the gas constant, 0.082 liter-atmospheres per mole-K.

T = temperature in absolute Kelvin

Air also behaves like an ideal gas. An assumption is made in this analysis that air makes up the internal free volume of the containers evaluated. The pressure in a sealed container will be the sum of the partial pressures of gases in the container: helium and air in the present case. For fixed values of V and T, pressure is directly proportional to the total moles of gas generated, so that the partial pressure of helium is directly proportional to the moles of helium generated by alpha decay. The atomic weight of helium is 4 grams per gram-atom (4 grams per mole).

The TB-1 and the TB-1 internal configurations were considered. From Table 1, the SC-1 and SC-2 quantities were less than the 831 g Electro-Refined (ER) Pu hollow cylinder. The 1300 gram Pu metal hollow cylinder represents an upper limit of the quantity of Pu metal considered for the PAT-1 and is presented for reference. Consequently, pressure calculations for alpha decay were only performed for the 831 and 1300 gram amounts. The temperatures considered were the "normal" extremes, -40°C (-40°F) NCT temperature (104°C), and a temperature of 136°C (276°F) in a HAC fire temperature, and 582°C (1080°F) in the accident conditions of plutonium air transport fire. A calculation at room temperature (21°C) was provided for reference.

Containments were assumed to be loaded at 1 atmosphere pressure (14.7 psi). Table 1 presents RT/V at these temperatures and volumes.

A 1300 g evaluation is provided for reference in Tables 1, 3, and 5; 831 g is the maximum plutonium content for this addendum. Helium generation was calculated from the mass loss of the Pu isotopic mixture. Table 2 shows the helium generation, per g of plutonium isotopic mixture, for the first year.

Table 1. RT/V for TB-1 Containment

	Maximum Plutonium Mass (g)	676 g SC-2	523 g SC-1	831 g Pu Hollow Cylinder	1300 g Pu Hollow Cylinder
		Void Volume TB-1 Containment Boundary (liters)			
		1.103	1.112	1.275	1.252
Deg C	K	P=RT/V(atm/mole)^a			
104.00	377.00	27.80	27.84	24.25	24.69
-40.00	233.00	17.18	17.21	14.99	15.26
136.00	409.00	30.16	30.21	26.31	26.79
20.00	294.00	21.64	21.62	18.85	19.19

	Maximum Plutonium Mass (g)	676.00	523.00	831.00	1300.00
		Void Volume TB-1 Containment Boundary (liters)			
		1.1103	1.1112	1.2749	1.2519
Deg C	Deg K	P=RT/V(atm/mole)^a			
104	377	27.84	27.82	24.25	24.69
-40	233	17.21	17.19	14.99	15.26
136	409	30.21	30.18	26.31	26.79
20	293	21.64	21.62	18.85	19.19
562	855	63.15	63.09	54.99	56.00

^aR=0.082 liter-atm/mole-deg

Table 2. Helium Generation Per Gram of Pu Isotopic Mixture for One Year

Time (weeks)	gm Pu	gm He	moles He	Time (weeks)	gm Pu	gm He	moles He
0	1.00E+00	0.00E+00	0.00E+00	28	1.00E+00	6.92E-05	1.73E-05
2	1.00E+00	5.01E-06	1.25E-06	30	1.00E+00	7.41E-05	1.85E-05
4	1.00E+00	1.00E-05	2.50E-06	32	1.00E+00	7.90E-05	1.97E-05
6	1.00E+00	1.50E-05	3.75E-06	34	1.00E+00	8.39E-05	2.10E-05
8	1.00E+00	2.00E-05	5.00E-06	36	1.00E+00	8.88E-05	2.22E-05
10	1.00E+00	2.50E-05	6.25E-06	38	1.00E+00	9.37E-05	2.34E-05
12	1.00E+00	3.00E-05	7.49E-06	40	1.00E+00	9.85E-05	2.46E-05
14	1.00E+00	3.49E-05	8.73E-06	42	1.00E+00	1.03E-04	2.59E-05
16	1.00E+00	3.99E-05	9.97E-06	44	1.00E+00	1.08E-04	2.71E-05
18	1.00E+00	4.48E-05	1.12E-05	46	1.00E+00	1.13E-04	2.83E-05
20	1.00E+00	4.98E-05	1.24E-05	48	1.00E+00	1.18E-04	2.95E-05
22	1.00E+00	5.47E-05	1.37E-05	50	1.00E+00	1.23E-04	3.08E-05
24	1.00E+00	5.93E-05	1.48E-05	52	1.00E+00	1.28E-04	3.20E-05
26	1.00E+00	6.42E-05	1.61E-05				

Time (weeks)	gm Pu	gm He	moles He	Time (weeks)	gm Pu	gm He	moles He
0	1.00E+00	0.00E+00	0.00E+00	28	1.00E+00	3.06E-07	7.65E-08
2	1.00E+00	2.19E-08	5.46E-09	30	1.00E+00	3.28E-07	8.20E-08
4	1.00E+00	4.37E-08	1.09E-08	32	1.00E+00	3.50E-07	8.74E-08
6	1.00E+00	6.56E-08	1.64E-08	34	1.00E+00	3.72E-07	9.29E-08
8	1.00E+00	8.74E-08	2.19E-08	36	1.00E+00	3.93E-07	9.83E-08
10	1.00E+00	1.09E-07	2.73E-08	38	1.00E+00	4.15E-07	1.04E-07
12	1.00E+00	1.31E-07	3.28E-08	40	1.00E+00	4.37E-07	1.09E-07
14	1.00E+00	1.53E-07	3.82E-08	42	1.00E+00	4.59E-07	1.15E-07
16	1.00E+00	1.75E-07	4.37E-08	44	1.00E+00	4.81E-07	1.20E-07
18	1.00E+00	1.97E-07	4.92E-08	46	1.00E+00	5.03E-07	1.26E-07
20	1.00E+00	2.19E-07	5.46E-08	48	1.00E+00	5.24E-07	1.31E-07
22	1.00E+00	2.40E-07	6.01E-08	50	1.00E+00	5.46E-07	1.37E-07
24	1.00E+00	2.62E-07	6.56E-08	52	1.00E+00	5.68E-07	1.42E-07
26	1.00E+00	2.84E-07	7.10E-08				

The partial pressure of helium and the total pressure in the containment depend on the containment volume and on the temperature. The total pressure is the sum of the partial pressure of helium and the air pressure at which the containment was loaded; the latter is assumed to be one atmosphere (14.7 psi).

The container was assumed to be filled at ambient temperature (294 K or 21 deg. C) and to reach the indicated temperature quickly. At two weeks the indicated temperature would have been reached. The helium pressure, shown in Table 1, is thus:

$$P_{\text{He}} = n_{\text{He}} \cdot (RT/V)$$

where $n_{\text{He}} = \text{gm}_{\text{He}}/4$

T= the final average temperature in Kelvin (absolute)

V = 1.252 liters

R = 0.082 l-atm/mole K, the gas constant.

Pressure in psi= 14.7*Pressure in atmospheres

Table 3 shows helium pressure increase in atm and psi in the TB-1 in weeks up to one year assuming 1300 g Pu content.

Table 3. Helium Pressure Increase Generation in TB-1, Void Volume 1.252 Liters, for 1300 g Pu

	deg C	104	-40	136	104	-40	136
	K	377	233	409	377	233	409
	RT/V	24.69	15.26	26.79	24.69	15.26	26.79
	gm Pu	1300.00	1300.00	1300.00	1300.00	1300.00	1300.00
weeks	mole He/gm	Atmospheres			PSI		
0	0.00E+00	0.000	0.000	0.000	0.000	0.000	0.000
2	1.25E-06	0.040	0.025	0.044	0.591	0.365	0.641
4	2.50E-06	0.080	0.050	0.087	1.181	0.730	1.282
6	3.75E-06	0.120	0.074	0.131	1.771	1.094	1.921
8	5.00E-06	0.161	0.099	0.174	2.359	1.458	2.560
10	6.25E-06	0.200	0.124	0.218	2.947	1.821	3.197
12	7.49E-06	0.240	0.149	0.261	3.534	2.184	3.834
14	8.73E-06	0.280	0.173	0.304	4.120	2.547	4.470
16	9.97E-06	0.320	0.198	0.347	4.706	2.908	5.105
18	1.12E-05	0.360	0.222	0.390	5.291	3.270	5.740
20	1.24E-05	0.400	0.247	0.434	5.874	3.631	6.373
22	1.37E-05	0.439	0.271	0.477	6.457	3.991	7.006
24	1.48E-05	0.476	0.294	0.516	6.997	4.324	7.591
26	1.61E-05	0.516	0.319	0.559	7.578	4.684	8.221
28	1.73E-05	0.555	0.343	0.602	8.159	5.042	8.851
30	1.85E-05	0.594	0.367	0.645	8.739	5.401	9.481
32	1.97E-05	0.634	0.392	0.688	9.318	5.759	10.109
34	2.10E-05	0.673	0.416	0.730	9.896	6.116	10.736
36	2.22E-05	0.712	0.440	0.773	10.474	6.473	11.363
38	2.34E-05	0.752	0.465	0.816	11.050	6.830	11.988
40	2.46E-05	0.791	0.489	0.858	11.626	7.186	12.613
42	2.59E-05	0.830	0.513	0.900	12.202	7.541	13.237
44	2.71E-05	0.869	0.537	0.943	12.776	7.896	13.860

46	2.83E-05	0.908	0.561	0.985	13.350	8.251	14.483
48	2.95E-05	0.947	0.585	1.027	13.922	8.605	15.104
50	3.08E-05	0.989	0.611	1.073	14.534	8.982	15.767
52	3.20E-05	1.028	0.635	1.115	15.105	9.336	16.387

	deg C	104	-40	136	582	104	-40	136	582	
	deg Kelvin	377	233	409	855	377	233	409	855	
	RT/V	24.69	15.26	26.79	56.18	24.69	15.26	26.79	56.18	
	gm Pu	1300.0	1300.0	1300.0	1300.0	1300.0	1300.0	1300.0	1300.0	
week s	mole He/gm	Atmospheres					PSI			
		0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	5.46E-09	1.75E-04	1.08E-04	1.90E-04	3.98E-04	2.58E-03	1.59E-03	2.80E-03	5.85E-03	
4	1.09E-08	3.51E-04	2.17E-04	3.81E-04	7.96E-04	5.16E-03	3.19E-03	5.59E-03	1.17E-02	
6	1.64E-08	5.26E-04	3.25E-04	5.71E-04	1.19E-03	7.74E-03	4.78E-03	8.39E-03	1.75E-02	
8	2.19E-08	7.02E-04	4.34E-04	7.61E-04	1.59E-03	1.03E-02	6.37E-03	1.12E-02	2.34E-02	
10	2.73E-08	8.77E-04	5.42E-04	9.51E-04	1.99E-03	1.29E-02	7.97E-03	1.40E-02	2.92E-02	
12	3.28E-08	1.05E-03	6.50E-04	1.14E-03	2.39E-03	1.55E-02	9.56E-03	1.68E-02	3.51E-02	
14	3.82E-08	1.23E-03	7.59E-04	1.33E-03	2.78E-03	1.80E-02	1.12E-02	1.96E-02	4.09E-02	
16	4.37E-08	1.40E-03	8.67E-04	1.52E-03	3.18E-03	2.06E-02	1.27E-02	2.24E-02	4.68E-02	
18	4.92E-08	1.58E-03	9.76E-04	1.71E-03	3.58E-03	2.32E-02	1.43E-02	2.52E-02	5.26E-02	
20	5.46E-08	1.75E-03	1.08E-03	1.90E-03	3.98E-03	2.58E-02	1.59E-02	2.80E-02	5.85E-02	
22	6.01E-08	1.93E-03	1.19E-03	2.09E-03	4.38E-03	2.84E-02	1.75E-02	3.08E-02	6.43E-02	
24	6.56E-08	2.10E-03	1.30E-03	2.28E-03	4.77E-03	3.09E-02	1.91E-02	3.36E-02	7.02E-02	
26	7.10E-08	2.28E-03	1.41E-03	2.47E-03	5.17E-03	3.35E-02	2.07E-02	3.64E-02	7.60E-02	
28	7.65E-08	2.46E-03	1.52E-03	2.66E-03	5.57E-03	3.61E-02	2.23E-02	3.92E-02	8.19E-02	
30	8.20E-08	2.63E-03	1.63E-03	2.85E-03	5.97E-03	3.87E-02	2.39E-02	4.20E-02	8.77E-02	
32	8.74E-08	2.81E-03	1.73E-03	3.04E-03	6.36E-03	4.13E-02	2.55E-02	4.48E-02	9.36E-02	
34	9.29E-08	2.98E-03	1.84E-03	3.23E-03	6.76E-03	4.38E-02	2.71E-02	4.76E-02	9.94E-02	
36	9.83E-08	3.16E-03	1.95E-03	3.43E-03	7.16E-03	4.64E-02	2.87E-02	5.03E-02	1.05E-01	
38	1.04E-07	3.33E-03	2.06E-03	3.62E-03	7.56E-03	4.90E-02	3.03E-02	5.31E-02	1.11E-01	
40	1.09E-07	3.51E-03	2.17E-03	3.81E-03	7.96E-03	5.16E-02	3.19E-02	5.59E-02	1.17E-01	
42	1.15E-07	3.68E-03	2.28E-03	4.00E-03	8.35E-03	5.41E-02	3.35E-02	5.87E-02	1.23E-01	
44	1.20E-07	3.86E-03	2.38E-03	4.19E-03	8.75E-03	5.67E-02	3.51E-02	6.15E-02	1.29E-01	
46	1.26E-07	4.03E-03	2.49E-03	4.38E-03	9.15E-03	5.93E-02	3.66E-02	6.43E-02	1.34E-01	
48	1.31E-07	4.21E-03	2.60E-03	4.57E-03	9.55E-03	6.19E-02	3.82E-02	6.71E-02	1.40E-01	

50	1.37E-07	4.38E-03	2.71E-03	4.76E-03	9.94E-03	6.45E-02	3.98E-02	6.99E-02	1.46E-01
52	1.42E-07	4.56E-03	2.82E-03	4.95E-03	1.03E-02	6.70E-02	4.14E-02	7.27E-02	1.52E-01

Table 4 shows the helium pressure increase in atm and psi in the TB-1, in weeks up to one year assuming an 831 g Pu content.

Table 4. Helium Pressure Generation Pressure in TB-1, Void Volume 1.275 Liters, for 831 g Pu

	deg C	104	-40	136	104	-40	136
	K	377	233	409	377	233	409
	RT/V	24.25	14.99	26.31	24.25	14.99	26.31
	gm Pu	831	831	831	831	831	831
weeks	mole He/gm	Atmospheres			PSI		
0	0.00E+00	0.000	0.000	0.000	0.000	0.000	0.000
2	1.25E-06	0.025	0.016	0.027	0.371	0.229	0.402
4	2.50E-06	0.050	0.031	0.055	0.741	0.458	0.804
6	3.75E-06	0.076	0.047	0.082	1.111	0.687	1.206
8	5.00E-06	0.101	0.062	0.109	1.481	0.915	1.607
10	6.25E-06	0.126	0.078	0.137	1.850	1.143	2.007
12	7.49E-06	0.151	0.093	0.164	2.218	1.371	2.407
14	8.73E-06	0.176	0.109	0.191	2.586	1.598	2.806
16	9.97E-06	0.201	0.124	0.218	2.954	1.826	3.204
18	1.12E-05	0.226	0.140	0.245	3.321	2.052	3.603
20	1.24E-05	0.251	0.155	0.272	3.687	2.279	4.000
22	1.37E-05	0.276	0.170	0.299	4.053	2.505	4.397
24	1.48E-05	0.299	0.185	0.324	4.392	2.714	4.764
26	1.61E-05	0.324	0.200	0.351	4.757	2.940	5.160
28	1.73E-05	0.348	0.215	0.378	5.121	3.165	5.556
30	1.85E-05	0.373	0.231	0.405	5.485	3.390	5.951
32	1.97E-05	0.398	0.246	0.432	5.849	3.615	6.345
34	2.10E-05	0.423	0.261	0.458	6.212	3.839	6.739
36	2.22E-05	0.447	0.276	0.485	6.574	4.063	7.132
38	2.34E-05	0.472	0.292	0.512	6.936	4.287	7.525
40	2.46E-05	0.496	0.307	0.539	7.298	4.510	7.917
42	2.59E-05	0.521	0.322	0.565	7.659	4.733	8.309
44	2.71E-05	0.546	0.337	0.592	8.019	4.956	8.700
46	2.83E-05	0.570	0.352	0.618	8.379	5.179	9.090
48	2.95E-05	0.594	0.367	0.645	8.739	5.401	9.481
50	3.08E-05	0.621	0.384	0.673	9.122	5.638	9.897
52	3.20E-05	0.645	0.399	0.700	9.481	5.860	10.286

	deg C	104	-40	136	582	104	-40	136	582
	deg Kelvin	377	233	409	855	377	233	409	855
	RT/V	24.69	15.26	26.79	56.18	24.69	15.26	26.79	56.18
	gm Pu	1300.0	1300.0	1300.0	1300.0	1300.0	1300.0	1300.0	1300.0
week s	mole He/gm	Atmospheres				PSI			
0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	5.46E-09	1.75E-04	1.08E-04	1.90E-04	3.98E-04	2.58E-03	1.59E-03	2.80E-03	5.85E-03
4	1.09E-08	3.51E-04	2.17E-04	3.81E-04	7.96E-04	5.16E-03	3.19E-03	5.59E-03	1.17E-02
6	1.64E-08	5.26E-04	3.25E-04	5.71E-04	1.19E-03	7.74E-03	4.78E-03	8.39E-03	1.75E-02
8	2.19E-08	7.02E-04	4.34E-04	7.61E-04	1.59E-03	1.03E-02	6.37E-03	1.12E-02	2.34E-02
10	2.73E-08	8.77E-04	5.42E-04	9.51E-04	1.99E-03	1.29E-02	7.97E-03	1.40E-02	2.92E-02
12	3.28E-08	1.05E-03	6.50E-04	1.14E-03	2.39E-03	1.55E-02	9.56E-03	1.68E-02	3.51E-02
14	3.82E-08	1.23E-03	7.59E-04	1.33E-03	2.78E-03	1.80E-02	1.12E-02	1.96E-02	4.09E-02
16	4.37E-08	1.40E-03	8.67E-04	1.52E-03	3.18E-03	2.06E-02	1.27E-02	2.24E-02	4.68E-02
18	4.92E-08	1.58E-03	9.76E-04	1.71E-03	3.58E-03	2.32E-02	1.43E-02	2.52E-02	5.26E-02
20	5.46E-08	1.75E-03	1.08E-03	1.90E-03	3.98E-03	2.58E-02	1.59E-02	2.80E-02	5.85E-02
22	6.01E-08	1.93E-03	1.19E-03	2.09E-03	4.38E-03	2.84E-02	1.75E-02	3.08E-02	6.43E-02
24	6.56E-08	2.10E-03	1.30E-03	2.28E-03	4.77E-03	3.09E-02	1.91E-02	3.36E-02	7.02E-02
26	7.10E-08	2.28E-03	1.41E-03	2.47E-03	5.17E-03	3.35E-02	2.07E-02	3.64E-02	7.60E-02
28	7.65E-08	2.46E-03	1.52E-03	2.66E-03	5.57E-03	3.61E-02	2.23E-02	3.92E-02	8.19E-02
30	8.20E-08	2.63E-03	1.63E-03	2.85E-03	5.97E-03	3.87E-02	2.39E-02	4.20E-02	8.77E-02
32	8.74E-08	2.81E-03	1.73E-03	3.04E-03	6.36E-03	4.13E-02	2.55E-02	4.48E-02	9.36E-02
34	9.29E-08	2.98E-03	1.84E-03	3.23E-03	6.76E-03	4.38E-02	2.71E-02	4.76E-02	9.94E-02
36	9.83E-08	3.16E-03	1.95E-03	3.43E-03	7.16E-03	4.64E-02	2.87E-02	5.03E-02	1.05E-01
38	1.04E-07	3.33E-03	2.06E-03	3.62E-03	7.56E-03	4.90E-02	3.03E-02	5.31E-02	1.11E-01
40	1.09E-07	3.51E-03	2.17E-03	3.81E-03	7.96E-03	5.16E-02	3.19E-02	5.59E-02	1.17E-01
42	1.15E-07	3.68E-03	2.28E-03	4.00E-03	8.35E-03	5.41E-02	3.35E-02	5.87E-02	1.23E-01
44	1.20E-07	3.86E-03	2.38E-03	4.19E-03	8.75E-03	5.67E-02	3.51E-02	6.15E-02	1.29E-01
46	1.26E-07	4.03E-03	2.49E-03	4.38E-03	9.15E-03	5.93E-02	3.66E-02	6.43E-02	1.34E-01
48	1.31E-07	4.21E-03	2.60E-03	4.57E-03	9.55E-03	6.19E-02	3.82E-02	6.71E-02	1.40E-01
50	1.37E-07	4.38E-03	2.71E-03	4.76E-03	9.94E-03	6.45E-02	3.98E-02	6.99E-02	1.46E-01
52	1.42E-07	4.56E-03	2.82E-03	4.95E-03	1.03E-02	6.70E-02	4.14E-02	7.27E-02	1.52E-01

Table 5 presents helium pressure increase for all four masses of Pu at ambient temperature (21°C; 294 K) with their respective void volumes.

Table 5. Helium Pressure Generation Increase in TB-1, Void Volume at 21 degrees C (294 K)

	V (liters)	1.103	1.112	1.275	1.252	1.103	1.112	1.275	1.252
	RT/V	21.71	21.70	18.91	19.26	21.71	21.70	18.91	19.26
	gm Pu	676.00	523.00	831.00	1300.00	676.00	523.00	831.00	1300.0
Weeks	mole He/gm	Atmospheres				PSI			
0	0.00E+00	0.00	0.00	0.00	0.00	0.000	0.000	0.000	0.000
2	1.25E-06	0.018	0.014	0.020	0.031	0.270	0.209	0.289	0.461
4	2.50E-06	0.037	0.028	0.039	0.063	0.540	0.418	0.578	0.921
6	3.75E-06	0.055	0.043	0.059	0.094	0.810	0.626	0.867	1.381
8	5.00E-06	0.073	0.057	0.079	0.125	1.079	0.834	1.155	1.840
10	6.25E-06	0.092	0.071	0.098	0.156	1.348	1.042	1.443	2.298
12	7.49E-06	0.110	0.085	0.118	0.187	1.616	1.249	1.730	2.756
14	8.73E-06	0.128	0.099	0.137	0.219	1.884	1.456	2.017	3.213
16	9.97E-06	0.146	0.113	0.157	0.250	2.152	1.663	2.303	3.670
18	1.12E-05	0.165	0.127	0.176	0.281	2.419	1.870	2.590	4.126
20	1.24E-05	0.183	0.141	0.196	0.312	2.686	2.076	2.875	4.581
22	1.37E-05	0.201	0.155	0.215	0.343	2.952	2.282	3.161	5.036
24	1.48E-05	0.218	0.168	0.233	0.371	3.199	2.473	3.425	5.456
26	1.61E-05	0.236	0.182	0.252	0.402	3.465	2.678	3.709	5.910
28	1.73E-05	0.254	0.196	0.272	0.433	3.730	2.884	3.994	6.363
30	1.85E-05	0.272	0.210	0.291	0.464	3.995	3.089	4.277	6.815
32	1.97E-05	0.290	0.224	0.310	0.494	4.260	3.293	4.561	7.266
34	2.10E-05	0.308	0.238	0.330	0.525	4.525	3.498	4.844	7.717
36	2.22E-05	0.326	0.252	0.349	0.556	4.789	3.702	5.127	8.168
38	2.34E-05	0.344	0.266	0.368	0.586	5.052	3.906	5.409	8.618
40	2.46E-05	0.362	0.280	0.387	0.617	5.316	4.109	5.691	9.067
42	2.59E-05	0.380	0.293	0.406	0.647	5.579	4.313	5.973	9.515
44	2.71E-05	0.397	0.307	0.425	0.678	5.841	4.516	6.254	9.963
46	2.83E-05	0.415	0.321	0.445	0.708	6.104	4.718	6.534	10.411
48	2.95E-05	0.433	0.335	0.464	0.739	6.366	4.921	6.815	10.857
50	3.08E-05	0.452	0.349	0.484	0.771	6.645	5.137	7.114	11.334
52	3.20E-05	0.470	0.363	0.503	0.801	6.906	5.339	7.394	11.780

	V (liters)	1.1103	1.1112	1.2749	1.2519	1.1103	1.1112	1.2749	1.2519
	RT/V	21.71	21.70	18.91	19.26	21.71	21.70	18.91	19.26
	gm Pu	676.00	523.00	831.00	1300.00	676.00	523.00	831.00	1300.0
Week	mole He/gm	Atmospheres				PSI			
0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	5.46E-09	8.02E-05	6.20E-05	8.59E-05	1.37E-04	1.18E-03	9.11E-04	1.26E-03	2.01E-03
4	1.09E-08	1.60E-04	1.24E-04	1.72E-04	2.74E-04	2.36E-03	1.82E-03	2.52E-03	4.02E-03
6	1.64E-08	2.41E-04	1.86E-04	2.58E-04	4.10E-04	3.54E-03	2.73E-03	3.79E-03	6.03E-03
8	2.19E-08	3.21E-04	2.48E-04	3.43E-04	5.47E-04	4.72E-03	3.65E-03	5.05E-03	8.04E-03
10	2.73E-08	4.01E-04	3.10E-04	4.29E-04	6.84E-04	5.89E-03	4.56E-03	6.31E-03	1.01E-02
12	3.28E-08	4.81E-04	3.72E-04	5.15E-04	8.21E-04	7.07E-03	5.47E-03	7.57E-03	1.21E-02
14	3.82E-08	5.61E-04	4.34E-04	6.01E-04	9.57E-04	8.25E-03	6.38E-03	8.83E-03	1.41E-02
16	4.37E-08	6.42E-04	4.96E-04	6.87E-04	1.09E-03	9.43E-03	7.29E-03	1.01E-02	1.61E-02
18	4.92E-08	7.22E-04	5.58E-04	7.73E-04	1.23E-03	1.06E-02	8.20E-03	1.14E-02	1.81E-02
20	5.46E-08	8.02E-04	6.20E-04	8.59E-04	1.37E-03	1.18E-02	9.11E-03	1.26E-02	2.01E-02
22	6.01E-08	8.82E-04	6.82E-04	9.44E-04	1.50E-03	1.30E-02	1.00E-02	1.39E-02	2.21E-02
24	6.56E-08	9.62E-04	7.44E-04	1.03E-03	1.64E-03	1.41E-02	1.09E-02	1.51E-02	2.41E-02
26	7.10E-08	1.04E-03	8.06E-04	1.12E-03	1.78E-03	1.53E-02	1.18E-02	1.64E-02	2.61E-02
28	7.65E-08	1.12E-03	8.68E-04	1.20E-03	1.91E-03	1.65E-02	1.28E-02	1.77E-02	2.81E-02
30	8.20E-08	1.20E-03	9.30E-04	1.29E-03	2.05E-03	1.77E-02	1.37E-02	1.89E-02	3.02E-02
32	8.74E-08	1.28E-03	9.92E-04	1.37E-03	2.19E-03	1.89E-02	1.46E-02	2.02E-02	3.22E-02
34	9.29E-08	1.36E-03	1.05E-03	1.46E-03	2.33E-03	2.00E-02	1.55E-02	2.15E-02	3.42E-02
36	9.83E-08	1.44E-03	1.12E-03	1.55E-03	2.46E-03	2.12E-02	1.64E-02	2.27E-02	3.62E-02
38	1.04E-07	1.52E-03	1.18E-03	1.63E-03	2.60E-03	2.24E-02	1.73E-02	2.40E-02	3.82E-02
40	1.09E-07	1.60E-03	1.24E-03	1.72E-03	2.74E-03	2.36E-02	1.82E-02	2.52E-02	4.02E-02
42	1.15E-07	1.68E-03	1.30E-03	1.80E-03	2.87E-03	2.48E-02	1.91E-02	2.65E-02	4.22E-02
44	1.20E-07	1.76E-03	1.36E-03	1.89E-03	3.01E-03	2.59E-02	2.00E-02	2.78E-02	4.42E-02
46	1.26E-07	1.84E-03	1.43E-03	1.97E-03	3.15E-03	2.71E-02	2.10E-02	2.90E-02	4.62E-02
48	1.31E-07	1.92E-03	1.49E-03	2.06E-03	3.28E-03	2.83E-02	2.19E-02	3.03E-02	4.83E-02
50	1.37E-07	2.00E-03	1.55E-03	2.15E-03	3.42E-03	2.95E-02	2.28E-02	3.16E-02	5.03E-02
52	1.42E-07	2.08E-03	1.61E-03	2.23E-03	3.56E-03	3.06E-02	2.37E-02	3.28E-02	5.23E-02

4.5.3.1 Reference

1. Caviness, M., LANL Content Description for PAT-1 PACKAGING, Updated August 9, 2007.

4.5.4 O-Ring Decomposition

LA-UR-09-05112

*Approved for public release;
distribution is unlimited.*

Title: Thermal Decomposition of Viton® O-rings for the PAT-1 Packaging Accident Scenario

Author(s): J.B. Rubin

Intended for: Support an amendment application to the US Nuclear Regulatory Commission for the PAT-1 packaging



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC02-06NA25396. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Form 836 (7/06)

Abstract

As part of the submission package to the NRC to amend the approved contents for the PAT-1 container, a calculation was necessary to determine the theoretical pressure rise in the PAT-1 containment vessel (TB-1) due to the thermal decomposition of o-rings within the container. These o-rings are composed of Viton A[®], whose number and mass are determined by the internal packing configuration. This report contains the calculations of the decomposition of these o-rings, in the theoretical accident conditions defined by the PAT-1 SARP, assuming both oxygen-deficient and oxygen-available environments. The results show that even for the case of complete thermal decomposition to gaseous products, the total pressure rise inside of the TB-1 containment vessel is less than the maximum allowable, as defined in the PAT-1 SARP.

The o-rings are treated as tori, with a volume given by

$$V = (2\pi R)(\pi r^2) \quad (1)$$

where r is the radius of the cross-sectional area of the torus and R is the distance from the center of the torus to the center of the cross sectional area, Figure 1 :

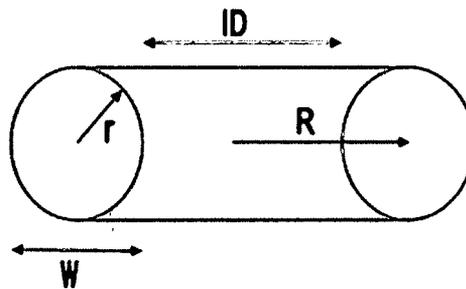


Figure 1. Cross section of a torus, showing the dimensional relations to Eq. (1).

Table 1. Dimensions and volumes of Viton A[®] o-rings contained within the TB-1 for the Packing Configurations described in Table 3 and shown schematically in Figure 2.

o-ring location	o-ring designation	w (in)	r (in)	ID (in)	R (in)	Volume (in ³)	Volume (cm ³)
T-ampoule	Parker 2-241	0.139	0.070	3.859	3.929	0.1906	3.1233
TB-1	Parker 2-242	0.139	0.070	3.984	2.062	0.1966	3.2209
SC-1/2	Parker 2-147	0.103	0.052	2.675	1.389	0.0727	1.1916
Packing Configuration #1							
TB-1	Parker 2-242	0.139	0.070	3.984	2.062	0.1966	3.2209
T-ampoule	Parker 2-241	0.139	0.070	3.859	3.929	0.1906	3.1233
					Total	0.3872	6.3442
Packing Configuration #2							
TB-1	Parker 2-242	0.139	0.070	3.984	2.062	0.1966	3.2209
T-ampoule	Parker 2-241	0.139	0.070	3.859	3.929	0.1906	3.1233
SC-2	Parker 2-147	0.103	0.052	2.675	1.389	0.0727	1.1916
SC-2	Parker 2-147	0.103	0.052	2.675	1.389	0.0727	1.1916
					Total	0.5326	8.7275
Packing Configuration #3							
TB-1	Parker 2-242	0.139	0.070	3.984	2.062	0.1966	3.2209
T-ampoule	Parker 2-241	0.139	0.070	3.859	3.929	0.1906	3.1233
SC-1	Parker 2-147	0.103	0.052	2.675	1.389	0.0727	1.1916
SC-1	Parker 2-147	0.103	0.052	2.675	1.389	0.0727	1.1916
					Total	0.6053	9.9192

Table 1 gives the relevant dimensions (w, r and R as defined in Figure 1) of the o-rings, taken from the o-ring supplier's (Parker) catalog. From these dimensions, the volume of each o-ring is calculated using Eq. (1) and compared to the values given in the supplier's product catalog (as verification that the volume of each o-ring is accurate). From these individual o-ring volumes, the total o-ring (volume) inventory in the TB-1, for each of the three packing configurations, is obtained.

Based on literature review, the reaction products produced by pyrolysis of Viton A[®] in air is similar to that of pyrolysis of PTFE in air, namely, CO, CO₂, HF, CF₄, C₂F₄, C₃F₆, C₃F₈, C₄F₈. Therefore, for gas generation calculations, we will assume that the maximum amount of HF (g) is formed, since this specie would form the greatest amount of product, on a molar basis, from the degradation products, and therefore represents the maximum pressure contribution of any (single) pyrolysis product. Then, it is assumed that any fluorine in excess of that taken up in the formation of HF(g) will react with carbon to form the maximum amount of CF₄(g).

In the following section, a calculation will be given of the pressure rise due to o-ring degradation for Packing Configuration #3, which includes five o-rings, as shown in Table 1.

Viton A^o is a vinylidene fluoride/hexafluoropropylene copolymer, manufactured by DuPont Corporation, with a nominal composition of 78 wt% CF₂CH₂ and 22 wt% C₃F₆. [1]. For packing configuration #3, the total elastomer volume is 9.9192 cm³ (Table 1). Assuming an elastomer specific gravity of 1.8 g/cm³, we have 17.855 g of elastomer material, or 13.927 g (0.217 moles) CF₂CH₂ and 3.928 g (0.026 moles) C₃F₆. The overall decomposition reaction, based on the assumed decomposition products is therefore



For the elastomer inventory in Packing Configuration #3, we have

$$13.927 \text{ g CF}_2\text{CH}_2 \left(\frac{37.996 \text{ g F}}{64.034 \text{ g CF}_2\text{CH}_2} \right) = 8.264 \text{ g F} \quad (3)$$

$$13.927 \text{ g CF}_2\text{CH}_2 \left(\frac{2.016 \text{ g H}}{64.034 \text{ g CF}_2\text{CH}_2} \right) = 0.438 \text{ g H} \quad (4)$$

$$13.927 \text{ g CF}_2\text{CH}_2 \left(\frac{24.022 \text{ g C}}{64.034 \text{ g CF}_2\text{CH}_2} \right) = 5.225 \text{ g C} \quad (5)$$

plus

$$3.928 \text{ g C}_3\text{F}_6 \left(\frac{113.988 \text{ g F}}{150.021 \text{ g C}_3\text{F}_6} \right) = 2.985 \text{ g F} \quad (6)$$

$$3.928 \text{ g C}_3\text{F}_6 \left(\frac{36.033 \text{ g C}}{150.021 \text{ g C}_3\text{F}_6} \right) = 0.943 \text{ g C} \quad (7)$$

or

$$11.249 \text{ g F} \quad (8)$$

$$6.168 \text{ g C} \quad (9)$$

$$0.438 \text{ g H} \quad (10)$$

If we assume that all available hydrogen and fluorine are liberated and form the maximum moles of gaseous products, we would have

$$\left(\frac{0.438 \text{ g H}}{1.008 \text{ g/mole H}} \right) = 0.435 \text{ moles hydrogen available for HF generation, and}$$

$$\left(\frac{11.249 \text{ g F}}{18.998 \text{ g/mole F}} \right) = 0.592 \text{ moles total fluorine minus the 0.435 moles of fluorine in HF, leaving}$$

0.157 moles of fluorine available for $\text{CF}_4(\text{g})$ generation, or 0.039 moles $\text{CF}_4(\text{g})$. If these reaction products add incrementally, and ideally, then we would have 0.435 mole $\text{HF}(\text{g}) + 0.039$ mole $\text{CF}_4(\text{g})$, or a total of 0.474 moles of gaseous [$\text{HF}(\text{g}) + \text{CF}_4(\text{g})$] reaction products. For an unoccupied internal TB-1 volume of 1103.01 cm^3 (see Packing Configuration #3 in Table 3), and $T = 1080^\circ\text{F}$ (582.2°C , 855.4 K) for the PAT-1 hypothetical accident condition, there would be a pressure increment of

$$P = \frac{(0.474 \text{ mole}) \left(82.056 \text{ atm cm}^3 / \text{mole K} \right) (855.4 \text{ K})}{1103.01 \text{ cm}^3} = 30.16 \text{ atm} \quad (11)$$

or 443.23 psi due to the assumed o-ring degradation products. Once the hydrogen and fluorine are consumed in the formation of $\text{HF}(\text{g})$ and $\text{CF}_4(\text{g})$, there is a theoretical excess of

$$\left(\frac{6.168 \text{ g C}}{12.011 \text{ g/mole}} \right) = 0.514 \text{ moles of carbon in the virgin elastomer minus 0.039 moles carbon in}$$

CF_4 , or 0.475 moles.

At this point we could assume that (1) the theoretical excess of carbon will remain as solid, unreactive char, or that (2) the excess carbon can be further reacted with oxygen to form $\text{CO}(\text{g})$ or $\text{CO}_2(\text{g})$ (the formation of either $\text{CO}(\text{g})$ or $\text{CO}_2(\text{g})$ would produce the same number of moles of gaseous reaction products).

The formation of residual carbon char, as opposed to the formation of $\text{CO}(\text{g})$ or $\text{CO}_2(\text{g})$, would be supported based on (a) any oxygen present at the time of initial packaging is scavenged completely by the formation of plutonium oxide, and (b) the TB-1 remains intact at the theoretical accident conditions. Solid char is experimentally observed, even in the oxidative thermal decomposition of fluoroelastomers.^{14, 15} Further, for studies of the thermal degradation of Viton A[®] in non-oxidizing environments, an incomplete volatilization of the polymer, as evidenced by a low yield of fluorine with respect to the theoretical quantity. The calculated amount of char represents 32% of the original elastomer mass and 93% of the carbon contained in the original elastomer.

However, for the purposes of a conservative estimate, we assume the case where additional oxygen were to be made available in the TB-1 and sample containers, in a quantity sufficient to react completely with the excess carbon from the elastomer, to produce CO(g) or CO₂(g). Such a reaction would increase the overall moles of gaseous reaction products to 0.474 moles (HF(g) + CF₄(g)) + 0.475 (moles CO(g) or CO₂(g)), thereby doubling the overall pressure rise from 30.16 atm to 60.32 atm, or 887.28 psi.

Table 2 summarizes the calculation given above, which, again, represents the elastomer inventory in Packaging Configuration #3, along with a similar calculation of the remaining two Packaging Configurations, which have a reduced elastomer loading.

Table 2. Calculation of elastomer degradation products for the three Packaging Configurations described in Table 1 and shown schematically in Figure 2. The top summation in the right-hand part of each row represents the total number of moles assuming that the excess carbon forms a solid char (i.e., no CO(g) or CO₂(g) formation), while the bottom summation in each row is the total number of moles assuming that the excess carbon reacts completely to form gaseous product, either CO(g) or CO₂(g).

Packing Configuration #1 (6.3442 cm ³ of Viton A [®])	8.907 g (0.139 moles) CF ₂ CH ₂ 2.512 g (0.017 moles) C ₃ F ₆	0.280 g (0.278 moles) H 7.194 g (0.379 moles) F 3.945 g (0.328 moles) C	0.278 moles HF(g) 0.025 moles CF ₄ (g) Σ = 0.303 moles 0.303 moles CO(g) Σ = 0.606 moles
Packing Configuration #2 (8.7277 cm ³ of Viton A [®])	12.254 g (0.191 moles) CF ₂ CH ₂ 3.456 g (0.023 moles) C ₃ F ₆	0.386 g (0.383 moles) H 9.897 g (0.521 moles) F 5.427 g (0.452 moles) C	0.383 moles HF(g) 0.035 moles CF ₄ (g) Σ = 0.418 moles 0.417 moles CO(g) Σ = 0.835 moles
Packing Configuration #3 (9.9192 cm ³ of Viton A [®])	13.927 g (0.217 moles) CF ₂ CH ₂ 3.928 g (0.026 moles) C ₃ F ₆	0.438 g (0.435 moles) H 11.249 g (0.592 moles) F 6.168 g (0.514 moles) C	0.435 moles HF(g) 0.039 moles CF ₄ (g) Σ = 0.474 moles 0.475 moles CO(g) Σ = 0.949 moles

Table 3 gives the overall pressure rise calculation for the three Packing Configurations, using the appropriate o-ring inventory (Table 1) and unoccupied TB-1 volume (Table 3) for each Configuration.

Table 3. Internal volume of the TB-1 container (top line), and solid volumes of T-ampoule, filler ring, sample containers (SC-1 or SC-2) and Pu metal payloads for each Packing Configuration (volume of optional tantalum foil and copper foam were neglected). Column 4 gives the resulting pressure rise for the case of char formation, while column 5 gives the result for the case of no char formation. Column 6 is a summation of the pressure rise from Column 5 plus an additional 2.9 atmospheres (42.62 psi), assumed originally present in the TB-1.

components	Volume (in ³)	Volume (cm ³)	Pressure rise (psi) – with char	Pressure rise (psi) – no char	Pressure rise (psia) – no char
Empty TB-1	89.10	1460.09			
Packing Configuration #1					
T-ampoule	7.83	128.31			
Filler ring	0.90	14.75			
Pu cylinder 831 g	2.57	42.11			
<i>Unoccupied TB-1 volume</i>	77.80	1274.91	245.10	490.20	532.83
Packing Configuration #2					
T-ampoule	7.83	128.31			
Filler ring	0.90	14.75			
SC-2	2.75	45.06			
SC-2	2.75	45.06			
SC-2 Cradle Assembly	4.90	80.30			
Pu cylinder 1.1" Ø x 1.1" h	1.05	17.21			
Pu cylinder 1.1" Ø x 1.1" h	1.05	17.21			
<i>Unoccupied TB-1 volume</i>	67.87	1112.19	387.59	774.26	816.89
Packing Configuration #3					
T-ampoule	7.83	128.31			
Filler ring	0.90	14.75			
SC-1	2.15	35.23			
SC-1	2.15	35.23			
SC-1	2.15	35.23			
SC-1 Cradle Assembly	5.02	82.26			
Pu cylinder 0.88"Ø x 0.88" h	0.53	8.69			
Pu cylinder 0.88"Ø x 0.88" h	0.53	8.69			
Pu cylinder 0.88"Ø x 0.88" h	0.53	8.69			
<i>Unoccupied TB-1 volume</i>	67.31	1103.01	443.17	887.28	929.91

¹. A.K. Burnham and R.K. Weese, "Kinetics of thermal degradation of explosive binders Viton A, Estane, and Kel-F", *Thermochimica Acta* 426 (2005) pp. 85-92.

². *Analytical Pyrolysis of Synthetic Organic Polymers*, ed. by Șerban Moldoveanu (2005) p.289.

³. I. Lee, R.R. Reed, V.L. Brady, and S.A. Finnegan, "Energy release in the reaction of metal powders with fluorine containing polymers", *J. Thermal Anal.* 49 (1997) pp. 1699-1705.

⁴. A.E. Venger, et al., "Thermogravimetric Study of the Thermal Decomposition of poly(tetrafluoroethylene) under Nonisothermal Conditions", *Vestsi Akademii Navuk BSSR, Seriya Fizika-Energetichnykh Navuk* 2 (1976) pp. 65.

⁵. G. J. Knight and W. W. Wright, "The Thermal Degradation of Hydrofluoro Polymers", *J. Appl. Polym. Sci.* 16 (1972) pp. 683-693.

LA-UR-10-05846

*Approved for public release;
distribution is unlimited.*

Title: Thermal Decomposition of Viton® O-rings for the PAT-1 Packaging Accident Scenario

Author(s): J.B. Rubin

Intended for: Support an amendment application to the US Nuclear Regulatory Commission for the PAT-1 packaging



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Form 836 (7/06)

Abstract

As part of the submission package to the NRC to amend the approved contents for the PAT-1 container, a calculation was necessary to determine the theoretical pressure rise in the PAT-1 containment vessel (TB-1) due to the thermal decomposition of O-rings within the container. These o-rings are composed of Viton A[®], whose number and mass are determined by the internal packing configuration. This report contains a conservative calculation of the decomposition of these O-rings, in the theoretical accident conditions defined by the PAT-1 SARP. The calculation assumes a scenario whereby the O-ring material is completely volatilized, using a reaction scheme which generates the maximum number of gaseous reaction products, and the maximum pressure rise within the TB-1. The results show that even for the case of complete thermal decomposition to gaseous products, the total pressure rise inside of the TB-1 containment vessel is less than the maximum allowable, as defined in the PAT-1 SARP.

The o-rings are treated as tori, with a volume given by

$$V = (2\pi R)(\pi r^2) \quad (1)$$

where r is the radius of the cross-sectional area of the torus and R is the distance from the center of the torus to the center of the cross sectional area, Figure 1 :

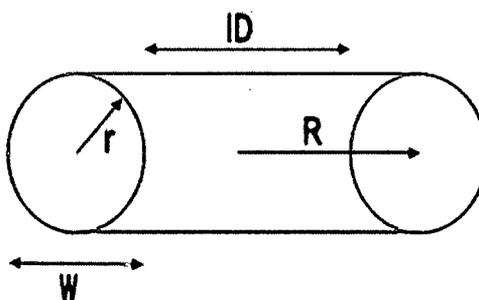


Figure 1. Cross section of a torus, showing the dimensional relations to Eq. (1).

Table 1. Dimensions and volumes of Viton A[®] O-rings contained within the TB-1 for the Packing Configurations described in Table 3 and shown schematically in Figure 2.

O-ring location	O-ring Size Standard ¹	w (in)	r (in)	ID (in)	R (in)	Volume (in ³)	Volume (cm ³)
T-Ampoule ^a	241	0.139	0.070	3.859	3.929	0.1906	3.1233
TB-1	242	0.139	0.070	3.984	2.062	0.1966	3.2209
SC-1/2	147	0.103	0.052	2.675	1.389	0.0727	1.1916
Packing Configuration #1							
T-Ampoule	241	0.139	0.070	3.859	3.929	0.1906	3.1233
					Total	0.1906	3.1233
Packing Configuration #2							
T-Ampoule	241	0.139	0.070	3.859	3.929	0.1906	3.1233
SC-2	147	0.103	0.052	2.675	1.389	0.0727	1.1916
SC-2	147	0.103	0.052	2.675	1.389	0.0727	1.1916
					Total	0.3360	5.5065
Packing Configuration #3							
T-Ampoule	241	0.139	0.070	3.859	3.929	0.1906	3.1233
SC-1	147	0.103	0.052	2.675	1.389	0.0727	1.1916
SC-1	147	0.103	0.052	2.675	1.389	0.0727	1.1916
SC-1	147	0.103	0.052	2.675	1.389	0.0727	1.1916
					Total	0.4087	6.6981

Table 1 gives the relevant dimensions (w, r and R as defined in Figure 1) of the O-rings, while the ID and w are provided from SAE AS568C "Aerospace Size Standard for O-rings". From these dimensions, the volume of each O-ring is calculated using Eq. (1) and compared to the values given in the SAE AS568C standard (as verification that the volume of each o-ring is accurate). From these individual O-ring volumes, the total O-ring (volume) inventory in the TB-1, for each of the three packing configurations, is obtained. *Note that the TB-1 O-ring is not used for the plutonium metal shipments and is not included in the volume calculation.*

Based on literature review, the reaction products produced by pyrolysis of Viton A[®] in air is similar to that of pyrolysis of PTFE in air, namely, CO, CO₂, COF₂, HF, CF₄, C₂F₄, C₃F₆, C₄F₈. This is to be expected since the atomic species present in the two fluoropolymers are nominally similar, both composed largely of carbon and fluorine. Once volatilized, these atomic species will re-form into other molecular species having stoichiometries determined by the prevailing thermodynamic conditions in the gas phase.

Viton A[®] is a vinylidene fluoride/hexafluoropropylene copolymer, manufactured by DuPont Corporation, with a nominal composition of 78 wt% CF₂CH₂ and 22 wt% C₃F₆. (2) (By comparison, PTFE has a nominal composition of 100 wt% C₂F₄. In the case of PTFE, the hydrogenous compounds observed on pyrolysis would obtain the necessary hydrogen from water vapor, which is invariably present during air oxidation.2) It is noted that air oxidation of

PTFE can result in significant fractions of higher molecular weight products, such as COF_2 ,^v relative to the oxidative pyrolysis of Viton A[®] (which produces larger fractions of HF and CF_4). In order to be *conservative*, we will assume that the pyrolysis products of Viton A[®] are composed of lower molecular weight products, resulting in the greatest number of moles of gaseous reaction product, and therefore the largest pressure increase. Consequently, for gas generation calculations, we will assume that the maximum amount of HF(g) is formed, since this specie would form the greatest amount of product, on a molar basis, from the degradation products, and therefore represents the maximum pressure contribution of any (single) pyrolysis product. It is further assumed that any fluorine in excess of that taken up in the formation of HF(g) will react with carbon to form the maximum amount of CF_4 (g).

It is known that Viton A[®] contains inorganic fillers, such as metal oxides and diatomaceous earth, to aid in processing.^{vi, vii} Again, to be *conservative*, no credit is given for any non-volatile components within the elastomer.

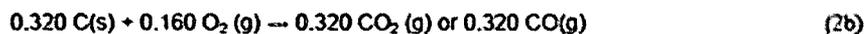
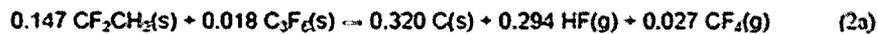
In the following section, a calculation will be given of the pressure rise due to O-ring degradation for Packing Configuration #3, which includes four O-rings, as shown in Table 1. Table 2 gives the results of this calculation, as well as the results for Packing Configurations 1 & 2.

The basis of the calculation assumes the sequential formation of

- (1) HF, to completely account for the hydrogen present in the original o-ring material, then
- (2) saturated fluorocarbon (CF_4), to account for the excess amount of fluorine over that taken up by HF formation, followed lastly by
- (3) either CO (g) or CO_2 (g), to account for the excess amount of carbon remaining after accounting for the hydrogen and fluorine present in the original o-ring(s).

This reaction scheme results in the maximum number of moles of gaseous reaction products, thereby generating the highest amount of internal pressure in the TB-1 unoccupied volume. This is the most conservative case.

For Packing Configuration #3, the total elastomer volume is 6.698 cm^3 (Table 1). Assuming an elastomer specific gravity of 1.8 g/cm^3 ,^{viii} we have 12.057 g of elastomer material, or 9.404 g (0.147 moles) CF_2CH_2 and 2.652 g (0.018 moles) C_3F_6 . The overall decomposition reaction, based on the assumed decomposition products is therefore



For the elastomer inventory in Packing Configuration #3, we have

$$9.404 \text{ g CF}_2\text{CH}_2 \left\{ \frac{37.996 \text{ g F}}{64.034 \text{ g CF}_2\text{CH}_2} \right\} = 5.580 \text{ g F} \quad (3)$$

$$9.404 \text{ g CF}_2\text{CH}_2 \left\{ \frac{2.016 \text{ g H}}{64.034 \text{ g CF}_2\text{CH}_2} \right\} = 0.296 \text{ g H} \quad (4)$$

$$9.404 \text{ g CF}_2\text{CH}_2 \left\{ \frac{24.022 \text{ g C}}{64.034 \text{ g CF}_2\text{CH}_2} \right\} = 3.528 \text{ g C} \quad (5)$$

plus

$$2.652 \text{ g C}_2\text{F}_6 \left\{ \frac{113.988 \text{ g F}}{150.021 \text{ g C}_2\text{F}_6} \right\} = 2.015 \text{ g F} \quad (6)$$

$$2.652 \text{ g C}_2\text{F}_6 \left\{ \frac{36.033 \text{ g C}}{150.021 \text{ g C}_2\text{F}_6} \right\} = 0.637 \text{ g C} \quad (7)$$

or

$$7.596 \text{ g F} \quad (8)$$

$$4.165 \text{ g C} \quad (9)$$

$$0.296 \text{ g H} \quad (10)$$

If we assume that all available hydrogen and fluorine are liberated and form the maximum moles of gaseous products, we would have

$$\left(\frac{0.296 \text{ g H}}{1.008 \text{ g/mole H}} \right) = 0.294 \text{ moles hydrogen available for HF generation, and}$$

$$\left(\frac{7.595 \text{ g F}}{18.998 \text{ g/mole F}} \right) = 0.400 \text{ moles total fluorine minus the 0.294 moles of fluorine in HF, leaving}$$

0.106 moles of fluorine available for $\text{CF}_4(\text{g})$ generation, or 0.027 moles $\text{CF}_4(\text{g})$. If these reaction products add incrementally, and ideally, then we would have 0.294 moles $\text{HF}(\text{g}) + 0.027 \text{ mole } \text{CF}_4(\text{g})$, or a total of 0.321 moles of gaseous [$\text{HF}(\text{g}) + \text{CF}_4(\text{g})$] reaction products. For an unoccupied internal TB-1 volume of 1103.01 cm^3 (see Packing Configuration #3 in Table 3), and $T = 1080^\circ\text{F}$ (582.2°C , 855.4 K) for the PAT-1 hypothetical accident condition, there would be a pressure increase of

$$P = \frac{(0.320 \text{ mole}) \left(82.056 \frac{\text{atm cm}^3}{\text{mole K}} \right) (855.4 \text{ K})}{1103.01 \text{ cm}^3} = 20.38 \text{ atm} \quad (11)$$

or 299.49 psi due to the assumed o-ring degradation products. Once the hydrogen and fluorine are consumed in the formation of HF(g) and CF₄(g), there is a theoretical excess of

$\left(\frac{4.165 \text{ g C}}{12.0119 \text{ mole}} \right) = 0.347$ moles of carbon in the virgin elastomer minus 0.027 moles carbon in CF₄ or 0.320 moles.

At this point we could assume that (1) the theoretical excess of carbon will remain as solid, unreactive char, or that (2) the excess carbon can be further reacted with oxygen to form CO(g) or CO₂(g) (the formation of either CO(g) or CO₂(g) would produce the same number of moles of gaseous reaction products and therefore, in the ideal gas case, an equal pressure contribution).

The formation of residual carbon char, as opposed to the formation of CO(g) or CO₂(g), would be supported based on (a) any oxygen present at the time of initial packaging is scavenged completely by the formation of plutonium oxide, and (b) the TB-1 remains intact at the theoretical accident conditions. Solid char is experimentally observed, even in the oxidative thermal decomposition of fluoroelastomers.^{4,6,8} Further, for studies of the thermal degradation of Viton A[®] in non-oxidizing environments, an incomplete volatilization of the polymer is evidenced by a low yield of fluorine with respect to the theoretical quantity.^{6,9} However, for the purposes of a conservative estimate, we assume the case where additional oxygen were to be made available in the TB-1 and sample containers, in a quantity sufficient to react completely with the excess carbon from the elastomer, to produce CO(g) or CO₂(g). Such a reaction would increase the overall moles of gaseous reaction products to 0.320 moles [HF(g) + CF₄(g)] + 0.320 moles [CO(g) or CO₂(g)], thereby (approximately) doubling the overall pressure rise from 20.38 atm to 40.76 atm, or 598.98 psi.

Table 2 summarizes the calculation given above, which, again, represents the elastomer inventory in Packaging Configuration #3, along with a similar calculation of the remaining two Packing Configurations, which have a reduced elastomer loading.

Table 2. Calculation of elastomer degradation products for the three Packing Configurations described in Table 1 and shown schematically in Figure 2. The summation in the right-hand column of each row is the total number of moles assuming that the excess carbon reacts completely to form gaseous product, either CO(g) or CO₂(g).

Packing Configuration #1 (3.1233 cm ³ of Viton A [®])	4.385 g (0.068 moles) CF ₂ CH ₂ 1.237 g (0.008 moles) C ₃ F ₆	0.138 g (0.137 moles) H 3.542 g (0.186 moles) F 1.942 g (0.162 moles) C	0.137 moles HF(g) 0.012 moles CF _x (g) 0.149 moles CO(g) $\Sigma = 0.299 \text{ moles}$
Packing Configuration #2 (5.5065 cm ³ of Viton A [®])	7.731 g (0.121 moles) CF ₂ CH ₂ 2.181 g (0.015 moles) C ₃ F ₆	0.243 g (0.241 moles) H 6.244 g (0.329 moles) F 3.424 g (0.285 moles) C	0.241 moles HF(g) 0.022 moles CF _x (g) 0.263 moles CO(g) $\Sigma = 0.527 \text{ moles}$
Packing Configuration #3 (6.6981 cm ³ of Viton A [®])	9.404 g (0.147 moles) CF ₂ CH ₂ 2.652 g (0.018 moles) C ₃ F ₆	0.296 g (0.294 moles) H 7.596 g (0.400 moles) F 4.165 g (0.347 moles) C	0.294 moles HF(g) 0.027 moles CF _x (g) 0.320 moles CO(g) $\Sigma = 0.640 \text{ moles}$

Table 3 gives the overall pressure rise calculation for the three Packing Configurations, using the appropriate O-ring inventory (Table 1) and unoccupied TB-1 volume (Table 3) for each Configuration.

Table 3. Internal volume of the TB-1 container (top line), and solid volumes of T-ampoule, filter ring, sample containers (SC-1 or SC-2) and Pu metal payloads for each Packing Configuration (volume of O-ring lubricant and optional tantalum foil are not included). The amount of lubricant on the O-ring would be minimal to permit joining the lid to the body of the T-Ampoule or sample containers. Column 4 gives the pressure rise for the case of complete volatilization of all contained o-ring materials. Column 5 is a summation of the pressure rise from Column 4 plus an additional 2.9 atmospheres, due to an initial 1 atm of pressure assumed to be present in the TB-1 at the time of packaging, and then heated from ambient to 582.2 K during the accident scenario.

components	Volume (in ³)	Volume (cm ³)	Pressure rise (psi)	Pressure rise (psia)
Empty TB-1	89.10	1460.09		
Packing Configuration #1				
T-ampoule	7.83	128.31		
Filter ring	0.90	14.75		
Pu cylinder 831 g	2.57	42.11		
<i>Unoccupied TB-1 volume</i>	<i>77.80</i>	<i>1274.91</i>	<i>241.63</i>	<i>284.25</i>
Packing Configuration #2				
T-ampoule	7.83	128.31		
Filter ring	0.90	14.75		
SC-2	2.75	45.06		
SC-2	2.75	45.06		
SC-2 Cradle Assembly	4.90	80.30		
Pu cylinder 1.1" Ø x 1.1" h	1.05	17.21		
Pu cylinder 1.1" Ø x 1.1" h	1.05	17.21		
<i>Unoccupied TB-1 volume</i>	<i>67.87</i>	<i>1112.19</i>	<i>488.33</i>	<i>530.94</i>
Packing Configuration #3				
T-ampoule	7.83	128.31		
Filter ring	0.90	14.75		
SC-1	2.15	35.23		
SC-1	2.15	35.23		
SC-1	2.15	35.23		
SC-1 Cradle Assembly	5.02	82.26		
Pu cylinder 0.88" Ø x 0.88" h	0.53	8.69		
Pu cylinder 0.88" Ø x 0.88" h	0.53	8.69		
Pu cylinder 0.88" Ø x 0.88" h	0.53	8.69		
<i>Unoccupied TB-1 volume</i>	<i>67.31</i>	<i>1103.01</i>	<i>598.94</i>	<i>641.56</i>

^v. From SAE AS568C, "Aerospace Size Standard for O-rings". ID, w, and Volume are provided from Table 1, r and R are derived.

^w. The TB-1 O-ring is not used for plutonium metal shipments.

^x. A.K. Burnham and R.K. Weese, "Kinetics of thermal degradation of explosive binders Viton A, Estane, and Kel-F", *Thermochimica Acta* 426 (2005) pp. 85-92.

^y. H. Arito and R. Soda "Pyrolysis Products of Polytetrafluoroethylene and Polytetrafluoroethylenepropylene with Reference to Inhalation Toxicology", *Korean J. Chem. Eng.* 12 (1995) pp. 247-255.

^z. L.D. Scheel, W.C. Lane and W.E. Coleman, "The Toxicity of Polytetraethylene Pyrolysis Products- Including Carbonyl Fluoride and a Reaction Product, Silicon Tetrafluoride", *Amer. Ind. Hygiene Ass.* 29 (1968) pp. 41-48.

^{aa}. J. F. Smith and G. T. Perkins, "The Mechanism of Post Cure of Viton A[®] Fluorocarbon Elastomer", *J. Appl. Polym. Sci.* 16 (1961) pp. 460-467.

^{ab}. Technical Information - Viton[®] fluor elastomer Fluid Resistance Guide (DuPont Dow Elastomers, 1998).

^{ac}. Technical Information - Viton[®] A-100 (DuPont Dow Elastomers, 2003).

^{ad}. The ideal gas law gives relates pressure, as a function of temperature and volume, as $P = nRT/V$. If temperature (T) is expressed in Kelvin, volume (V) is expressed in cm^3 , and mass (n) in moles, then the pressure can be expressed in units of atmospheres (atm) using a

conversion factor of $82.056 \text{ atm cm}^3 / \text{mole K}$.

^{ae}. Analytical Pyrolysis of Synthetic Organic Polymers, ed. by Șerban Moldoveanu (2005) p.289.

^{af}. I. Lee, R.R. Reed, V.L. Brady, and S.A. Finnegan, "Energy release in the reaction of metal powders with fluorine containing polymers", *J. Thermal Anal.* 49 (1997) pp. 1699-1705.

^{ag}. A.E. Venger, et al., "Thermogravimetric Study of the Thermal Decomposition of poly(tetrafluoroethylene) under Nonisothermal Conditions", *Vestsi Akademii Navuk BSSR, Seriya Fizika-Energetichnykh Navuk* 2 (1976) pp. 65.

^{ah}. G. J. Knight and W. W. Wright, "The Thermal Degradation of Hydrofluoro Polymers", *J. Appl. Polym. Sci.* 16 (1972) pp. 683-693.

4.5.5 Determination of A_2 for the PAT 1 Package with Plutonium Contents

Prepared by Monty L. Goins, LLC, and Reviewed by Drew Winder, LLC

DETERMINATION OF A_2 FOR THE PAT-1 PACKAGE WITH PLUTONIUM CONTENTS

Introduction

The containment criteria for radioactive, fissile material packages are given in 10 CFR 71.51(a)(1) for Normal Conditions of Transport (NCT) ($\leq 10^{-6}$ A_2/h), in 71.51(a)(2) for Hypothetical Accident Conditions (HAC) ($\leq A_2$ in a week), and 71.64(a)(1)(i) for Accident conditions for air transport of plutonium ($\leq A_2$ in a week). The A_2 value for this mixture of radioisotopes must be determined to establish the content containment criteria and to determine the maximum release quantity that is allowed by the regulations. These values for a mixture of isotopes are determined by the methodology given in 10 CFR 71, Appendix A, "Determination of A_1 and A_2 ," Sect. IV. The results of these analyses are used to demonstrate compliance of the PAT-1 package with the containment requirements of 10 CFR 71.

Scope

The A_2 value of the plutonium content to be shipped is evaluated based on the mass and weight percents of materials shown in Tables 4.5.5.1 and 4.5.5.2 defined in Sect. 1.2.2. The analysis documented in this section was conducted to establish the upper limit for the total activity and the maximum number of A_2 s proposed for transport in the PAT-1 package. The maximum activity [53.281 TBq (1440.02 Ci)] occurs at initial fabrication. However, the maximum activity-to- A_2 value (5.5708×10^3) of the contents occurs when the Pu-241 fully decays to Am-241. These values have been determined using a maximum of 1300 gram of plutonium. By applying the weight percents of isotopes shown in Tables 4.5.5.1 and 4.5.5.2, the maximum activity, minimum A_2 value, and the minimum leakage requirements were determined for the proposed contents and are summarized in Tables 4.5.5.4, 4.5.5.5, and 4.5.5.6. The mass and isotopic concentrations used for the proposed content do not take into consideration limits based on shielding, criticality or structural.

According to 10 CFR 71, Appendix A, parent and daughter nuclides are considered to be a mixture of different nuclides than those of the parent nuclide. The radioactive decay of uranium (refer to the decay chains presented by Dr. David C. Kocher, *Radioactive Decay Data Tables* [Kocher 1981]) creates isotopes that will accumulate enough activity to exceed their respective criteria for limited quantities (*Shippers--General Requirements for Shipments and Packagings* [49 CFR 173.425], Table 4, "Activity Limits for Limited Quantities, Instruments, and Articles") and for Type A quantities of radionuclides (10 CFR 71, Table A-1, " A_1 and A_2 Values for Radionuclides"). Furthermore, the A_2 value for the mixture will change over time as a result of radioactive decay. The analysis below shows that the A_2 value for this mixture reaches a minimum when the Pu-241 is fully decayed to Am-241.

Analysis

Mass Tables. The mass and weight fractions for the isotopes used in the containment calculations are presented in Tables 4.5.5.1 and 4.5.5.2.

Table 4.5.5. 1. Isotopic mass and weight percent for the Plutonium contents ^a

Nuclide	Weight percent	Mass (g)
Pu-238	0.050000	0.650000
Pu-239	92.350000	1200.550000
Pu-240	6.500000	84.500000
Pu-241	1.000000	13.000000
Pu-242	0.100000	1.300000
Am-241	0.000000	0.000000
Total	100.000000	1300.000000

^a Entire weight of contents is assumed to be plutonium. Maximum content mass is assumed to be 1300 grams.

Table 4.5.5.2. Isotopic mass and weight percent for the Plutonium contents with full Pu-241 decay to Am-241^b

Nuclide	Weight percent	Mass (g)
Pu-238	0.050000	0.650000
Pu-239	92.350000	1200.550000
Pu-240	6.500000	84.500000
Pu-241	0.000000	0.000000
Pu-242	0.100000	1.300000
Am-241	1.000000	13.000000
Total	100.000000	1300.000000

^b Entire weight of contents is assumed to be plutonium. Maximum content mass is assumed to be 1300 grams.

Table 4.5.5.3. A_2 value and activity calculation for 1300 g of radioactive material at 0 years

Isotope	Mass (g)	Specific activity (TBq/g)	Activity (TBq)	A_2 (TBq)	$f(i)$ (TBq/TBq)	$f(i) / A_2$ (1/TBq)
Pb-210	0.00000	2.5000E+00	0.0000E+00	5.0000E-02	0.0000E+00	0.0000E+00
Pb-212	0.00000	5.1000E+04	0.0000E+00	2.0000E-01	0.0000E+00	0.0000E+00
Bi-210	0.00000	4.6000E+03	0.0000E+00	6.0000E-01	0.0000E+00	0.0000E+00
Bi-212	0.00000	5.4000E+05	0.0000E+00	6.0000E-01	0.0000E+00	0.0000E+00
Po-210	0.00000	1.7000E+02	0.0000E+00	2.0000E-02	0.0000E+00	0.0000E+00
Rn-222	0.00000	5.7000E+03	0.0000E+00	4.0000E-03	0.0000E+00	0.0000E+00
Ra-223	0.00000	1.9000E+03	0.0000E+00	7.0000E-03	0.0000E+00	0.0000E+00
Ra-224	0.00000	5.9000E+03	0.0000E+00	2.0000E-02	0.0000E+00	0.0000E+00
Ra-225	0.00000	1.5000E+03	0.0000E+00	4.0000E-03	0.0000E+00	0.0000E+00
Ra-226	0.00000	3.7000E-02	0.0000E+00	3.0000E-03	0.0000E+00	0.0000E+00
Ra-228	0.00000	1.0000E+01	0.0000E+00	2.0000E-02	0.0000E+00	0.0000E+00
Ac-225	0.00000	2.1000E+03	0.0000E+00	6.0000E-03	0.0000E+00	0.0000E+00
Ac-227	0.00000	2.7000E+00	0.0000E+00	9.0000E-05	0.0000E+00	0.0000E+00
Ac-228	0.00000	8.4000E+04	0.0000E+00	5.0000E-01	0.0000E+00	0.0000E+00
Th-227	0.00000	1.1000E+03	0.0000E+00	5.0000E-03	0.0000E+00	0.0000E+00
Th-228	0.00000	3.0000E+01	0.0000E+00	1.0000E-03	0.0000E+00	0.0000E+00
Th-229	0.00000	7.9000E-03	0.0000E+00	5.0000E-04	0.0000E+00	0.0000E+00
Th-230	0.00000	7.6000E-04	0.0000E+00	1.0000E-03	0.0000E+00	0.0000E+00
Th-231	0.00000	2.0000E+04	0.0000E+00	2.0000E-02	0.0000E+00	0.0000E+00
Th-232	0.00000	4.0000E-09	0.0000E+00	1.0000E+75	0.0000E+00	0.0000E+00
Pa-231	0.00000	1.7000E-03	0.0000E+00	4.0000E-04	0.0000E+00	0.0000E+00
Pa-233	0.00000	7.7000E+02	0.0000E+00	7.0000E-01	0.0000E+00	0.0000E+00
U-232	0.00000	8.3000E-01	0.0000E+00	1.0000E-03	0.0000E+00	0.0000E+00
U-233	0.00000	3.6000E-04	0.0000E+00	6.0000E-03	0.0000E+00	0.0000E+00
U-234	0.00000	2.3000E-04	0.0000E+00	6.0000E-03	0.0000E+00	0.0000E+00
U-235	0.00000	8.0000E-03	0.0000E+00	1.0000E+75	0.0000E+00	0.0000E+00
U-236	0.00000	2.4000E-06	0.0000E+00	6.0000E-03	0.0000E+00	0.0000E+00
Np-237	0.00000	2.6000E-05	0.0000E+00	2.0000E-03	0.0000E+00	0.0000E+00
Pu-236	0.00000	2.0000E+01	0.0000E+00	3.0000E-03	0.0000E+00	0.0000E+00
Pu-238	0.65000	6.3000E-01	4.0950E-01	1.0000E-03	7.6857E-03	7.6857E-03
Pu-239	1200.5500	2.3000E-03	2.7613E+00	1.0000E-03	5.1825E-02	5.1825E-01
Pu-240	84.50000	8.4000E-03	7.0950E-01	1.0000E-03	1.3322E-02	1.3322E-01
Pu-241	13.00000	3.5000E+00	4.9400E+01	6.0000E-02	9.2716E-01	1.5453E-01
Pu-242	1.30000	1.5000E-04	1.9500E-04	1.0000E-03	3.6599E-06	3.6599E-03
Mass =	1300.0000	ACTIVITY SUM =	5.3281E+01		SUM OF $f_i A_2$ =	8.8289E-01

$$(\text{mixture}) = \frac{1}{\sum f(i) / A_2} = \frac{1}{8.8289 \times 10^1 (1/\text{TBq})} = 1.1326 \times 10^{-2} \text{ TBq}$$

Table 4.5.5.4. A₂ value and activity calculation for 1300 g of radioactive material with full Pu-241 decay to Am-241

Isotope	Mass (g)	Specific activity (TBq/g)	Activity (TBq)	A ₂ (TBq)	f(i) (TBq/TBq)	f(i) / A ₂ (1/TBq)
Pb-210	0.0000	2.8000E+00	0.0000E+00	5.0000E-02	0.0000E+00	0.0000E+00
Pb-212	0.0000	5.1000E+04	0.0000E+00	2.0000E-01	0.0000E+00	0.0000E+00
Bi-210	0.0000	4.6300E+03	0.0000E+00	6.0000E-01	0.0000E+00	0.0000E+00
Bi-212	0.0000	5.4000E+05	0.0000E+00	6.0000E-01	0.0000E+00	0.0000E+00
Po-210	0.0000	1.7000E+02	0.0000E+00	2.0000E-02	0.0000E+00	0.0000E+00
Rn-222	0.0000	5.7000E+03	0.0000E+00	4.0000E-03	0.0000E+00	0.0000E+00
Ra-223	0.0000	1.9000E+03	0.0000E+00	7.0000E-03	0.0000E+00	0.0000E+00
Ra-224	0.0000	5.9000E+03	0.0000E+00	2.0000E-02	0.0000E+00	0.0000E+00
Ra-226	0.0000	1.5000E+03	0.0000E+00	4.0000E-03	0.0000E+00	0.0000E+00
Ra-228	0.0000	3.7000E+02	0.0000E+00	3.0000E-03	0.0000E+00	0.0000E+00
Ra-228	0.0000	1.0000E+01	0.0000E+00	2.0000E-02	0.0000E+00	0.0000E+00
Ac-225	0.0000	2.1000E+03	0.0000E+00	6.0000E-03	0.0000E+00	0.0000E+00
Ac-227	0.0000	2.7000E+00	0.0000E+00	9.0000E-05	0.0000E+00	0.0000E+00
Ac-228	0.0000	8.4000E+04	0.0000E+00	5.0000E-01	0.0000E+00	0.0000E+00
Tb-227	0.0000	1.1000E+03	0.0000E+00	5.0000E-03	0.0000E+00	0.0000E+00
Tb-228	0.0000	3.0000E-01	0.0000E+00	1.0000E-03	0.0000E+00	0.0000E+00
Tb-229	0.0000	7.9000E-03	0.0000E+00	5.0000E-04	0.0000E+00	0.0000E+00
Tb-230	0.0000	7.6000E-04	0.0000E+00	1.0000E-03	0.0000E+00	0.0000E+00
Tb-231	0.0000	2.0000E+04	0.0000E+00	2.0000E-02	0.0000E+00	0.0000E+00
Tb-232	0.0000	4.0000E-09	0.0000E+00	1.0000E-75	0.0000E+00	0.0000E+00
Po-231	0.0000	1.7000E-03	0.0000E+00	4.0000E-04	0.0000E+00	0.0000E+00
Po-233	0.0000	7.7000E+02	0.0000E+00	7.0000E-01	0.0000E+00	0.0000E+00
U-232	0.0000	8.3000E-01	0.0000E+00	1.0000E-03	0.0000E+00	0.0000E+00
U-233	0.0000	3.6000E-04	0.0000E+00	6.0000E-03	0.0000E+00	0.0000E+00
U-234	0.0000	2.3000E-04	0.0000E+00	6.0000E-03	0.0000E+00	0.0000E+00
U-235	0.0000	8.0000E-03	0.0000E+00	1.0000E-75	0.0000E+00	0.0000E+00
U-235	0.0000	2.4000E-06	0.0000E+00	6.0000E-03	0.0000E+00	0.0000E+00
Np-237	0.0000	2.6000E-05	0.0000E+00	2.0000E-03	0.0000E+00	0.0000E+00
Pu-236	0.0000	2.0000E+01	0.0000E+00	3.0000E-03	0.0000E+00	0.0000E+00
Pu-238	0.65000	6.3000E-01	4.0950E-01	1.0000E-03	7.3509E-02	7.3509E-01
Pu-239	1200.5500	2.3000E-03	2.7613E+00	1.0000E-03	4.9567E-01	4.9567E+02
Pu-240	84.50000	8.4000E-03	7.0950E-01	1.0000E-03	1.2742E-01	1.2742E+02
Pu-241	0.0000	3.8000E+00	0.0000E+00	6.0000E-02	0.0000E+00	0.0000E+00
Pu-242	1.30000	1.5000E-04	1.9500E-04	1.0000E-03	3.5004E-05	3.5004E-02
Am-241	13.0000	1.3000E-01	1.6900E+00	1.0000E-03	3.0337E-01	3.0337E+02
Mass =	1300.0000	Activity sum =	5.5708E+00		Sum of f_iA₂ =	1.0000E+03

$$A_2(\text{mixture}) = \frac{1}{\sum f(i) / A_2} = \frac{1}{1.0000 \times 10^3 (1/\text{TBq})} = 1.0000 \times 10^3 \text{ TBq}$$

The total number of A₂ proposed for shipment is equal to the ratio of total activity divided by the A₂ of

this particular mixture as shown in Table 4.5.5.5.

Table 4.5.5.5. Activity, A_2 value, and number of A_2 proposed for transport

Isotopic distribution	Activity (TBq)	A_2 (TBq)	Act / A_2
Full Pu-241 (see Table 4.5.5.1)	5.3281E+01	1.1326E-02	4.7042E+03
Full Am-241 (see Table 4.5.5.2)	5.5708E+00	1.0000E-03	5.5708E+03

4.5.6 Calculation of the PAT-1 Containment Vessel's Regulatory Reference Air Leakage Rates

Prepared by Monty L. Goins, LLC, and Reviewed by Drew Winder, LLC

CALCULATION OF THE PAT-1 CONTAINMENT VESSEL'S REGULATORY REFERENCE AIR LEAKAGE RATES

Introduction

The PAT-1 leak-testing requirements of the containment boundary are based on the smallest maximum allowable leakage rate generated from the maximum plutonium content defined in Tables 4.5.5.1 and 4.5.5.2. Section 5 of ANSI N14.5-1997 defines the maximum allowable leakage rate based on the maximum allowable release rate. These leakage rates, L_N , L_A , and L_{PA} , are the maximum allowable seal leakage rates for Normal Conditions of Transport (NCT), Hypothetical Accident Conditions (HAC), and Accident condition for air transport of plutonium (ACATP). The worst-case maximum allowable leakage rates are used to calculate an equivalent leakage hole diameter following ANSI N14.5-1997, Appendix B, for each condition of transport. This leakage hole diameter is used to calculate a reference air and a helium leakage rate for leak testing. A bounding mass for the plutonium content of 1300 gram is used in this calculation to certify the PAT-1 package for shipment. The maximum allowable leakage rates are calculated using this maximum content mass in a much more dispersive form (oxide powder) at the highest calculated pressures and temperatures. This section shows the following procedure used to calculate the leak criteria for the plutonium constituents at initial fabrication. Table 4.5.6.1 shows the results of using this procedure for both set of isotopic distributions.

Plutonium Content with no Pu-241 decay

Calculate R_N , R_A , and R_{PA} :

where

- R_N = allowable release rate for normal conditions of transport;
- R_A = allowable release rate for hypothetical accident condition, and
- R_{PA} = allowable release rate for accident condition for air transport of plutonium.

The maximum allowable release rate is based on using A_2 .

$$A_2 = 1.1326 \times 10^{-2} \text{ TBq} \text{ (} 3.0611 \times 10^{-1} \text{ Ci)} \quad \text{Table 4.5.5.5}$$

The containment requirements for NCT, HAC, and ACATP are:

$$\begin{aligned} R_N &= A_2 \times 10^{-6} \text{ TBq/h} = A_2 \times 2.78 \times 10^{-10} \text{ TBq/s}, && \text{ANSI N14.5-1997 (Eq. 1)} \\ &= 1.1326 \times 10^{-2} \times 2.78 \times 10^{-10} \text{ TBq/s}, \\ &= 3.1488 \times 10^{-12} \text{ TBq/s, (} 8.5102 \times 10^{-11} \text{ Ci/s)}. \end{aligned}$$

$$\begin{aligned} R_A &= A_2 \text{ (TBq/week)}, \\ &= A_2 \times 1.65 \times 10^{-6} \text{ (TBq/s)}, && \text{ANSI N14.5-1997 (Eq. 2)} \\ &= 1.1326 \times 10^{-2} \times 1.65 \times 10^{-6} \text{ TBq/s}, \\ &= 1.8689 \times 10^{-8} \text{ TBq/s, (} 5.0510 \times 10^{-7} \text{ Ci/s)}. && \text{or limited to } 10 \text{ } A_2 \text{/week of } ^{87}\text{Kr} \end{aligned}$$

$$\begin{aligned} R_{PA} &= A_2 \text{ (TBq/week)}, \\ &= A_2 \times 1.65 \times 10^{-6} \text{ (TBq/s)}, && \text{ANSI N14.5-1997 (Eq. 2)} \\ &= 1.1326 \times 10^{-2} \times 1.65 \times 10^{-6} \text{ TBq/s}, \\ &= 1.8689 \times 10^{-8} \text{ TBq/s, (} 5.0510 \times 10^{-7} \text{ Ci/s)}. \end{aligned}$$

Following ANSI N14.5-1997, the medium aerosol activity must be calculated to determine the leakage rates.

m = total nuclide mass in the package available for release (g),
 $TotA$ = total activity in the package available for release (TBq),
 TSA = total specific activity in the package available for release (TBq/g).

For the plutonium content:

TSA = $TotA / m$,
 TSA = 5.3281×10^4 (TBq) / 1300 (g), Table 4.4
 TSA = 4.0985×10^{-2} TBq/g.

ρ_p = 9×10^{-6} g/cm³. The maximum density of powder aerosols in the fill gas
 Curren, W.D. and R.D. Bond, 1980, *Leakage of Radioactive Powders from Containers*.

For the packaging arrangement:

C_N = activity per unit volume of medium that could escape from the containment system (TBq/cm³),
 C_N = $TSA \times \rho_p$,
 C_N = 4.0985×10^{-2} (TBq/g) $\times 9 \times 10^{-6}$ (g/cm³),
 C_N = 3.6887×10^{-7} TBq/cm³. NCT

Using Curren's maximum aerosol density, $C_A = C_N = C_{PA}$:

C_A = activity per unit volume of exiting gas (TBq/cm³), HAC
 C_A = 3.6887×10^{-7} TBq/cm³.

C_{PA} = activity per unit volume of exiting gas (TBq/cm³), ACATP
 C_{PA} = 3.6887×10^{-7} TBq/cm³.

Section 6.1 of ANSI N14.5-1997 calculates L_N with (Eq. 3) and L_A , and L_{PA} with (Eq. 4). L_N , L_A , and L_{PA} are the maximum allowable leakage rates for the containment vessel fill gas aerosol during NCT, HAC, and ACATP, respectively.

L_N = maximum allowable leakage rate for the medium for NCT (TBq/cm³),
 L_N = R_N / C_N , ANSI N14.5-1997 (Eq. 3)
 L_N = 3.1488×10^{-12} (TBq/s) / 3.6887×10^{-7} (TBq/cm³),
 L_N = 8.5363×10^{-6} cm³/s.

L_A = maximum allowable leakage rate for the medium for HAC (TBq/cm³),
 L_A = R_A / C_A ,
 L_A = 1.8689×10^{-5} (TBq/s) / 3.6887×10^{-7} (TBq/cm³),
 L_A = 5.0665×10^{-2} cm³/s.

L_{PA} = maximum allowable leakage rate for the medium for ACATP (TBq/cm³),
 L_{PA} = R_{PA} / C_{PA} ,
 L_{PA} = 1.8689×10^{-5} (TBq/s) / 3.6887×10^{-7} (TBq/cm³),
 L_{PA} = 5.0665×10^{-2} cm³/s.

L_N , L_A , and L_{PA} correspond to the upstream volumetric leakage rate (L_u) at the upstream pressure (P_u)

in the ANSI N14.5-1997 formulas for use later in this section. The reference air leakage rates L_{RN} , L_{RA} , and L_{RPA} for NCT, HAC, and ACATP based on the L_N , L_A , and L_{PA} are then calculated using the maximum temperatures and pressure combinations from Sections 4.2, 4.3, and 4.3.1.

Determination of the Leakage Test Procedure Requirements for the Plutonium Content

This calculation will examine the most conservative effects of a fully loaded containment vessel with a plutonium mass of 1300 gram. The smallest allowable leakage values are shown in Table 4.5.6.1. The A_2 value and the maximum content activity-to- A_2 value ratio for this mixture were calculated in Section 4.5.5 and summarized in Table 4.5.5.5. As calculated in Section 4.5.5, the A_2 value and the maximum content activity-to- A_2 ratio used in the following calculations occur at initial fabrication and are 1.1326×10^{-2} TBq (3.0611×10^{-3} Ci) and 4.7042×10^3 respectively. These values are used to determine the leakage test procedural requirements when packaging the TB-1 containment vessel.

The following analysis determines the maximum allowable seal air reference leakage rate for NCT, HAC, and ACATP. The ANSI N14.5-1997 recommended method using a straight circular tube to model the leakage path is applied. Using this "standard" leakage hole model permits the calculation of equivalent reference leakage rates from which leak-test requirements can be established. Viscosity data for air and helium used in the following analyses were obtained from curve fitting routines at specific temperatures based on viscosity data for air (Handbook of Chemistry and Physics, 55th ed.) and helium (NBS Technical Note 631).

L_N and L_A correspond to the upstream volumetric leakage rate (L_D) at the upstream pressure (P_D).

$$\begin{aligned} L_N &= 8.5363 \times 10^{-6} \text{ cm}^3/\text{s}, \\ L_A &= 5.0665 \times 10^{-2} \text{ cm}^3/\text{s}, \\ L_{PA} &= 5.0665 \times 10^{-2} \text{ cm}^3/\text{s}. \end{aligned}$$

Find the maximum pressure and temperature in the containment vessel:
Converting the temperature to degrees Kelvin:

$$\begin{aligned} T &= 273.15 + T(^{\circ}\text{C}), \\ T &= 273.15 + 5/9 (^{\circ}\text{F} - 32) \text{ (K)}. \\ \\ T_N &= 273.15 + 5/9 (218.00^{\circ}\text{F} - 32) \text{ (K)}, & (T = 218.00^{\circ}\text{F}) \\ T_N &= 376.48 \text{ K}, & \text{NCT (Section 4.2)} \\ \\ T_A &= 273.15 + 5/9 (276.00^{\circ}\text{F} - 32) \text{ (K)}, & (T = 276.00^{\circ}\text{F}) \\ T_A &= 408.71 \text{ K}, & \text{HAC (Section 4.3)} \\ \\ T_{PA} &= 273.15 + 5/9 (1080.00^{\circ}\text{F} - 32) \text{ (K)}, & (T = 1080^{\circ}\text{F}) \\ T_{PA} &= 855.37 \text{ K}, & \text{ACATP (Section 4.3.1)} \end{aligned}$$

Converting the pressures from psia to atmospheres:

$$\begin{aligned} P_N &= P \text{ (psia)} / 14.696 \text{ (psia/atm)}, & \text{where P is the pressure in Section 4.2} \\ P_N &= 18.872 \text{ (psia)} / 14.696 \text{ (psia/atm)}, & \text{for NCT} \\ P_N &= 1.2842 \text{ atm}. \\ \\ P_A &= P \text{ (psia)} / 14.696 \text{ (psia/atm)}, & \text{where P is the pressure in Section 4.3} \\ P_A &= 20.486 \text{ (psia)} / 14.696 \text{ (psia/atm)}, & \text{for HAC} \\ P_A &= 1.3940 \text{ atm}. \end{aligned}$$

For ACATP conditions, two different pressures will be analyzed:

$$\begin{aligned}
 P_{PA1} &= P \text{ (psia)} / 14.696 \text{ (psia/atm)}, && \text{where } P \text{ is the pressure in Section 4.3.1} \\
 P_{PA1} &= 613 \text{ (psia)} / 14.696 \text{ (psia/atm)}, && \text{for ACATP} \\
 P_{PA1} &= 41.7120 \text{ atm.} \\
 \\
 P_{PA2} &= P_{MAX} / 14.696 \text{ (psia/atm)}, && \text{where } P_{MAX} \text{ is the maximum design pressure of the} \\
 &&& \text{TB-1 containment vessel} \\
 P_{PA2} &= 1125 \text{ (psia)} / 14.696 \text{ (psia/atm)}, \\
 P_{PA2} &= 76.55 \text{ atm.}
 \end{aligned}$$

The molar gas percentages, determined later in this section for ACATP at 613 psia, will be used for both the P_{PA1} and P_{PA2} analysis during ACATP.

NCT Leakage Hole Diameter for the Plutonium Content

The following calculations determine the leakage hole diameter that generates the maximum allowable leakage rate during NCT. To keep these calculations conservative, the maximum values for temperature and pressure were used as steady-state conditions for NCT. According to Sect. 4.1.1, the gas inside the containment vessel may consist of nitrogen/helium/argon with a maximum 100 parts per million of oxygen. Based on sample calculations, the lowest regulatory leakage rate was predicted with 100 percent helium in the void volumes of the TB-1 containment vessel and T-Ampoule. The leak path length was assumed to be 0.022 inches (0.056 cm) based on the length of the copper gasket seal compression.

Input data for NCT with 100% helium gas:

$$\begin{aligned}
 L_N &= 8.5363 \times 10^{-6} \text{ cm}^3/\text{s}, && \text{Maximum upstream leakage} \\
 P_u &= 1.2842 \text{ atm}, && \text{Upstream pressure} = 18.872 \text{ psia} \\
 P_d &= 0.2382 \text{ atm}, && \text{Downstream pressure} = 3.5 \text{ psia, per 10 CFR 71.71(3)} \\
 a &= 0.056 \text{ cm}, && \text{Leak path length (copper gasket seal compression)} \\
 T &= 376.48 \text{ K}, && \text{Fill gas temperature} = 218.00^\circ\text{F} \\
 \mu &= 0.02310 \text{ cP}, && \text{Viscosity at temperature} \\
 M &= 4.0 \text{ g/g-mole.} && \text{Molecular weight of fill gas}
 \end{aligned}$$

The average pressure is:

$$\begin{aligned}
 P_s &= (P_u + P_d)/2, \\
 &= (1.2842 + 0.2382) / 2, \\
 P_s &= 0.7612 \text{ atm.} && \text{Average pressure during NCT}
 \end{aligned}$$

According to ANSI N14.5-1997, the flow leakage hole diameter is unknown. Therefore, the mass-like leakage flow rate must be calculated to calculate the average leakage flow rate. Q is the mass-like leakage for flow using the upstream leakage, L_u , and pressure, P_u :

$$\begin{aligned}
 Q &= P_u L_u, && \text{(Eq. B1)} \\
 L_u &= L_N, && \text{NCT leakage} \\
 \\
 Q &= (1.2842)(\text{atm})(8.5363 \times 10^{-6})(\text{cm}^3/\text{s}), \\
 Q &= 1.0962 \times 10^{-5} \text{ atm-cm}^3/\text{s}, && \text{NCT mass-like leakage rate} \\
 \\
 Q &= P_s L_s, && \text{(Eq. B1)}
 \end{aligned}$$

$$L_a = Q / P_a = 1.0962 \times 10^{-5} \text{ (atm-cm}^3\text{/s)} / (0.7612 \text{ atm}),$$

$$L_a = 1.4403 \times 10^{-5} \text{ cm}^3\text{/s.} \quad \text{NCT average leakage rate}$$

Solve equations B2 B4 from ANSI N14.5-1997:

$$L_a = (F_c + F_m) (P_a - P_d) \text{ cm}^3\text{/s.} \quad \text{(Eq. B2)}$$

$$L_a = (F_c + F_m) (1.2842 - 0.2382),$$

$$L_a = (1.0460) (F_c + F_m) \text{ cm}^3\text{/s.}$$

$$F_c = (2.49 \times 10^5) D^3 / (a \mu) \text{ (cm}^3\text{/atm-s)}, \quad \text{(Eq. B3)}$$

$$F_c = (2.49 \times 10^5) D^3 / ((0.056) (0.02310)),$$

$$F_c = (1.9245 \times 10^8) D^3 \text{ cm}^3\text{/atm-s.}$$

$$F_m = (3.81 \times 10^5) D^3 (\bar{T} / M)^3 / (a P_d) \text{ (cm}^3\text{/atm-s)}, \quad \text{(Eq. B4)}$$

$$F_m = (3.81 \times 10^5) D^3 (376.48 / 4.0)^3 / ((0.056) (0.7612)),$$

$$F_m = (8.6717 \times 10^8) D^3 \text{ cm}^3\text{/atm-s.}$$

From the mass-like leakage calculation:

$$L_a = 1.4403 \times 10^{-5} \text{ cm}^3\text{/s.} \quad \text{NCT average leakage rate}$$

Find the leakage hole diameter that sets:

$$L_2 = L_a$$

Using the equations:

$$L_2 = (1.0460) (F_c + F_m) \text{ cm}^3\text{/s.}$$

$$F_c = (1.9245 \times 10^8) D^3 \text{ cm}^3\text{/atm-s.}$$

$$F_m = (8.6717 \times 10^8) D^3 \text{ cm}^3\text{/atm-s.}$$

To get a better guess on a new D use:

$$D = D_2 (L_a / L_2)^{0.252}$$

Now a guess must be made for D₂ to solve Eq. B2 for NCT:

$$D_2 = 0.001 \text{ cm. and solve for } L_a = 1.4403 \times 10^{-5} \text{ cm}^3\text{/s.} \quad \text{NCT average leakage rate}$$

Diameter	F _c	F _m	L ₂	L _a / L ₂
1.0000E-03	1.9245E-03	8.6717E-04	2.9201E-03	0.0049
2.6221E-04	9.0966E-06	1.5632E-05	2.5867E-05	0.5568
2.2623E-04	5.0410E-06	1.0041E-05	1.5775E-05	0.9129
2.2110E-04	4.5987E-06	9.3723E-06	1.4614E-05	0.9855
2.2028E-04	4.5315E-06	9.2693E-06	1.4436E-05	0.9976
2.2015E-04	4.5207E-06	9.2528E-06	1.4407E-05	0.9996
2.2013E-04	4.5190E-06	9.2502E-06	1.4403E-05	0.9999
2.2013E-04	4.5187E-06	9.2498E-06	1.4402E-05	1.0000

The NCT leakage hole diameter for the plutonium content:

$$D = 2.2013 \times 10^{-4} \text{ cm.} \quad \text{NCT diameter}$$

NCT Reference Air Leakage Rate for the Plutonium Content

The leakage hole diameter found for the maximum allowable leakage rate for NCT will be used to determine the reference air leakage rate. O-ring seal leakage testing must ensure that no leakage is greater than the leakage generated by the hole diameter $D = 2.2013 \times 10^{-4}$ cm. Therefore, the NCT reference leakage flow rate ($L_{R,Air}$) must be calculated to determine the allowable test leakage rate.

Input data for NCT reference air leakage rate:

D	=	2.2013×10^{-4} cm,	From NCT
a	=	0.056 cm,	Leak path length (copper gasket seal compression),
P_u	=	1.0 atm,	Upstream pressure
P_d	=	0.01 atm,	Downstream pressure
T	=	298 K,	Fill gas temperature, 77°F
M	=	29 g/g-mole,	Molecular weight of air
μ	=	0.0185 cP,	Viscosity of air at reference temperature

Calculate P_a :

$$P_a = (P_u + P_d) / 2, \\ = (1.0 + 0.01) / 2, \\ P_a = 0.505 \text{ atm.} \quad \text{NCT average pressure}$$

$$F_c = (2.49 \times 10^6) D^4 / (a \mu) \text{ (cm}^3/\text{atm-s)}, \quad \text{(Eq. B3)} \\ F_c = (2.49 \times 10^6) (2.2013 \times 10^{-4})^4 / ((0.056) (0.0185)), \\ F_c = (2.4035 \times 10^6) (2.2013 \times 10^{-4})^4, \\ F_c = 5.6433 \times 10^{-6} \text{ cm}^3/\text{atm-s.}$$

$$F_m = (3.81 \times 10^3) D^3 (T / M)^{1/2} / (a P_a) \text{ (cm}^3/\text{atm-s)}, \quad \text{(Eq. B4)} \\ F_m = (3.81 \times 10^3) (2.2013 \times 10^{-4})^3 (298 / 29)^{1/2} / ((0.056) (0.505)), \\ F_m = (4.3187 \times 10^3) (2.2013 \times 10^{-4})^3, \\ F_m = 4.6066 \times 10^{-6} \text{ cm}^3/\text{atm-s.}$$

$$L_a = (F_c + F_m) (P_u - P_d) (P_a / P_d) \text{ (cm}^3/\text{s)}, \quad \text{(Eq. B5)} \\ L_a = (5.6433 \times 10^{-6} + 4.6066 \times 10^{-6}) (\text{cm}^3/\text{atm-s}) (1.0 - 0.01) (\text{atm}) (0.505 / 1.0), \\ L_a = (1.0250 \times 10^{-5}) (\text{cm}^3/\text{atm-s}) (0.49995) (\text{atm}), \\ L_a = 5.1244 \times 10^{-6} \text{ cm}^3/\text{s.}$$

The reference air leakage rate as defined in ANSI N14.5-1997, Sect. B.3, is the upstream leakage in air.

$$L_{R,Air} = 5.1244 \times 10^{-6} \text{ ref-cm}^3/\text{s.} \quad \text{plutonium content}$$

The same equations can be used to calculate an allowable leakage rate using helium for leak testing.

M	=	4 g/g-mole,	Molecular weight of helium
μ	=	0.0198 cP,	Viscosity of helium at temperature

$$\begin{aligned}
 F_c &= (2.49 \times 10^6) D^4 / (a \mu) \text{ (cm}^3\text{/atm-s)}, & \text{(Eq. B3)} \\
 F_c &= (2.49 \times 10^6) (2.2013 \times 10^{-7})^4 / ((0.056) (0.0198)), \\
 F_c &= (2.2457 \times 10^6) (2.2013 \times 10^{-7})^4, \\
 F_c &= 5.2728 \times 10^{-6} \text{ cm}^3\text{/atm-s.} \\
 \\
 F_m &= (3.81 \times 10^5) D^3 (T/M)^{3/2} / (a P_d) \text{ (cm}^3\text{/atm-s)}, & \text{(Eq. B4)} \\
 F_m &= (3.81 \times 10^5) (2.2013 \times 10^{-7})^3 (298/4.0)^{3/2} / ((0.056) (0.505)), \\
 F_m &= (1.1629 \times 10^6) (2.2013 \times 10^{-7})^3, \\
 F_m &= 1.2404 \times 10^{-5} \text{ cm}^3\text{/atm-s.} \\
 \\
 L_a &= (F_c + F_m) (P_u - P_d) (P_u / P_d) \text{ (cm}^3\text{/s)}, & \text{(Eq. B5)} \\
 L_a &= (5.2728 \times 10^{-6} + 1.2404 \times 10^{-5}) (\text{cm}^3\text{/atm-s}) (1.0 - 0.01) (\text{atm}) (0.505 / 1.0), \\
 L_a &= (1.7676 \times 10^{-5}) (\text{cm}^3\text{/atm-s}) (0.49995) (\text{atm}), \\
 L_a &= 8.8373 \times 10^{-6} \text{ cm}^3\text{/s.}
 \end{aligned}$$

The allowable leakage rate using helium for leak testing is:

$$L_{2N-H_2} = 8.8373 \times 10^{-6} \text{ cm}^3\text{/s.} \quad \text{NCT helium test value}$$

HAC Leakage Hole Diameter for the Plutonium Content

The calculation of a maximum allowable leakage rate hole diameter is based on the temperature and pressure of the fill gas aerosol for HAC, assuming the content is in an oxide powder form. Keeping this calculation conservative, the maximum values for temperature and pressure were used as steady-state conditions for a week. The maximum values were generated during the 30-min burn test for HAC.

Input data for HAC:

L_A	=	$5.0665 \times 10^{-2} \text{ cm}^3\text{/s.}$	Maximum exit leakage
P_u	=	1.3940 atm.	Upstream pressure = 20.486 psia
P_d	=	1.0 atm.	Downstream pressure
T	=	408.71 K.	Fill gas temperature = 276°F
μ	=	0.02442 cP.	Viscosity of gas mixture at temperature
M	=	29 g/g-mole.	Molecular weight of gas mixture
a	=	0.056 cm.	Leak path length (copper gasket seal compression)
P_a	=	$(P_u + P_d) / 2$	
	=	$(1.3940 + 1.0) / 2.$	HAC average pressure
P_a	=	1.1970 atm.	

Q is the mass-like leakage for flow using the upstream leakage, L_a , and pressure, P_u :

$$\begin{aligned}
 Q &= P_u L_a & \text{(Eq. B1)} \\
 L_a &= L_a & \text{HAC leakage} \\
 \\
 Q &= (1.3940)(\text{atm}) (5.0665 \times 10^{-2})(\text{cm}^3\text{/s}), \\
 Q &= 7.0626 \times 10^{-2} \text{ atm-cm}^3\text{/s.} & \text{HAC mass-like leakage rate} \\
 \\
 Q &= P_a L_a & \text{(Eq. B1)}
 \end{aligned}$$

$$\begin{aligned}
 L_a &= Q / P_a \\
 L_a &= 7.0626 \times 10^{-2} \text{ (atm-cm}^3\text{/s)} / (1.1970)\text{(atm)}, \\
 L_a &= 5.9003 \times 10^{-2} \text{ cm}^3\text{/s.} \qquad \text{HAC average leakage rate}
 \end{aligned}$$

Solve equations B2 -B4 from ANSI N14.5-1997:

$$\begin{aligned}
 L_a &= (F_c + F_m) (P_a - P_d) \text{ (cm}^3\text{/s)}, & \text{(Eq B2)} \\
 L_a &= (F_c + F_m) (1.3940 - 1.0), \\
 L_a &= 0.3940 (F_c + F_m) \text{ cm}^3\text{/s.}
 \end{aligned}$$

$$\begin{aligned}
 F_c &= (2.49 \times 10^6) D^4 / (a \mu) \text{ (cm}^3\text{/atm-s)}, & \text{(Eq B3)} \\
 F_c &= (2.49 \times 10^6) D^4 / ((0.056) (0.02442)), \\
 F_c &= (1.8211 \times 10^8) D^4 \text{ cm}^3\text{/atm-s.}
 \end{aligned}$$

$$\begin{aligned}
 F_m &= (3.81 \times 10^3) D^3 (T / M)^{1/2} / (a P_d) \text{ (cm}^3\text{/atm-s)}, & \text{(Eq B4)} \\
 F_m &= (3.81 \times 10^3) D^3 (408.71 / 4.0)^{1/2} / ((0.056) (1.1970)), \\
 F_m &= (5.7454 \times 10^5) D^3 \text{ cm}^3\text{/atm-s.}
 \end{aligned}$$

From the mass-like leakage calculation:

$$L_a = 5.9003 \times 10^{-2} \text{ cm}^3\text{/s.} \qquad \text{HAC average leakage rate}$$

Find the leakage hole diameter that sets:

$$L_2 = L_a$$

Using the equations:

$$\begin{aligned}
 L_2 &= 0.3940 (F_c + F_m) \text{ cm}^3\text{/s.} \\
 F_c &= (1.8211 \times 10^8) D^4 \text{ cm}^3\text{/atm-s.} \\
 F_m &= (5.7454 \times 10^5) D^3 \text{ cm}^3\text{/atm-s.}
 \end{aligned}$$

To get a better guess on a new D use:

$$D = D_2 (L_a / L_2)^{0.232}$$

Now a guess must be made for D₂ to solve Eq. B2 for HAC:

$$D_2 = 0.001 \text{ (cm)}, \text{ and solve for } L_a = 5.9003 \times 10^{-2} \text{ (cm}^3\text{/s)}. \text{ HAC average leakage rate}$$

Diameter	F _c	F _m	L ₂	L _a / L ₂
1.0000E-02	1.8211E+01	5.7454E-01	7.4014E-01	0.00797
2.9593E-03	1.3967E-02	1.4890E-02	6.0896E-02	0.96891
2.9359E-03	1.3530E-02	1.4539E-03	5.9034E-02	0.99948
2.9355E-03	1.3523E-02	1.4533E-03	5.9004E-02	0.99999
2.9355E-03	1.3523E-02	1.4533E-03	5.9003E-02	1.00000

The HAC leakage hole diameter for the Plutonium content is:

$$D = 2.9355 \times 10^{-3} \text{ cm.} \quad \text{HAC diameter}$$

HAC Reference Air Leakage Rate for Plutonium Content

The leakage hole diameter found for the maximum allowable leakage rate for HAC will be used to determine the reference air leakage rate. O-ring seal leakage testing must assure that no leakage is greater than the leakage generated by the hole diameter $D = 2.9355 \times 10^{-3}$ cm. Therefore, the HAC reference air leakage rate ($L_{R,A}$) must be calculated to determine the acceptable test leakage rate for post-HAC leakage testing.

Input data for HAC reference air leakage rate:

D	=	2.9355×10^{-3} cm,	From the HAC of transport
a	=	0.056 cm,	Leak path length (copper gasket seal compression)
P_u	=	1.0 atm,	Upstream pressure
P_d	=	0.01 atm,	Downstream pressure
T	=	298 K,	Fill gas temperature, 77°F
M	=	29 g/g-mole,	Molecular weight of air
μ	=	0.0185 cP,	Viscosity at temperature

Calculate P_a :

$$P_a = (P_u + P_d) / 2 = 0.505 \text{ atm.} \quad \text{HAC average pressure}$$

$$F_c = (2.49 \times 10^6) D^4 / (a \mu) (\text{cm}^3/\text{atm-s}), \quad \text{(Eq. B3)}$$

$$F_c = (2.49 \times 10^6) (2.9355 \times 10^{-3})^4 / ((0.056) (0.0185)),$$

$$F_c = (2.4035 \times 10^3) (2.9355 \times 10^{-3})^4,$$

$$F_c = 1.7847 \times 10^{-1} \text{ cm}^3/\text{atm-s.}$$

$$F_m = (3.81 \times 10^3) D^3 (T/M)^{1/2} / (a P_a) (\text{cm}^3/\text{atm-s}), \quad \text{(Eq. B4)}$$

$$F_m = (3.81 \times 10^3) (2.9355 \times 10^{-3})^3 (298/29)^{1/2} / ((0.056) (0.505)),$$

$$F_m = (4.3187 \times 10^3) (2.9355 \times 10^{-3})^3,$$

$$F_m = 1.0924 \times 10^{-2} \text{ cm}^3/\text{atm-s.}$$

$$L_a = (F_c + F_m) (P_u - P_d) (P_u / P_a) (\text{cm}^3/\text{s}), \quad \text{(Eq. B5)}$$

$$L_a = (1.7847 \times 10^{-1} + 1.0924 \times 10^{-2}) (\text{cm}^3/\text{atm-s}) (1.0 - 0.01) (\text{atm}) (0.505 / 1.0),$$

$$L_a = (1.8939 \times 10^{-1}) (\text{cm}^3/\text{atm-s}) (0.49995) (\text{atm}),$$

$$L_a = 9.4686 \times 10^{-2} \text{ cm}^3/\text{s.}$$

The HAC reference air leakage rate as defined in ANSI N14.5-1997, Sect. B.3, is the upstream leakage in air.

$$L_{R,A,Pl} = 9.4686 \times 10^{-2} \text{ ref-cm}^3/\text{s.} \quad \text{for plutonium content}$$

The same equations can be used to calculate an allowable leakage rate using helium for leak testing.

M	=	4 g/g-mole,	Molecular weight of helium
μ	=	0.0198 cP,	Viscosity of helium at temperature

$$F_c = (2.49 \times 10^6) D^4 / (a \mu) (\text{cm}^3/\text{atm-s}), \quad \text{(Eq. B3)}$$

$$\begin{aligned}
 F_c &= (2.49 \times 10^6) (2.9355 \times 10^{-3} \text{ cm})^4 / ((0.056) (0.0198)), \\
 F_c &= (2.2457 \times 10^9) (2.9355 \times 10^{-3} \text{ cm})^4, \\
 F_c &= 1.6675 \times 10^{-1} \text{ cm}^3/\text{atm-s.} \\
 \\
 F_{\text{in}} &= (3.81 \times 10^3) D^3 (T/M)^{0.5} / (a P_2) (\text{cm}^3/\text{atm-s}), & (\text{Eq B4}) \\
 F_{\text{in}} &= (3.81 \times 10^3) (2.9355 \times 10^{-3} \text{ cm})^3 (298/4)^{0.5} / ((0.056) (0.505)), \\
 F_{\text{in}} &= (1.1629 \times 10^6) (2.9355 \times 10^{-3} \text{ cm})^3, \\
 F_{\text{in}} &= 2.9415 \times 10^{-2} \text{ cm}^3/\text{atm-s.} \\
 \\
 L_a &= (F_c + F_{\text{in}}) (P_e - P_d) (P_s / P_d) (\text{cm}^3/\text{s}), & (\text{Eq B5}) \\
 L_a &= (1.6675 \times 10^{-1} + 2.9415 \times 10^{-2}) (\text{cm}^3/\text{atm-s}) (1.0 - 0.01) (\text{atm}) (0.505 / 1.0), \\
 L_a &= (1.9617 \times 10^{-1}) (\text{cm}^3/\text{atm-s}) (0.49995) (\text{atm}), \\
 L_a &= 9.8072 \times 10^{-2} \text{ cm}^3/\text{s.}
 \end{aligned}$$

The allowable leakage rate using helium for leak testing for HAC is:

$$L_{\text{R,A-He}} = 9.8072 \times 10^{-2} \text{ cm}^3/\text{s.} \quad \text{HAC helium test value}$$

Accident Condition for Air Transport of Plutonium (ACATP)

The calculation of a maximum allowable leakage rate hole diameter is based on the temperature and pressure of the fill gas aerosol for ACATP, assuming the content is in an oxide powder form. Keeping this calculation conservative, the maximum values for temperature and pressure were used as steady-state conditions for a week. The maximum values were generated during the 60-min burn test for ACATP (10 CFR 71.74(a)(5)). In accordance with Section 4.5.3, 1.42×10^{-7} moles of He gas are generated per gram of plutonium in one year. Therefore, using 1300 grams of plutonium, 1.846×10^{-4} moles of helium is generated in one year. The original assumption for packaging assumed that the glove box was filled with helium gas. However, for air transport accident conditions, the contents are conservatively assumed to be loaded inside the T-Ampoule and T-Ampoule inside the TB-1 containment in an air environment. Therefore, the 1103.01 cm^3 of void volume would contain 0.00897 moles of oxygen and 0.0337 moles of nitrogen. According to the o-ring decomposition and pyrolysis of ancillary high density polyethylene analysis shown in Section 4.5.3, the following molar quantity of gases are created during ACATP: 0.009286 moles of CO_2 ; 0.29540 moles of HF; 0.03493 moles of N_2 ; 0.02711 moles of CF_4 ; and, 0.28866 moles of hydrocarbon gas. The gases are assumed perfectly mixed generating the following gas percentages:

1. 1.417 % of CO_2 $[(0.009286/0.65557) \times 100\%]$
2. 45.060 % of HF $[(0.2954/0.65557) \times 100\%]$
3. 5.328 % of N_2 $[(0.03493/0.65557) \times 100\%]$
4. 4.135 % of CF_4 $[(0.02711/0.65557) \times 100\%]$
5. 44.032 % of hydrocarbon gas mixture $[(0.28866/0.65557) \times 100\%]$
6. 0.028 % of He $[(0.00018/0.65557) \times 100\%]$

The molar gas percentages, determined above for 613 psia, will be used for both the 613 psia and 1125 psia analysis during ACATP. The hydrocarbon gas is a mixture of approximately seventy three different gases. The mixture has an average molecular weight of approximately 240 g/g-mole. The corresponding hydrocarbon gas with this molecular weight is $\text{C}_{17}\text{H}_{36}$. Therefore, the viscosity of $\text{C}_{17}\text{H}_{36}$ will be used for the hydrocarbon gas mixture in the following leakage calculations for ACATP. Equations shown in *Perry's Chemical Engineers' Handbook*, 7th Edition, provide a method of determining the viscosity of this hydrocarbon gas as a function of temperature. Normally, the leakage hole length, a , is assumed to be the basic diameter of the O-ring seal. In this case where the seal is created by deformation into a copper gasket, the value for " a " is the indentation depth into the copper gasket of 0.022 inches (0.056 cm). Varying this value by a factor of 10 will increase the leakage rates by approximately the same factor. The following

calculations are shown for the case where the Pu-241 has not decayed to Am-241. Table 4.5.6.1 summarizes the results for both decay conditions.

Input data for ACATP:

L_{PA}	=	$5.0665 \times 10^{-2} \text{ cm}^3/\text{s}$,	Maximum exit leakage
P_c	=	41.7120 atm,	Upstream pressure = 613.00 psia (P_{PA1})
P_d	=	1.0 atm,	Downstream pressure
T	=	855.37 K,	Fill gas temperature = 1080°F
μ	=	0.03694 cP,	Viscosity of gas mixture at temperature
M	=	120.44 g/g-mole,	Molecular weight of gas mixture
a	=	0.056 cm.	Leak path length (copper gasket seal compression)
P_a	=	$(P_c + P_d) / 2$	ACATP average pressure
	=	$(41.7120 + 1.0) / 2$,	
P_a	=	21.3560 atm.	

Q is the mass-like leakage for flow using the upstream leakage, L_a , and pressure, P_a :

Q	=	$P_a L_a$	(Eq. B1)
L_a	=	L_{PA}	ACATP leakage
Q	=	$(41.7120)(\text{atm})(5.0665 \times 10^{-2})(\text{cm}^3/\text{s})$,	ACATP mass-like leakage rate
Q	=	2.1134 atm-cm ³ /s.	
Q	=	$P_a L_a$	(Eq. B1)
L_a	=	Q / P_a	ACATP average leakage rate
L_a	=	$2.1134 (\text{atm-cm}^3/\text{s}) / (21.3560)(\text{atm})$,	
L_a	=	$9.8958 \times 10^{-2} \text{ cm}^3/\text{s}$.	

Solve equations B2-B4 from ANSI N14.5-1997:

L_a	=	$(F_c + F_m) (P_a - P_d) (\text{cm}^3/\text{s})$,	(Eq. B2)
L_a	=	$(F_c + F_m) (41.7120 - 1.0)$,	$L_a = 40.7120 (F_c + F_m) \text{ cm}^3/\text{s}$.
L_a	=	$40.7120 (F_c + F_m) \text{ cm}^3/\text{s}$.	
F_c	=	$(2.49 \times 10^6) D^4 / (a \mu) (\text{cm}^3/\text{atm-s})$,	(Eq. B3)
F_c	=	$(2.49 \times 10^6) D^4 / ((0.056)(0.03694))$,	
F_c	=	$(1.2037 \times 10^9) D^4 \text{ cm}^3/\text{atm-s}$.	
F_m	=	$(3.81 \times 10^3) D^3 (T/M)^{1/2} / (a P_a) (\text{cm}^3/\text{atm-s})$,	(Eq. B4)
F_m	=	$(3.81 \times 10^3) D^3 (855.37 / 120.44)^{1/2} / ((0.056)(21.3560))$,	
F_m	=	$(8.4899 \times 10^6) D^3 \text{ cm}^3/\text{atm-s}$.	

From the mass-like leakage calculation:

L_a	=	$9.8958 \times 10^{-2} \text{ cm}^3/\text{s}$.	ACATP average leakage rate
-------	---	---	----------------------------

Find the leakage hole diameter that sets:

$$L_2 = L_a$$

Using the equations:

$$\begin{aligned} L_2 &= 40.7120(F_c + F_m) \text{ cm}^3/\text{s}, \\ F_c &= (1.2037 \times 10^6) D^3 \text{ cm}^3/\text{atm-s}, \\ F_m &= (8.4899 \times 10^7) D^3 \text{ cm}^3/\text{atm-s}. \end{aligned}$$

To get a better guess on a new D use:

$$D = D_2 (L_1 / L_2)^{0.222}.$$

Now a guess must be made for D_2 to solve Eq. B2 for ACATP:

$$D_2 = 0.01 \text{ (cm)}, \text{ and solve for } L_1 = 9.8958 \times 10^{-2} \text{ (cm}^3/\text{s)}. \quad \text{ACATP average leakage rate}$$

Diameter	F_c	F_m	L_2	L_1 / L_2
1.0000E-02	1.2037E-01	8.4899E-03	4.9042E-02	0.00020
1.1717E-03	2.2691E-03	1.3658E-05	9.2937E-02	1.06478
1.1904E-03	2.4173E-03	1.4322E-05	9.8899E-02	0.99959
1.1903E-03	2.4163E-03	1.4318E-05	9.8958E-02	1.00000

The ACATP leakage hole diameter for the Plutonium content is:

$$D = 1.1903 \times 10^{-3} \text{ cm.} \quad \text{ACATP diameter}$$

ACATP Reference Air Leakage Rate for Plutonium Content

The leakage hole diameter found for the maximum allowable leakage rate for ACATP will be used to determine the reference air leakage rate. O-ring seal leakage testing must assure that no leakage is greater than the leakage generated by the hole diameter $D = 1.1903 \times 10^{-3} \text{ cm}$. Therefore, the ACATP reference air leakage rate ($L_{R, PA, ATR}$) must be calculated to determine the acceptable test leakage rate for post- ACATP leakage testing.

Input data for ACATP reference air leakage rate:

D	$= 1.1903 \times 10^{-3} \text{ cm.}$	From the ACATP of transport
a	$= 0.056 \text{ cm.}$	Leak path length (copper gasket seal compression)
P_u	$= 1.0 \text{ atm.}$	Upstream pressure
P_d	$= 0.01 \text{ atm.}$	Downstream pressure
T	$= 298 \text{ K.}$	Fill gas temperature, 77°F
M	$= 29 \text{ g/g.mole.}$	Molecular weight of air
μ	$= 0.0185 \text{ cP.}$	Viscosity at temperature

Calculate P_a :

$$\begin{aligned} P_a &= (P_u + P_d) / 2 \\ &= 0.505 \text{ atm.} \end{aligned} \quad \text{ACATP average pressure}$$

$$\begin{aligned}
 F_c &= (2.49 \times 10^6) D^4 / (a \mu) (\text{cm}^3/\text{atm-s}), & (\text{Eq. B3}) \\
 F_c &= (2.49 \times 10^6) (1.1903 \times 10^{-3})^4 / ((0.056) (0.0185)), \\
 F_c &= (2.4035 \times 10^6) (1.1903 \times 10^{-3})^4, \\
 F_c &= 4.8246 \times 10^3 \text{ cm}^3/\text{atm-s}. \\
 \\
 F_m &= (3.81 \times 10^3) D^3 (T/M)^{0.5} / (a P_d) (\text{cm}^3/\text{atm-s}), & (\text{Eq. B4}) \\
 F_m &= (3.81 \times 10^3) (1.1903 \times 10^{-3})^3 (298/29)^{0.5} / ((0.056) (0.505)), \\
 F_m &= (4.3187 \times 10^3) (1.1903 \times 10^{-3})^3, \\
 F_m &= 7.2832 \times 10^{-4} \text{ cm}^3/\text{atm-s}. \\
 \\
 L_a &= (F_c + F_m) (P_a - P_d) (P_1 / P_d) (\text{cm}^3/\text{s}), & (\text{Eq. B5}) \\
 L_a &= (4.8246 \times 10^3 + 7.2832 \times 10^{-4}) (\text{cm}^3/\text{atm-s}) (1.0 - 0.01) (\text{atm}) (0.505 / 1.0), \\
 L_a &= (5.5529 \times 10^3) (\text{cm}^3/\text{atm-s}) (0.49995) (\text{atm}), \\
 L_a &= 2.7762 \times 10^{-3} \text{ cm}^3/\text{s}.
 \end{aligned}$$

The ACATP reference air leakage rate as defined in ANSI N14.5-1997, Sect. B.3, is the upstream leakage in air.

$$L_{R,PA-AIR} = 2.7762 \times 10^{-3} \text{ ref-cm}^3/\text{s} \quad \text{for plutonium content}$$

The same equations can be used to calculate an allowable leakage rate using helium for leak testing.

$$\begin{aligned}
 M &= 4 \text{ g/g-mole}, & \text{Molecular weight of helium} \\
 \mu &= 0.0198 \text{ cP}, & \text{Viscosity of helium at temperature} \\
 \\
 F_c &= (2.49 \times 10^6) D^4 / (a \mu) (\text{cm}^3/\text{atm-s}), & (\text{Eq. B3}) \\
 F_c &= (2.49 \times 10^6) (1.1903 \times 10^{-3} \text{ cm})^4 / ((0.056) (0.0198)), \\
 F_c &= (2.2457 \times 10^6) (1.1903 \times 10^{-3} \text{ cm})^4, \\
 F_c &= 4.5078 \times 10^3 \text{ cm}^3/\text{atm-s}. \\
 \\
 F_m &= (3.81 \times 10^3) D^3 (T/M)^{0.5} / (a P_d) (\text{cm}^3/\text{atm-s}), & (\text{Eq. B4}) \\
 F_m &= (3.81 \times 10^3) (1.1903 \times 10^{-3} \text{ cm})^3 (298/4)^{0.5} / ((0.056) (0.505)), \\
 F_m &= (1.1629 \times 10^6) (1.1903 \times 10^{-3} \text{ cm})^3, \\
 F_m &= 1.9611 \times 10^{-3} \text{ cm}^3/\text{atm-s}. \\
 \\
 L_a &= (F_c + F_m) (P_a - P_d) (P_1 / P_d) (\text{cm}^3/\text{s}), & (\text{Eq. B5}) \\
 L_a &= (4.5078 \times 10^3 + 1.9611 \times 10^{-3}) (\text{cm}^3/\text{atm-s}) (1.0 - 0.01) (\text{atm}) (0.505 / 1.0), \\
 L_a &= (6.4689 \times 10^3) (\text{cm}^3/\text{atm-s}) (0.49995) (\text{atm}), \\
 L_a &= 3.2341 \times 10^{-3} \text{ cm}^3/\text{s}.
 \end{aligned}$$

The allowable leakage rate using helium for leak testing for ACATP is:

$$L_{R,PA-He} = 3.2341 \times 10^{-3} \text{ cm}^3/\text{s} \quad \text{ACATP helium test value}$$

In accordance with Table 4.2 of the SAR, the highest measured air leakage rate following the ACATP conditions was 4.5×10^{-3} cc/sec at atmosphere conditions (atm cc/s). This leakage rate is considerably lower than the calculated maximum allowable regulatory leakage rate requirement of 1.3152×10^{-3} ref cc/s shown in Table 4.5.6.1. Therefore, the TB-1 containment vessel inside the PAT-1 shipping package maintains containment for NCT, HAC, and ACATP conditions.

Mass Release During ACATP

To determine the amount of material that leaks out of the containment boundary in one week under ACATP conditions, the measured volumetric leakage rate shown in Table 4.2 ($4.5 \times 10^{-5} \text{ cm}^3/\text{s}$) is multiplied by the aerosol mass density ($9.0 \times 10^{-6} \text{ g/cm}^3$) and by time ($6.048 \times 10^5 \text{ sec/week}$). You obtain a mass release of approximately 2.45×10^{-4} grams in one week. This release amount disregards orifice size and particle size limits.

The regulatory release mass limit for the material in the containment vessel is calculated by using the regulatory activity limit of an A_2 in one week divided by the specific activity of the mixture. Assuming a homogenous mixture, the material leaving the containment vessel has a specific activity determined by dividing the total activity (TBq) by the total mass (grams) or TBq/gram. Therefore, the allowable mass release is then the A_2 in a week (TBq/week) divided by the specific activity of the mixture (TBq/gram) or grams/week. Using this approach for the material that has no Pu241 decay and Table 4.5.5.3, you obtain an activity release rate of 1.1326×10^{-2} TBq/week; total activity of 53.2808 TBq; total mass of 1300 grams; a specific activity of 4.0985×10^{-2} TBq/g; and finally an allowable mass release of 2.7634×10^{-1} grams. Again using this approach for the material with total Pu241 decay to Am241 and Table 4.5.5.4, you obtain an allowable mass release of 2.3336×10^{-1} grams. Since both of these material conditions release much less than the regulatory allowable mass release, the TB-1 containment vessel inside the PAT-1 shipping package maintains containment during ACATP conditions.

Table 4.5.6.1 Regulatory Leakage Criteria for 1300 g plutonium

Isotopic Distribution	NCT @: 218°F - 18.872 psia		HAC @: 276°F - 20.486 psia		ACATP @: 1080°F - 613 psia (P _{PA1})		ACATP @: 1080°F - 1135 psia (P _{PA2})	
	L _{R,N-air} (ref-cm ³ /s)	L _{R,N-He} (cm ³ /s)	L _{R,PA-air} (ref-cm ³ /s)	L _{R,PA-He} (cm ³ /s)	L _{R,A-air} (ref-cm ³ /s)	L _{R,A-He} (cm ³ /s)	L _{R,PA-air} (ref-cm ³ /s)	L _{R,PA-He} (cm ³ /s)
No Pu-241 decay	5.1244E-06	8.8373 E-05	9.4686 E-02	9.8072 E-02	2.7762 E-03	3.2341 E-03	1.5478 E-03	1.8527 E-03
Complete Pu-241 decay to Am-241	4.2787 E-06	1.4737 E-06	7.9317 E-02	8.3003 E-02	2.3570 E-03	2.7663 E-03	1.3152 E-03	1.5870 E-03

4.5.7 References for Sections 4.5.5 and 4.5.6

10 CFR 71, *Packaging and Transportation of Radioactive Material*, Jan. 1, 2010.

49 CFR 173, *Shippers—General Requirements for Shipments and Packagings*, Oct. 1, 2010.

ANSI N14.5-1997, *Radioactive Materials—Leakage Tests on Packages for Shipment*, American Natl. Standards Institute, Feb. 5, 1998.

Curren, W. D. and R. D. Bond, *Leakage of Radioactive Powders from Containers*, Proceedings of the Sixth International Symposium on Packaging and Transportation of Radioactive Material: PATRAM '80, West Berlin, F.R.G., November 10–14, 1980, pp. 463–471.

Kocher, D. C., *Radioactive Decay Data Tables, A Handbook of Decay Data for Application to Radiation Dosimetry and Radiological Assessments*, DOE/TIC-11026, U.S. DOE, Office of Scientific and Technical Information, 1981.

R.H. Perry, D.W. Green, and J.O. Maloney, *Perry's Chemical Engineers' Handbook*, 7th edition, 1997, p. 2-363)

R.D. McCarty Cryogenics Division, National Bureau of Standards Technical Note 631, *Thermophysical Properties of Helium-43 from 2 to 1500 K with Pressures to 100 Atmospheres*, pg 49, Nov. 1972.

Robert C. Weast, Ph. D., *Handbook of Chemistry and Physics*, 55th ed., pg. F-13, 1974.

5. SHIELDING EVALUATION

This section describes the shielding evaluation for incorporating plutonium (Pu) metal contents as a new payload into the PAT-1 package. The Pu metal is packed in an inner container (*T-Ampoule Assembly*,⁴ Drawing 2A0261, designated the T-Ampoule) that replaces the PC-1 inner container. The T-Ampoule and associated Pu metal content packing configurations are described in Section 1.2.1 and Section 1.2.2 of this addendum, respectively.

To demonstrate compliance with the dose rate limits of 10 CFR 71.47(a) (non-exclusive use) for normal conditions of transport (NCT) and 10 CFR 71.51(a)(2) for hypothetical accident conditions (HAC), an evaluation of the shielding performance of the Plutonium Air Transportation (PAT-1) package has been completed. The evaluation assumes a package loaded with up to 1.3 kg* of Pu metal or plutonium/beryllium (Pu/Be) sources with a total mass of 200 g* or less of Pu; a combined Pu/Be contact surface area of 91 cm² or less; and an isotopic Pu composition, including allowance for decay, such that the total neutron source from the (α ,n) reaction with beryllium (Be) metal does not exceed 363 n/s/cm² (see Table 5-13). A detailed description of the shielding characteristics of the PAT-1 packaging is provided in Section 5.4 of the SAR.¹

5.1 Description of Shielding Design

5.1.1 Design Features

The shielding design features of the PAT-1 include the stainless steel overpack drum (*Overpack, AQ*,⁴ Drawing 1002 in the SAR,¹ designated the AQ-1); the stainless steel (PH13-8Mo) TB-1 *Containment Vessel* (Drawing 1017, designated the TB-1); and the titanium ampoule (*T-Ampoule Assembly*, Drawing 2A0261, designated the T-Ampoule), which secures the contents inside the containment vessel. In addition, the aluminum (Al) load spreader assembly, the copper heat conductor tube, and the redwood assemblies (both inner and outer) provide minimal additional shielding. While these additional features are largely designed for other purposes, they perform a dual role as shielding features. The lid and the bottom of the overpack drum, the containment vessel, and the T-Ampoule provide shielding in the axial direction. Shielding credit is not taken for the T-Ampoule (or for packing materials contained therein), the inner redwood assembly, or the thicker portions of the TB-1 vessel.

The stainless steel 304 materials are fabricated with a density of 7.9 g/cm³ with the exception of the TB-1 containment vessel, which is fabricated with a PH13-8Mo material² with a density of 7.5 g/cm³. The copper tube is fabricated from pure copper metal with a density of 8.94 g/cm³, and the Al load spreader is fabricated from Al 6061 with a density of 2.6989 g/cm³. The redwood is assumed to be cellulose (C₆H₁₀O₅)^{3,4} with a density of 0.36 g/cm³.

^A The drawing titles are in italics and are used interchangeably with the designated names in this addendum. See Section 1.3.2 in this addendum and Chapter 9 of the SAR¹ for drawing number, title, and revision.

* The plutonium quantities analyzed in this shielding section represent a conservative upper bound for analysis and are higher than the payload quantities shown in Table 1-1 of Section 1 of this addendum.

The shielding design requirements for these packages are minimal due to high purification and relatively low specific activity of the desired contents. Thus, with generous bounding assumptions on the source magnitude, the dose rates are still demonstrated to be small fractions of the regulatory limits.

5.1.2 Summary Table of Maximum Radiation Levels

The dose rates shown in Table 5-1 indicate that the PAT-1 meets regulatory dose limits as specified in the respective 10 CFR sections under NCT and HAC for nonexclusive use. The analysis for the limiting contents is based on the natural radioactivity produced from the decay of 1300 g of plutonium metal under bounding conditions that include peak dose rates due to decay (Pu shelf-life after separation), worst-case scenario for the various isotopes of Pu, and (α,n) production from an oxide matrix instead of a metal matrix. Details of the source generation and shielding analyses for the limiting contents are described in Sections 5.2 and 5.3, respectively. Description of an alternate content of Pu/Be sources is described in Section 5.5.3. It is shown in this section that Pu/Be is not the limiting content.

Table 5-1. Summary Table of External Radiation Levels (Non-Exclusive Use)

NCT	Package Surface mSv/h (mrem/h)			1 Meter from Package Surface mSv/h (mrem/h)		
	Top	Side	Bottom	Top	Side	Bottom
Gamma	0.060 (6.0) ^a	0.277 (27.7)	0.055 (5.5) ^a	0.006 (0.6) ^a	0.015 (1.5)	0.006 (0.6) ^a
Neutron	0.036 (3.6) ^a	0.319 (31.9)	0.038 (3.8) ^a	0.003 (0.3) ^a	0.014 (1.4) ^a	0.003 (0.3) ^a
Total	0.096 (9.6) ^a	0.596 (59.6)	0.093 (9.3) ^a	0.009 (0.9) ^a	0.029 (2.9)	0.009 (0.9) ^a
10 CFR 71.47(a) Limit	2 (200)	2 (200)	2 (200)	0.1 (10) ^b	0.1 (10) ^b	0.1 (10) ^b

^a Monte Carlo statistics of 5% or less; all others 1% or less.

^b Transport index may not exceed 10.

HAC	1 Meter from Package Surface mSv/h (mrem/h)		
	Top	Side	Bottom
Gamma	0.024 (2.4)	0.035 (3.5)	0.021 (2.1)
Neutron	0.015 (1.5)	0.018 (1.8)	0.014 (1.4)
Total	0.039 (3.9)	0.053 (5.3)	0.035 (3.5)
10 CFR 71.51(a)(2) Limit	10 (1000)	10 (1000)	10 (1000)

5.2 Source Specification

Because of the variety of contents envisioned for the PAT-1, a procedure to determine and generate bounding sources was developed that allows for a great deal of flexibility of allowed package contents. The gamma and neutron sources are based on a limiting Pu isotopic vector (see Table 5-2) that should allow for almost any form of plutonium metal to be loaded into the package, subject only to the mass and heat constraints of 1300 g of Pu and 25 watts, respectively.

The Pu isotopic distribution (Pu isotope versus mass fraction seen in Table 5-2) was generated through simulation of all conceivable routes of Pu production from different reactor types. The package was limited to 1300 g and a heat load of 25 watts although the isotopes for the radiation source are based on 2197 g with a heat load of 40 watts. For each isotope, the largest weight percent was selected across all the reactor types; taking the largest weight percent for each isotope regardless of other restrictions results in a total that exceeds 100 weight percent (wt %). The source definition is the upper bound of the actual source and therefore, yields an overestimate of the expected package doses. The analysis to support these Pu isotopic values is further described in Section 5.5.2.

Table 5-2. Plutonium Isotopics Used for Source Generation

Isotope	Mass Fraction	Mass (g)
Pu-236	2.0E-07	0.00026
Pu-238	0.04	52
Pu-239	1.00	1300
Pu-240	0.40	520
Pu-241	0.15	<195 ^a
Pu-242	0.10	130
Am-241	0.15 ^a	<195 ^a
Total	1.69 ^b	2197

^a The initial Am-241 is assumed to be zero, with 195 g of Pu-241. The time-varying source is optimized such that the maximum dose is computed with respect to the decay of Pu-241 to Am-241.

^b As a conservative assumption, the mass fractions used to generate the radiation source are allowed to exceed unity. The package is limited to 831 g (1300 g was used as an upper bound), although the isotopics for the radiation source are based on 2197 g. In addition, the allowed heat load is limited to 25 watts, while the radiation source used in this analysis is based on isotopics that would generate about 40 watts of heat.

5.2.1 Gamma Source

The gamma source arises from the beta and gamma decay of the Pu isotopes, each of which has distinct time and energy characteristics. The specific radiation characteristics of each of these isotopes are discussed further in Section 5.5.2. From this analysis, a gamma source is derived that bounds all realistic forms of plutonium metal. This source is given in Table 5-3 in the SCALE 18 group structure. This source corresponds to 2197 g of Pu (1300 g of Pu with the mass fractions specified in Table 5-2) and a decay time since Pu separation of 18.0 years (referred to as the shelf-life). While this decay time does not represent the peak source, it does represent the peak dose rate due to the dominance of the high-energy photons from the decay of Pu-236, which peaks at 18.0 years. In contrast, the lower-energy photons from predominately Pu/Am-241 have a very broad peak of about 75 years (see Figure 5-3).

5.2.2 Neutron Source

The neutron source consists of spontaneous fission and (α ,n) components, as shown in Table 5-4. The spontaneous fission component is invariant relative to the Pu matrix material (oxide or metal), is uniquely defined for each isotope, and decreases slightly with decay time. The (α ,n) component is a function of the impurities in the Pu matrix and exhibits a broad peak with decay

due to the variation of the Pu/Am-241 concentrations (see Figure 5-3). The (α ,n) component of the neutron spectrum, shown in Table 5-4, is based on an oxide matrix and represents a bound of the contents for a metal matrix (see Section 5.5.2). Both components of the neutron source shown are for a Pu decay time of 30 years, which corresponds to the peak source and dose with respect to the decay time.

Table 5-3. Gamma-Ray Source Used in the Shielding Analysis (2197 g Pu)

Energy Group	Energy Boundaries (MeV)	Photons/s
1	10	6.691E+02
2	8	3.182E+03
3	6.5	1.645E+04
4	5	4.162E+04
5	4	1.255E+05
6	3	6.089E+07
7	2.5	2.481E+05
8	2	7.277E+05
9	1.66	3.519E+06
10	1.33	2.546E+06
11	1	1.201E+07
12	0.8	1.396E+08
13	0.6	1.404E+08
14	0.4	4.397E+08
15	0.3	1.636E+09
16	0.2	7.217E+09
17	0.1	4.048E+12
18	0.05	5.459E+12
Total		9.517E+12

5.3 *Shielding Model*

5.3.1 Configuration of Source and Shielding

A slice of the three-dimensional shielding model used for the NCT evaluation is shown in Figure 5-1. This model is constructed with the dimensions given in Table 5-5 and contains the materials as described in Table 5-6. The dimensions correspond to those from the reference drawings with nominal dimensions used where given. The use of nominal dimensions is appropriate for this analysis since the package materials are not designed as shielding bodies and, therefore, produce minimal shielding effects. In addition, the inner redwood assembly, inner can assembly, T-Ampoule, and thicker regions along the side of the TB-1 containment vessel are assumed to be void in the shielding model. Since the geometry of the source material is variable, analyses were

performed to conservatively bound the configuration and magnitude of the source. The bounding of the source magnitude was previously discussed in Section 5.2.

Table 5-4. Neutron Source Used in the Shielding Analysis (2197 g Pu)

Energy Group	Energy Boundaries (eV)	Spontaneous Fission (neutrons/s)	(α ,n) Source (neutrons/s)	Total (neutrons/s)
1	2.000E+7	1.161E+04	0.0	1.161E+04
2	6.434E+6	1.632E+05	2.658E+05	4.290E+05
3	3.000E+6	2.024E+05	5.305E+05	7.330E+05
4	1.850E+6	1.154E+05	1.185E+05	2.340E+05
5	1.400E+6	1.486E+05	7.443E+04	2.231E+05
6	9.000E+5	1.517E+05	5.428E+04	2.060E+05
7	4.000E+5	7.012E+04	2.719E+04	9.731E+04
8	1.000E+5	1.034E+04	4.798E+03	1.513E+04
9	1.700E+4	7.403E+02	3.497E+02	1.090E+03
10	3.000E+3	5.486E+01	2.255E+01	7.740E+01
11	5.500E+2	4.314E+00	1.855E+00	6.169E+00
12	1.000E+2	3.031E-01	1.385E-01	4.415E-01
13	3.000E+1	4.813E-02	2.516E-03	5.065E-02
14	1.000E+1	9.546E-03	8.739E-04	1.042E-02
15	3.05	1.081E-03	1.607E-04	1.242E-03
16	1.77	3.179E-04	5.900E-05	3.769E-04
17	1.30	1.025E-04	2.134E-05	1.238E-04
18	1.13	7.345E-05	1.632E-05	8.976E-05
19	1.00	1.040E-04	2.510E-05	1.291E-04
20	0.80	1.698E-04	5.021E-05	2.200E-04
21	0.40	2.504E-05	9.414E-06	3.445E-05
22	0.33	2.923E-05	1.255E-05	4.179E-05
23	0.23	2.847E-05	8.945E-06	3.742E-05
24	0.10	8.138E-06	0.0	8.138E-06
25	0.05	2.565E-06	0.0	2.565E-06
26	0.03	2.095E-06	0.0	2.095E-06
27	0.01	1.121E-06	0.0	1.121E-06
Total		8.743E+05	1.076E+06	1.950E+06

The shape of the source in this scenario determines the (1) degree to which the source particles are self-shielded for gamma emissions and (2) the magnitude of the neutron source multiplication due to fission. The bounding source geometry is determined from a series of three assumed source geometries (see Section 5.4.4):

- A full-density, solid sphere with a radius of 2.63 cm
- A reduced-density, smeared source that completely fills the central region shown in Figure 5-1
- A full-density, thin, hollow cylinder with inner and outer radii of 5.249 and 5.4 cm, respectively, and a height of 15.11 cm (the central cylindrical region shown in Figure 5-1).

Each of these three geometries is assumed to contain 1300 g of plutonium metal. The full-density models assume the use of plutonium metal with a density of 17.0 g/cm³ (see Table 5-6 for material reference and discussion below). The bounding source geometry for the neutron dose is the solid, maximum-density sphere with the sphere moved outward so that it touches the inside surface of the TB-1 vessel. The bounding source geometry for the gamma doses is the smeared geometry, which minimizes the self-shielding effect and also moves the source material closer to the detector locations. The maximum total side dose (neutron plus gamma components) is simulated using the smeared geometry model for the gamma contribution and an intermediate full-density off-center sphere (density of 17 g/cm³) for the neutron contribution; the predicted total doses using this hybrid approach are some 20% greater than those using consistent neutron/gamma contributions for the various geometry/density models. The top and bottom dose values reported in Table 5-1 are based on the reduced-density, smeared Pu source model only since these values are not limiting.

Spot checks were completed for the top and bottom geometries to ensure that the peak source geometries were evaluated. The shielding source model for the HAC is the same as the NCT reduced-density smeared source model with only the central Pu region and the TB-1 containment vessel remaining.

5.3.2 Material Properties

The constituents of the materials used in the shielding calculations are shown in Table 5-6. All materials are used at their stated densities, although the plutonium metal density is modified by the ratio of the full-density volume to the smeared-density volume used in the reduced-density source model that bounds the shielding results. The density for this case follows.

The volume of the bottom curved region (204.2 cm³) is taken from Section 6.9.2. The cylindrical volume is given below and differs from that in Section 6.9.2 since a minimum thickness of the TB-1 lid is assumed here.

$$\text{Smeared-plutonium-source density} = 1300 \text{ g} / ([\pi * 5.4^2 * 15.11] + 204.2) \text{ cm}^3 = 0.818 \text{ g/cm}^3$$

The non-Pu materials use the SCALE standard definitions for the isotopic compositions, while selecting the minimal density from other sources, if available. The references used for each material are also presented in Table 5-6.

5.4 Shielding Evaluation

5.4.1 Methods

The shielding evaluation is performed by calculating the dose rates at the top, bottom, and radial directions of the PAT-1 package to verify compliance with the 10 CFR Part 71 nonexclusive dose rates during NCT. The dose rates are 2 mSv/h (200 mrem/h) at the package surface and 0.01mSv/h (10 mrem/h) at 1m from the accessible package surface under NCT, and 10 mSv/h (1000 mrem/h) at 1m, the 10 CFR Part 71 dose rate limit, under HAC.

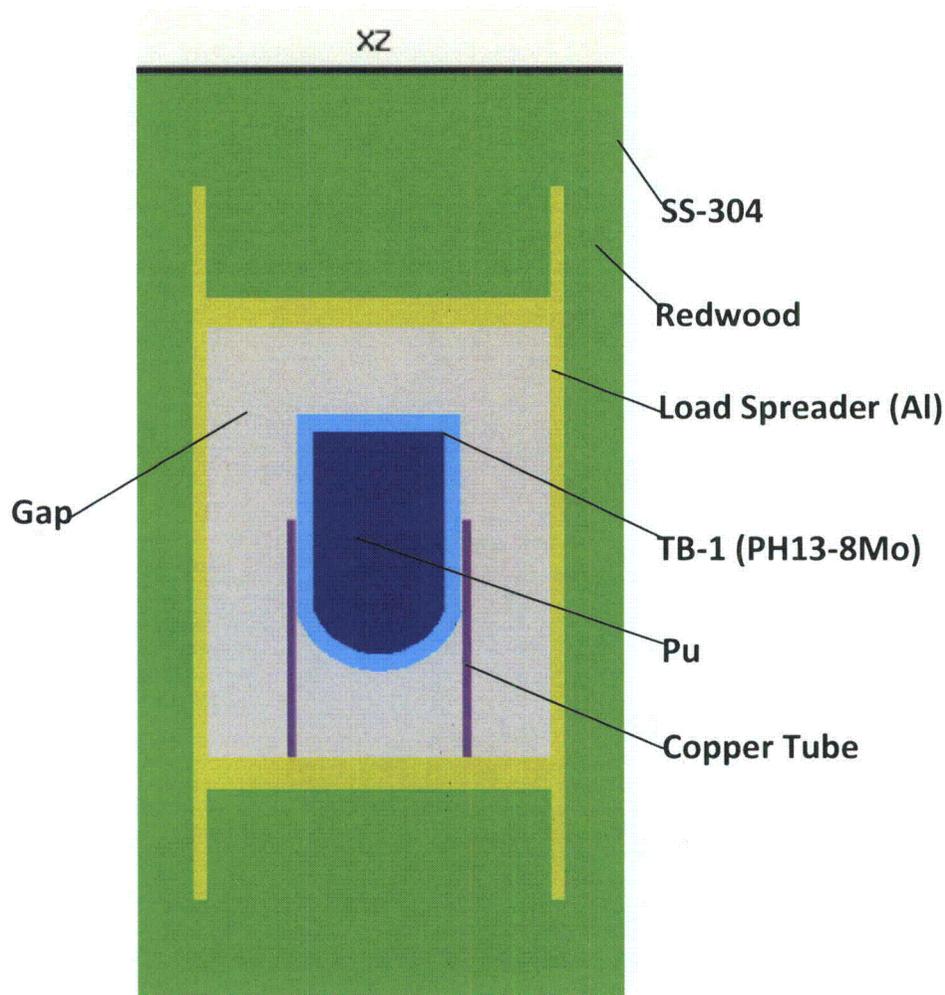


Figure 5-1. Cylindrical Shielding Model of PAT-1 Used in This Analysis (see Table 5-6 for Dimensional Information)

The evaluation has been performed for the PAT-1 package containing up to 1300g of plutonium metal. The Shielding Analysis Sequence #4 (SAS4)³ code was utilized to determine the dose rate at the surface and at 1 m from the surface, in both the axial and radial directions, for

bounding gamma and neutron sources. The dose locations evaluated in this scenario are shown in Figure 5-2. As shown in Table 5-1, the surface side dose is the most restrictive and is composed almost equally of gamma and neutron dose components.

The spatial distribution for each source used in these analyses was uniform within each of the defining cylindrical or spherical volumes (i.e., reduced-density, smeared cylinder; full-density annular cylinder; full-density sphere), as described in Section 5.3.1.

Table 5-5. Dimensions of Materials Regions Used in Shielding Analyses

Body	Radius (cm)	Bottom location (cm)	Height (cm)	Description
1 – cylinder	5.40	-5.64	15.11	cylindrical inside of TB-1
2 – sphere	5.72	-3.74 ^a	—	curved inside of TB-1
3 – cylinder	6.795	-5.64	16.71	outside of TB-1
4 – sphere	7.12	-3.74 ^a	—	curved outside of TB-1
5 – cylinder	10.0	-5.64	16.71	dummy piece for geometry
6 – cylinder	6.875	-10.86	21.93	void outside TB-1
7 – cylinder	6.875	-18.25	7.39	wood block below TB-1
8 – cylinder	7.52	-18.25	20.32	copper tube
9 – cylinder	8.74	2.07	9.00	void for thicker TB-1 region
10 – cylinder	13.97	-18.25	36.79	wood inside Al spreader
11 – cylinder	13.97	-20.79	41.87	upper and lower Al spreader
12 – cylinder	13.97	-30.35	60.81	top and bottom wood inside Al
13 – cylinder	15.24	-30.35	60.81	Al on outside of spreader
14 – cylinder	28.58	-48.69	99.13	wood inside drum
15 – cylinder	28.73	-48.84	99.43	steel drum

^a For spherical bodies, this value is the z location of the sphere; all bodies shown are centered at x and y = 0.

All shielding calculations were performed with the SCALE 5.1 version of the SAS4. This sequence consists of multiple codes executed from a single input stream. The individual modules used are the:

- BONAMI and NITAWL codes, which process the cross sections into formats the subsequent shielding codes can utilize.
- XSDRNPM one-dimensional discrete ordinates code, which is run in the adjoint mode to automatically generate biasing parameters for the final shielding analysis.
- MORSE-SGC, which is the Monte Carlo shielding code that quantifies the fluxes and dose rates at desired locations in the geometry.

Unless otherwise noted, all results reported in Table 5-1 are converged to a Monte Carlo statistical value of 1% or less at the 1 sigma level, indicating that the results are well converged.

This degree of convergence is aided by the automated bias generation built into the SAS4 sequence. Automated biasing as implemented in SAS4 gives rise to some inherent geometry limitations (e.g., axially symmetric models). Section 5.5.4 contains a discussion of how these limitations were overcome.

Table 5-6. Elemental Compositions Used in Shielding Analysis

Material	Density (g/cm ³)	Composition, wt % (atoms/barn-cm)	
		Element	Value
PH13-8Mo ²	7.74 (7.5 used)	Cr	12.75 (1.10753E-02)
		Ni	8.00 (6.15690E-03)
		Al	1.13 (1.88319E-03)
		Mo	2.25 (1.05924E-03)
		Fe	75.88 (6.13662E-02)
Redwood ^{3,4}	0.36	H	6.2 (1.33725E-02)
		C	44.4 (8.02350E-03)
		O	49.4 (6.68625E-02)
Aluminum ^{3,5}	2.6989	Al	100.0 (6.02375E-02)
304 Stainless Steel ^{3,5}	7.9	C	0.080 (3.16873E-04)
		Si	1.000 (1.69394E-03)
		Cr	19.000 (1.73846E-02)
		Mn	2.000 (1.73195E-03)
		Fe	68.375 (5.82497E-02)
		Ni	9.500 (7.70121E-03)
		P	0.045 (6.91181E-05)
Copper ⁵	8.94	Cu	100.0 (8.47233E-02)
Plutonium metal ⁶	15-19.7 (17.0 used)	Pu-239	100.0 (4.28259E-02)

The following is a complete list of the conservative assumptions and techniques used in this analysis to ensure that the results generated bound those of the actual contents under any circumstances.

1. The source is generated based on an extremely pessimistic representation of the Pu isotopes. The use of a burned reactor-grade Pu vector allows for isotopes other than Pu-239 to contribute significantly to the total source. The expected use of components more in line with weapons-grade Pu (higher Pu-239; lower for other isotopes) should produce radiation levels much lower than those assumed in this analysis. See estimates of this effect in Section 5.5.2.
2. The metal matrix anticipated for shipments using this package should have a neutron source that is significantly lower than the oxide matrix that was used for all source calculations (see Section 5.5.2).

3. The source generation scenario is based on a Pu mass 60% greater than allowed and a heat generation rate also 60% greater than the allowed rate, ensuring that doses are bounding. However, the actual mass of Pu in the package for self-shielding purposes is only 1300 g.
4. The shape of the source was varied to determine the configuration that produced the maximum dose for the bounding source spectrum described above and in Section 5.2.
5. The time variation of the source spectrum and magnitude was analyzed to select a decay time that produced bounding dose rates over any possible decay time.
6. The shielding analysis assumed the minimum Pu density expected for the various forms of plutonium metal.
7. The T-Ampoule, the thicker steel portions of the TB-1 containment vessel, and the inner redwood assembly were omitted from the shielding analysis. The structural material densities were the minimum values found in the literature.

In the model, the dose at a given location is obtained by assuming “point detectors,” which allow the dose at a specific point in space to be tabulated. Dose estimation via point detectors is less efficient than that based on radiation tracking across a specified surface length or area, but it allows for greater detail in the reported results. In each case, a series of point detectors were placed side-by-side to determine the location of the peak dose. In most cases, the peak dose was at the location corresponding to or in alignment with the center of the source region. The point locations shown in Figure 5-2 indicate where the point detectors were placed for the various locations reported in Table 5-1. The use of point detectors directly on the outermost shielding surface is limited; standard practice is to move the point detectors about 1 cm off the surface. The 1-m detectors are located precisely 1 m from the outermost shielding surface. For the HAC cases, only the contents and the TB-1 containment vessel were modeled, with the 1-m detectors placed at a distance of precisely 1 m from the outermost surface of the TB-1 body.

The cross section set used for all analyses was the SCALE 27N-18COUPLE library. This is the recommended library for all shielding calculations using the SCALE system.

5.4.2 Input and Output Data

A listing of the input data for the ORIGEN-S source generation is shown in Section 5.5.4. The output of this source generation calculation is automatically written onto a file named *ft71f001* and subsequently read in by the shielding analysis modules. SAS4 inputs for the shielding study of the radial neutron and gamma doses are also given in Section 5.5.4. SAS4 utilizes an automated bias parameter generator, which typically allows for both neutron and gamma problems to converge rapidly. In all cases, the results given in Table 5-1 are converged to 1% or less unless otherwise noted.

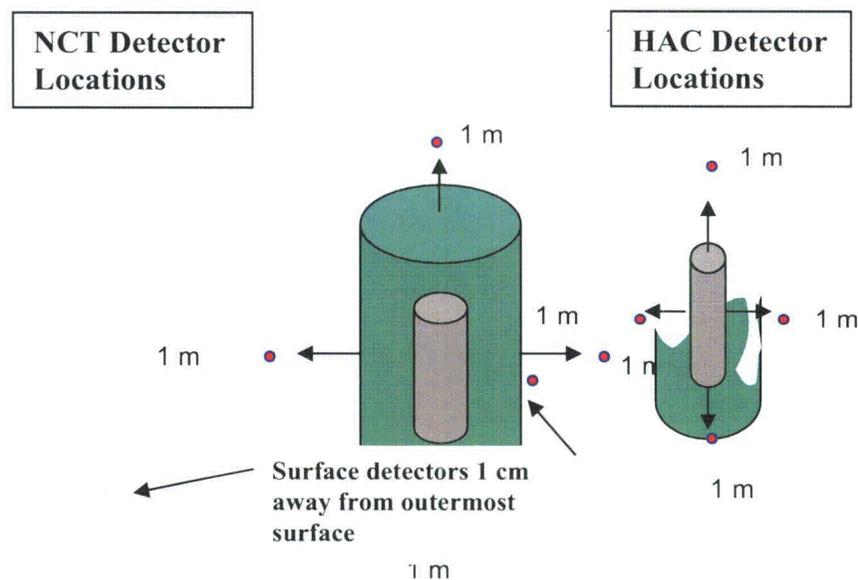


Figure 5-2. Dose Locations Analyzed for the PAT-1 Package

5.4.3 Flux-to-Dose-Rate Conversion

ANSI/ANS-6.1.1-1977 flux-to-dose-rate conversion factors are used in the SAS4 shielding calculations. These factors are provided in Tables 5-7 and 5-8 for neutrons in the SCALE 27 neutron group structure and gamma radiation in the SCALE 18 group gamma structure.

5.4.4 External Radiation Levels

Radiation levels corresponding to up to 1300 g of plutonium metal loaded in the PAT-1 package have been predicted in this section. The methods and techniques are based on current-generation, well-known, and approved codes and procedures and should be accurate to within 10–20%. A number of bounding approximations included in each phase of the analysis should ensure that the predicted results are larger than any actual radiation levels and, therefore, allow a high level of assurance that an actual shipment should pass the dose-measurement tests at the time approved contents are shipped. While no measurements of sufficient quality exist to serve as benchmarks for expected dose rates near plutonium metal components, the results reported herein are consistent with previous analyses⁷ performed prior to certification of Pu oxide contents in the same PAT-1 package. The sources and final dose predictions from that study differ only within a factor of 2 from those in this study, even though the techniques and underlying data sets have been updated since the previous study.

A comparison of dose predictions at the top, side, and bottom package locations (both at the surface and at 1 m) indicates very consistent relative dose values: the package surface values are a factor of 5 greater along the side than those along the top and bottom. At 1 m, this factor of 5 is reduced to approximately 3 (as expected), as the distributed Pu source will begin to approximate a point source as the distance from the package increases. The top and bottom doses are also consistent with each other as expected from a visual examination of Figure 5-1, which shows similar top and bottom geometries and similar distances from the package contents to the exterior surface locations.

Although not included in the analyses, the effect of ground scatter during the loading process should only be approximately 10–20%, which is readily bounded by the conservatism included in the analysis.

The bounding source configuration was found to be the reduced-density, smeared Pu source that completely filled the inside of the TB-1 containment vessel volume. This conclusion is based on the analysis of five other source configurations described as follows:

Table 5-7. Neutron Flux-to-Dose Conversion Factors Used in Shielding Analysis

Group Number	Energy Bounds (eV)	Dose Factor (rem/h/neutrons/cm ² /s)
1	2.000E+07	1.492E-04
2	6.434E+06	1.446E-04
3	3.000E+06	1.270E-04
4	1.850E+06	1.281E-04
5	1.400E+06	1.298E-04
6	9.000E+05	1.028E-04
7	4.000E+05	5.118E-05
8	1.000E+05	1.232E-05
9	1.700E+04	3.837E-06
10	3.000E+03	3.725E-06
11	5.500E+02	4.015E-06
12	1.000E+02	4.293E-06
13	3.000E+01	4.474E-06
14	1.000E+01	4.568E-06
15	3.050E+00	4.558E-06
16	1.770E+00	4.519E-06
17	1.300E+00	4.488E-06
18	1.130E+00	4.466E-06
19	1.000E+00	4.435E-06
20	8.000E-01	4.327E-06
21	4.000E-01	4.197E-06
22	3.250E-01	4.098E-06
23	2.250E-01	3.839E-06
24	1.000E-01	3.675E-06
25	5.000E-02	3.675E-06
26	3.000E-02	3.675E-06
27	1.000E-02	3.675E-06

- A full-density, solid sphere of radius 2.63 cm located at the center of the TB-1 volume
- A solid sphere moved to the TB-1 vessel inner wall
- Three hollow cylindrical configurations with various radii and heights

The three hollow cylindrical sources are described as a small cylinder; a large cylinder; and a large, thin cylinder. The first two are actual components under consideration for loading. The

third is a hypothetical cylinder with an outer radius of 5.4 cm, which coincides with the inner radius of the TB-1 vessel, and a height of 15.11 cm, which is the complete height of the cylindrical section inside the TB-1 vessel. The inner radius was calculated to be 5.249 cm, which corresponds to 1300 g of plutonium metal at a density of 17.0 g/cm³. The complete set of results for the side surface of the package is shown in Table 5-9. These results show that the reduced-density, smeared cylinder is the bounding source geometry; however, the results also show very little sensitivity of the total dose to the source configuration. Hence, for the top and bottom dose locations, only the reduced-density, smeared cylinder source configuration was analyzed.

Table 5-8. Gamma Flux-to-Dose Conversion Factors Used in Shielding Analysis

Group Number	Energy Bounds (eV)	Dose Factor (rem/h/photon/cm ² /s)
1	1.000E+07	8.772E-06
2	8.000E+06	7.478E-06
3	6.500E+06	6.375E-06
4	5.000E+06	5.414E-06
5	4.000E+06	4.622E-06
6	3.000E+06	3.960E-06
7	2.500E+06	3.469E-06
8	2.000E+06	3.019E-06
9	1.660E+06	2.628E-06
10	1.330E+06	2.205E-06
11	1.000E+06	1.833E-06
12	8.000E+05	1.523E-06
13	6.000E+05	1.172E-06
14	4.000E+05	8.759E-07
15	3.000E+05	6.306E-07
16	2.000E+05	3.834E-07
17	1.000E+05	2.669E-07
18	5.000E+04	9.347E-07

Table 5-9. Source Geometry Optimization Dose Results (at PAT-1 Side Surface)

Source Configuration	Neutron Dose (mrem/h)	Gamma Dose (mrem/h)	Total Dose (mrem/h)
reduced-density, smeared cylinder	18.9	27.7	46.6
centered sphere	26.1	10.3	36.4
off-center sphere	31.9	11.1	43.0
large cylinder	20.3	20.5	40.8
small cylinder	20.3	16.9	37.2
Large, thin cylinder	20.2	25.6	45.8

Dose profiles were generated for each separate analysis. In all cases the peak dose occurs at the center point of the source region or just off the center point (due to the influence of the copper pipe in the radial calculations). These are the expected results for a uniformly distributed source and indicate no streaming through various regions of the PAT-1 geometry.

5.5 Appendix

5.5.1 References

1. United States. Nuclear Regulatory Commission. NUREG-0361, "Safety Analysis Report for the Plutonium Air Transportable Package, Model PAT-1." Washington, D.C. 1978.
2. Brown, Jr., W. F. and S. J. Setlak. *Aerospace Structural Metals Handbook, 37th Edition*, CINDAS/USAF CRDA Handbooks Operation, Purdue University, West Lafayette, IN. 2001.
3. SCALE-5.1, "A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation for Workstations and Personal Computers, CCC-545," Oak Ridge National Laboratory. Oak Ridge, TN.
4. United States. Dept. of Agriculture. Alden, H. A., "Softwoods of North America," September 1997.
5. Davis, J.R., ed. *ASM Specialty Handbook: Copper and Copper Alloys*. p. 446-452, ASM International, 2001.
6. "LANL Content Description for PAT-1 Packaging," Los Alamos National Laboratory. Los Alamos, NM: August 9, 2007.
7. United States. Nuclear Regulatory Commission. NUREG/CR-0030 (SAND76-0587), "PARC (Plutonium Accident Resistant Container) Program Research, Design, and Development." Reprinted January 1983.
8. PAT-1 Content impurity description transmitted from SNL to ORNL on October 18, 2007.
9. Wilson, W.B., et al. "SOURCES 4C: A Code for Calculating (α ,n), Spontaneous Fission, and Delayed Neutron Sources and Spectra," LA-UR-02-1839: Los Alamos National Laboratory. Los Alamos, NM: April 2002.
10. Caviness, M. L., and J.B. Rubin. "Authorized Contents Proposed for the Plutonium Air Transporter (PAT-1) Packaging (U)," LA-UR-08-05154. Los Alamos National Laboratory. Los Alamos, NM: August 7, 2008.

5.5.2 Summary of Source Bounding Analyses

The isotopes of concern in generating a radioactive source for Pu are Pu-236, Pu-238, Pu-239, Pu-240, Pu-241, and Pu-242. Each of these have very different behaviors with respect to neutron and photon emissions and their variation over time since purification of the Pu product (referred to as either decay time or shelf-life). The key parameters of the neutron source, photon source, and decay heat per gram of each of these isotopes are given in Figures 5-3 through 5-5.

These values indicate that the primary contributors (per unit mass) to the photon source are, in order, Pu-236, Pu-238, and Pu-241. Of these, Pu-241 is typically the most abundant isotope. The primary contributors to the neutron source are the same three isotopes. The specific decay heat values from Figure 5-5 are 18.2, 0.57, 1.9E-3, 7.1E-3, 0.10, and 1.2E-4 watts/g for Pu-236,

Pu-238, Pu-239, Pu-240, Pu-241, and Pu-242, respectively. The value for Pu-241 corresponds to the peak time-varying value and can be used per gram of both Pu-241 and Am-241.

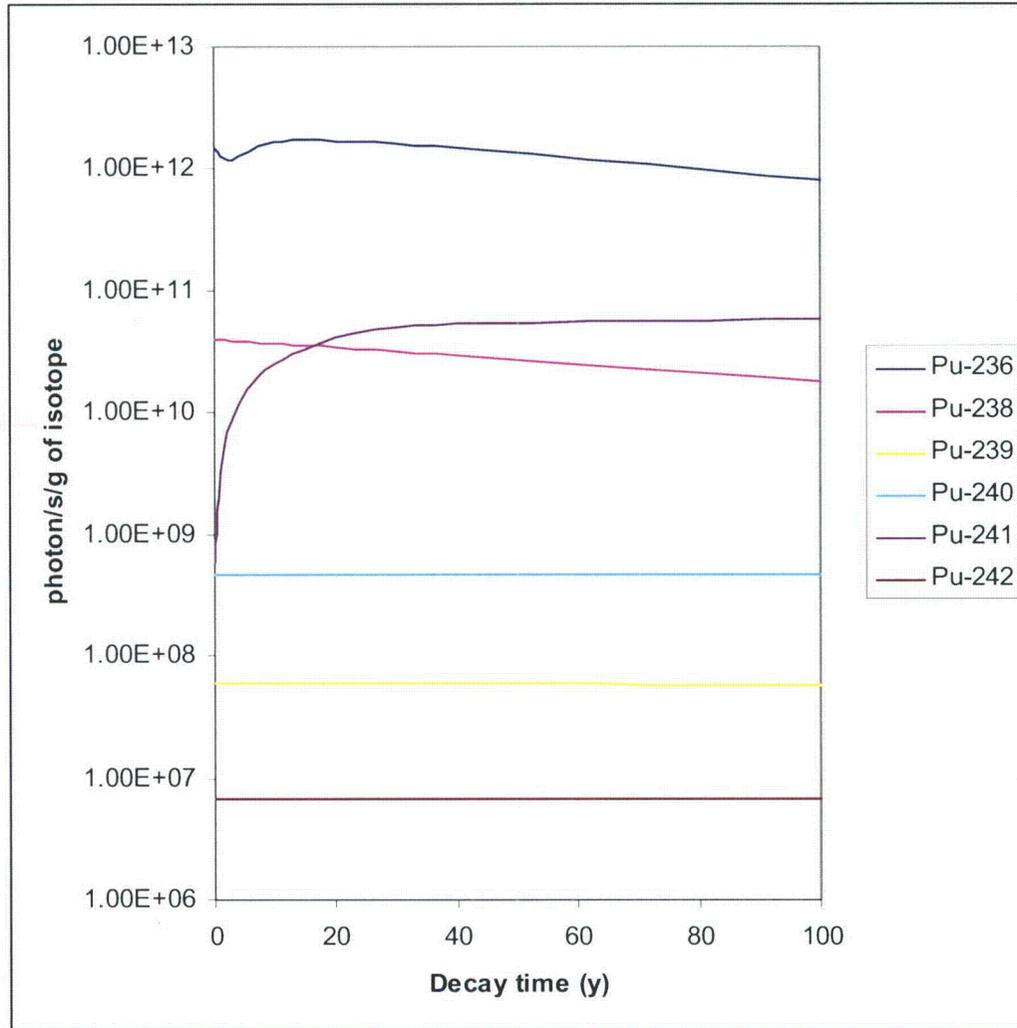


Figure 5-3. Photon Source per Gram of Each Isotope of Pu Initially Present (Note That Pu-241 Data Includes Buildup of Am-241)

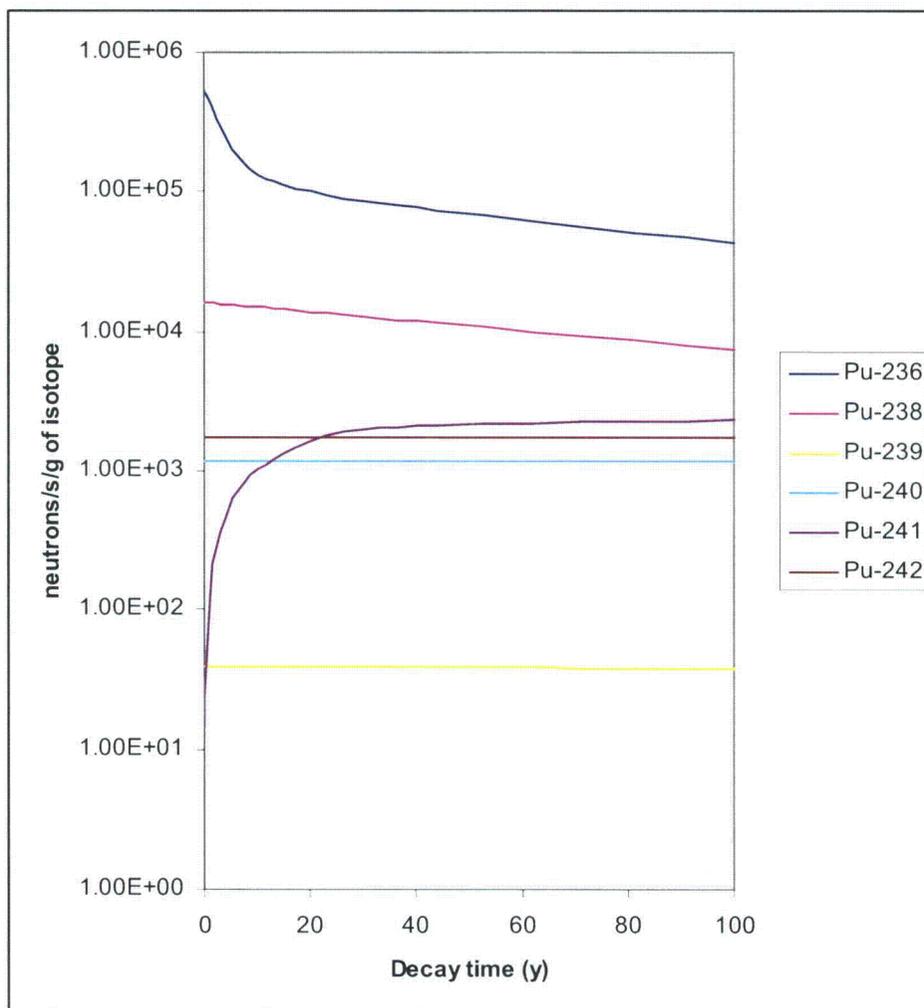
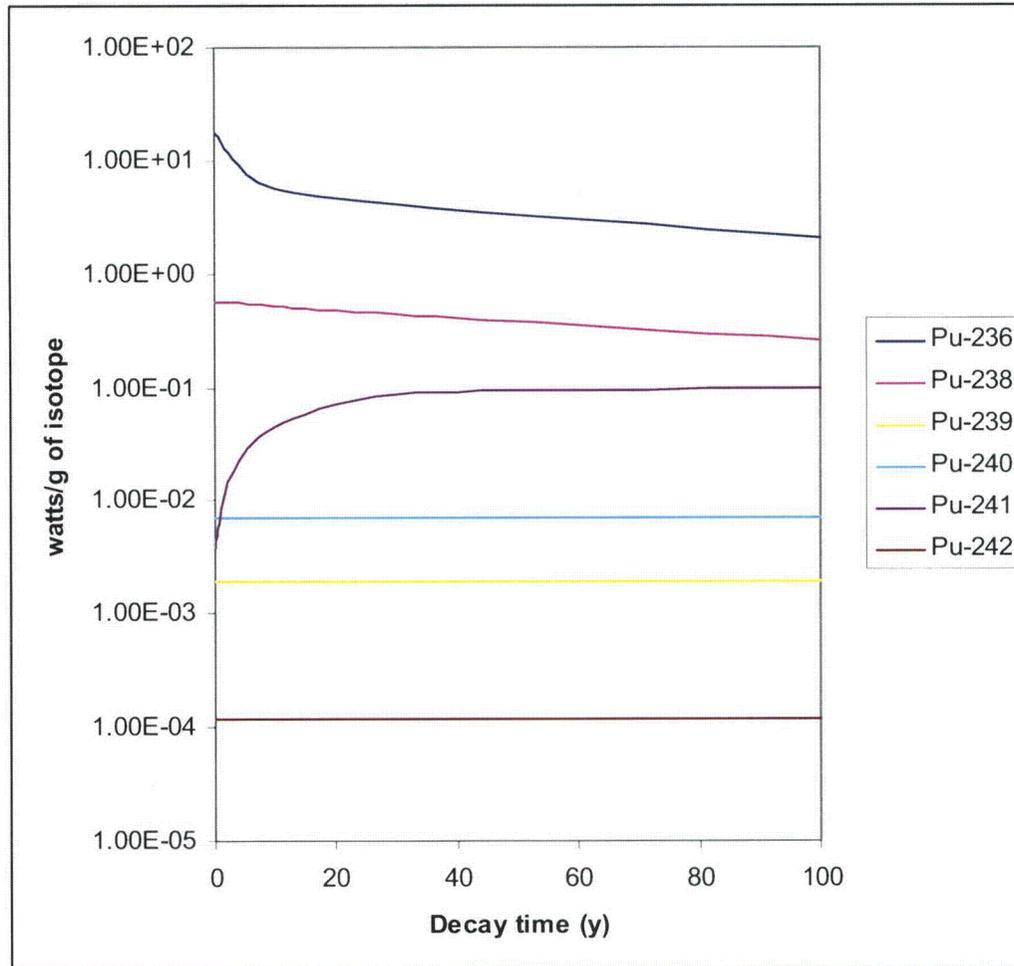


Figure 5-4. Neutron Source per Gram of Each Isotope of Pu Initially Present (Includes Both Spontaneous Fission and (α,n) Components with an Oxide Matrix; Also Note That Pu-241 Data Includes Buildup of Am-241)



**Figure 5-5. Watts per Gram of Each Isotope of Pu Initially Present
(Note That Pu-241 Data Includes Buildup of Am-241)**

In order to bound the Pu sources in this study, a series of seven depletion calculations were performed using the SCALE depletion code ORIGEN-ARP.³ The ORIGEN-ARP code uses the same ORIGEN-S code used to generate the neutron, photon, and decay heat values presented in Figures 5-3 to 5-5. The ARP portion of ORIGEN-ARP takes reactor-based cross sections tabulated for each reactor system and automatically interpolates to the desired burnup and enrichment values appropriate for a given level of depletion. Three reactor systems were selected for this study: a pressurized water reactor (PWR, Westinghouse 17×17 lattice), a CANDU (Canadian design power reactor), and the Hanford N Reactor (a government reactor primarily designed for Pu production). A total of seven depletion scenarios were performed for these systems as defined in Table 5-10, corresponding to medium and high burnups for the PWR and CANDU designs and to a low, medium, and high burnup for the N reactor. The goal of these studies is to predict the full range of Pu isotopes that would result from these scenarios. The resulting Pu isotope values are given in Table 5-10 for each scenario.

Table 5-10. Pu Isotope Wt % Under Various Depletion Scenarios

Isotope	PWR (35 GWd/t)	PWR (60 GWd/t)	CANDU (5 GWd/t)	CANDU (10 GWd/t)	N_Reactor (2 GWd/t)	N_Reactor (5 GWd/t)	N_Reactor (10 GWd/t)
Pu-236	2.4E-6	1.6E-5	8.5E-8	2.5E-7	2.0E-8	1.0E-7	2.2E-7
Pu-238	0.49	3.6	0.05	0.15	0.01	0.05	0.12
Pu-239	74.9	49.3	75.4	59.5	93.6	83.9	76.7
Pu-240	15.2	23.7	20.2	30.7	5.8	12.8	17.6
Pu-241	8.4	15.2	3.7	6.9	0.6	3.0	5.0
Pu-242	1.1	8.2	0.6	2.8	0.02	0.2	0.6
Total	100	100	100	100	100	100	100

From these individual results, the following Pu isotope definition is generated that bounds all the above scenarios. The maximum weight percent from each isotope in Table 5-10 is used to define the mass fractions given in Table 5-11 (for Pu-236, the value of 1.6E-5 is divided by 100 and rounded to 2E-7). The use of this Pu isotope definition should allow any realistic Pu production scenario to be accounted for.

In order to estimate the amount of overprediction for the bounding radiation sources, the bounding neutron and gamma sources are presented in Table 5-12 along with predicted sources based on the "N_Reactor 2 GWd/t" case shown in Table 5-10. The Pu isotopic distributions from this case correspond closely with typical weapons-grade plutonium metal along with corresponding impurities.^{6,8}

5.5.3 Analysis of Pu/Be Source Contents

An alternate content of Pu/Be sources is desired for the PAT-1 package. This section separately analyzes the shielding concerns related to this content.

The radiation emitted from a Pu/Be source, both neutron source magnitude and energy spectrum, is estimated using the SOURCE4C⁹ code. The source configuration used in this study is an interface source, where α particles emitted from the Pu and americium (Am) materials produce neutrons via interaction with the Be material along a common interface. The source from such a calculation is tabulated as n/s/cm², with the source directly proportional to the contact surface area between the two materials. For the materials expected to be shipped in this package, there is also an alpha barrier, which places another material between the Pu and Be, effectively making the neutron source much smaller. The influence of alpha barriers is conservatively ignored in these source estimates.

The neutron source used in the Pu/Be source study is given in Tables 5-13 and 5-14. The assumed Pu and Am isotopes are taken from Reference 10 and correspond to the expected material to be shipped; as a bound on the source magnitude, the Pu-241 is assumed to be completely decayed to Am-241. The neutron source spectrum is shown in Table 5-14.

The impurity content of the plutonium metal used for the Pu/Be sources is given in Reference 10; however, for this study the impurities were replaced with plutonium metal to maximize the quantity of α -producing material present in the calculations.

Table 5-11. Bounding Pu Isotope Mass Fraction Used in This Study

Isotope	Mass Fraction	Mass (g)
Pu-236	2E-7	0.00026
Pu-238	0.04	52
Pu-239	1.00	1300
Pu-240	0.40	520
Pu-241	0.15	<195 ^a
Pu-242	0.10	130
Am-241	0.15 ^a	<195 ^a
Total	1.69 ^b	2197

^a The initial Am-241 is assumed to be zero, with 195 g of Pu-241. The time-varying source is optimized such that the maximum dose is computed with respect to the decay of Pu-241 to Am-241.

^b As a conservative assumption, the mass fractions are allowed to exceed unity. The package is limited to 1300 g, although the source is based on 2197 g. In addition, the heat load is limited to 25 watts, while the source is based on a heating of about 40 watts.

Table 5-12. Estimation of Degree of Overprediction in Bounding Pu Source Used in This Study

Case	Neutron Source (neutrons/s)	Gamma Source (photons/s)
Bounding source	1.950E+6	9.517E+12
Typical source ^a	3.241E+5	2.623E+11
Ratio bounding/typical	6.0	36.3

^a Case based on 1300 g of Pu with isotopic distribution corresponding to source scenario "N_Reactor 2 GWd/t" in Table 5-12 with the following impurities: 200 ppm each of Be, Li, B, F, Al, and Si; 300 ppm of Na; 500 ppm each of C and Mg.

In order to arrive at the total neutron source to be used in these shielding studies, the per-unit-area sources given in Table 5-13 require a bounding contact surface area. The value used in this study assumes that the diameter of the TB-1 container (a radius of 5.4 cm is given in Table 5-5) provides a bounding surface area of 91 cm². Thus, the sources loaded into the PAT-1 package under this analysis must have total contact surface areas equal to or less than this area.

Table 5-13. Pu/Be Source Specification Used in This Study

Isotope	Mass Fraction	Atom Fraction	Neutron Source for Pure Isotope (n/s/cm ²)
Pu-238	0.0005	0.0005	65,000
Pu-239	0.9235	0.9238	171.85
Pu-240	0.0650	0.0648	637.58
Pu-241	0.0000 ^a	0.0000	5.36
Pu-242	0.0010	0.0010	8.53
Am-241	0.0100	0.0099	13,000
Total	1.0000	1.0000	363 ^b

^a The Pu-241 is assumed to be completely decayed to Am-241 to bound the source for the typical material isotopes expected to be shipped.

^b This neutron source value is the basis for the Pu/Be source shielding calculations in this section. The value is obtained by multiplying the mass fraction values in column 2 by the neutron source for pure isotope values in column 4 and summing over all isotopes. A source with mass fractions that differ from those in this table can be shipped if the estimated source is less than this value with allowance for decay. Typical Pu/Be source materials should fit this specification provided the Pu-238 content is 0.4 wt % or less.

The mass of Pu material loaded into the package must also be bounded: the same value used in the criticality analysis, 200 g of plutonium metal, is assumed. Using a mass of 200 g and the default full density of α -phase plutonium metal (Reference 2 gives a density of 19.84 g/cc), the dimensions of this sphere can be calculated for use in the shielding studies: a sphere of full-density, α -phase plutonium metal with a mass of 200 g will have a radius of 1.34 cm. A spherical source of this dimension with offset distances corresponding to the package surface and 1 m from the package surface was used in the shielding analyses.

As described above, the shielding model for the Pu/Be source study was a sphere with radius of 1.34 cm containing full-density, α -phase plutonium metal. The rest of the PAT-1 package is conservatively omitted from the analysis. The offset distances used for the package surface and 1-m dose values were determined from the values in Table 5-5; the minimum distance from a source to the surface detector along the cask side is specified as the difference in radii for bodies 15 and 1 (28.73 – 5.4 = 23.33 cm). Along the cask bottom, the minimum source-to-detector distance is specified as the difference in bottom locations for bodies 11 and 15 (48.84 – 20.79 = 28.05 cm). Along the cask top, the minimum source-to-detector distance is specified as the differences in the top boundaries for bodies 11 and 15 (99.43 – 48.84 – 41.87 + 20.79 = 29.51 cm). These top and bottom distances assume that the source rests on the Al spacer material, which is conservative. In addition, because the side detector locations are closer to the source than the top and bottom locations, the side locations are used for side, top, and bottom dose estimates. The 1-m dose location for side, top, and bottom locations is therefore 123.33 cm. These locations are actually minimum distances from the outer surface of the spherical source touching these named bodies, but for conservatism, the code input assumes these distances are from the source center, not the edge.

Table 5-14. Neutron Source Spectrum Used in the Pu/Be Source Shielding Analysis

Energy Group	Energy Boundaries (eV)	(α,n) Source Spectrum
1	2.000E+7	2.90211E-01
2	6.434E+6	4.11765E-01
3	3.000E+6	2.26912E-01
4	1.850E+6	1.91999E-02
5	1.400E+6	2.54550E-02
6	9.000E+5	2.39615E-02
7	4.000E+5	2.58964E-03
8	1.000E+5	8.56173E-05
9	1.700E+4	3.16844E-06
10	3.000E+3	4.29906E-08
11	5.500E+2	0.0
12	1.000E+2	0.0
13	3.000E+1	0.0
14	1.000E+1	0.0
15	3.05	0.0
16	1.77	0.0
17	1.30	0.0
18	1.13	0.0
19	1.00	0.0
20	0.80	0.0
21	0.40	0.0
22	0.33	0.0
23	0.23	0.0
24	0.10	0.0
25	0.05	0.0
26	0.03	0.0
27	0.01	0.0
	0.00001	
Total		1.000E+00

The SAS1 module of the SCALE system, version 5.1³ was used to quantify the dose rates from a Pu/Be source using the source and geometry described above. Briefly, the SAS1 shielding model for both NCT and HAC consisted of an unshielded Pu sphere with a mass of 200 g. The NCT and HAC dose locations were specified as the minimum source-to-detector locations possible. The SAS1 code explicitly accounts for both secondary gamma radiation and subcritical source multiplication. The cross section library was the same SCALE 27N-18COUPLE library used for the other source configurations described in Section 5.4. The flux-to-dose conversion

factors were also the same used for the other source calculations, the ANSI/ANS 6.1.1-1977 standard. See Section 5.5.4 for a listing of the inputs for SAS1 and SOURCES4C.

The results for the Pu/Be source analysis are given in Table 5-15. The full-density results under conservative conditions show that the doses from the Pu/Be sources described herein are well below those of the other contents considered in Sections 5.2 through 5.4. The maximum total doses for the Pu/Be sources shown in Table 5-15 are 28, 41, and 88 times less than the limiting cases shown in Table 5-1 for NCT surface, NCT 1-m, and HAC 1-m locations respectively. The plutonium metal used in the Pu/Be sources also has a natural component of radiation; however, the Pu mass limit of 200 g for the Pu/Be sources is a factor of 6 lower in mass than the metal-only limits. The conservatisms built into this Pu/Be source analysis include the following:

1. PAT-1 packaging is ignored.
2. Both sides of a Pu/Be disk are assumed to have contact surface areas.
3. Complete decay of Pu-241 to Am-241 is assumed.
4. The minimum source-to-detector distance is used for the surface and 1-m dose locations. The center of the source is assumed to contact the innermost package boundary.
5. No α barrier is included in the calculations, although one is physically present in the sources to be shipped.
6. Comparisons of void source material to full-density sources in the shielding analysis indicate that doses for full-density material are higher due to source multiplication. Comparison of α - and δ -phase Pu also indicated that higher densities produced higher dose estimates.
7. In the shielding model, the source containing Pu was assumed to contain 100% Pu-239 to maximize the source subcritical multiplication.

It can therefore be concluded that the addition of Pu/Be sources as allowable contents of the PAT-1 package have no influence on the limiting dose results given in Table 5-1.

Table 5-15. Dose Results for Pu/Be Source Content

Case description	Detector location for top, bottom, or side geometry	Neutron dose (gamma dose) mrem/h	Total dose, doubled ^a mrem/h
Full-density, α -phase Pu	surface	0.838 (0.004)	1.68
	1 m	0.030 (0.0001)	0.06
Voided source	surface	0.680 (1e-8)	1.36
	1 m	0.024 (1e-9)	0.05

^a Dose rates for a doubled case are given to account for the possible rearrangement of multiple Pu/Be sources such that both sides of the Pu surface come in contact with the Be material, doubling the radiation emitted. The comparison of doubled doses to regulatory limits effectively allows the summing of contact surface areas from multiple disks without regard to possible restacking. For example, while a single disk would only have a surface area corresponding to the actual contact area between the Pu and Be, two disks could properly align such that there were three contact surfaces, and three disks could properly align such that there were five contact surfaces. By applying a factor of two, only the actual contact areas for individual sources or multiple sources need to be considered.

5.5.4 List of Various Code Inputs

The ORIGEN-S computer code calculates the neutron and gamma source based on the initial loadings of each isotope as specified in Table 5-2. The code then generates the neutron and gamma spectrum in the specified SCALE 27 neutron and 18 gamma group structures for a series of decay times. The case below determines the sources at the following decay times: 0.1, 0.3, 1, 3, 10, 18, 30, 50, 75, and 100 years.

Code Listing 5-1 ORIGEN-S Input

```
'This SCALE input file was generated by
'OrigenArp Version 5.1 October 27, 2006
#origens
0$$$ all 71 e t
Decay Case
3$$$ 21 1 1 27 a16 2 a33 18 e t
35$$$ 0 t
54$$$ a8 1 a11 0 e
56$$$ a2 10 a6 1 a10 0 a13 6 a14 5 a15 3 a17 2 e
57** 0 a3 1e-05 e
95$$$ 0 t
Case 1
0 MTU
60** 0.1 0.3 1 3 10 18 30 50 75 100
61** f0.05
65$$$
'Gram-Atoms Grams Curies Watts-All Watts-Gamma
3z 1 0 0 3z 3z 3z 6z
3z 1 0 0 3z 3z 3z 6z
3z 1 0 0 3z 3z 3z 6z
81$$$ 2 0 26 1 a7 200 e
82$$$ 2 2 2 2 2 2 2 2 2 e
83**
1.0000000e+07 8.0000000e+06 6.5000000e+06 5.0000000e+06 4.0000000e+06
```

```

3.0000000e+06 2.5000000e+06 2.0000000e+06 1.6600000e+06 1.3300000e+06
1.0000000e+06 8.0000000e+05 6.0000000e+05 4.0000000e+05 3.0000000e+05
2.0000000e+05 1.0000000e+05 5.0000000e+04 1.0000000e+04 e
84**
2.0000000e+07 6.4340000e+06 3.0000000e+06 1.8500000e+06
1.4000000e+06 9.0000000e+05 4.0000000e+05 1.0000000e+05 1.7000000e+04
3.0000000e+03 5.5000000e+02 1.0000000e+02 3.0000000e+01 1.0000000e+01
3.0499900e+00 1.7700000e+00 1.2999900e+00 1.1299900e+00 1.0000000e+00
8.0000000e-01 4.0000000e-01 3.2500000e-01 2.2500000e-01 9.9999850e-02
5.0000000e-02 3.0000000e-02 9.999980e-03 1.0000000e-05 e
73$$ 942360 942380 942390 942400 942410 942420
74** 0.00026 52 1300 520 195 130
75$$ 2 2 2 2 2 2
t
56$$ 0 0 a10 1 e t
56$$ 0 0 a10 2 e t
56$$ 0 0 a10 3 e t
56$$ 0 0 a10 4 e t
56$$ 0 0 a10 5 e t
56$$ 0 0 a10 6 e t
56$$ 0 0 a10 7 e t
56$$ 0 0 a10 8 e t
56$$ 0 0 a10 9 e t
56$$ 0 0 a10 10 e t
56$$ f0 t
end
=opus
LIBUNIT=21
TYPARAMS=NUCLIDES
UNITS=WATTS
LIBTYPE=ALL
TIME=YEARS
NPOSITION=1 2 3 4 5 6 7 8 9 10 end
End
=shell
[command to copy file ft71f001 to a local directory]
end

```

The Shielding Analysis Sequence #4 (SAS4) code reads the shielding problem definitions from a single input stream, then proceeds to automatically execute the BONAMI, NITAWL, XSDRNPM, and MORSE-SCG computer codes in sequence. The SCALE driver software reads the single input stream and prepares individual inputs for each of the above codes, automatically executes each code, and then collects all output into a common output file. The source file written by the ORIGEN-S code with the input stream shown in Code Listing 5-1 is copied into the ft30f001 file just prior to execution as described in the first =shell input shown in Code Listing 5-2.

The input options for SAS4 were carefully chosen to ensure accurate dose estimates. The radial calculations along the package side utilize the IDR=0 option with full automated biasing as well as point detectors because the code is fully applicable under these conditions. The axial calculations for the package top and bottom used the IDR=2 option and effectively turned off the automated biasing (note all void materials in the one-dimensional adjoint model). The axial biasing produces inaccurate results for a nonsymmetric axial model because the SAS4 code is designed to bias particles in opposite directions above and below the model axial centerline. The effective removal of the automated biasing allows the underlying MORSE-SCG code to run

without the axial symmetry requirement. The accuracy of these results was tested by comparison to another SCALE module under development that removes these limitations.

Code Listing 5-2 SAS4 Input Stream for NCT Reduced-Density Smearred Cylinder Source (radial side gamma)

```
=shell
[copy ORIGEN-S ft71f001 output file previously saved to file named ft30f001]
end
'Input generated by Espn 5.1 Compiled on 8-07-2006
=sas4      parm=size=1000000
pat-1 pu large cyl 3d case
27n-18couple infhommedium
pu 1 den=0.818 1 300 end
redwood 3 den=0.36 1 300 end
aluminum 4 den=2.6989 1 300 end
ss304 5 den=7.9 1 300 end
copper 6 den=8.94 1 300 end
mgconcrete 7 1 300 end
arbmph13-8mo 7.5 5 0 0 24000 12.75 28000 8 13000 1.125 42000 2.25
26000 75.875 2 1 300 end
end comp
izm=6 mhw=2 frd=5.4 end
5.4 6.8 13.97 15.24 28.58 28.73 end
1 2 0 4 3 5 end
xend
ran=000003600621 tim=1200 nst=4000 nmt=12000 nit=900 nco=4 ist=0 ipr=0
iso=0 nod=16 sfa=9.517e+12 igo=4 inb=0 ine=0 mfu=2 isp=6 ipf=0 isd=4
nda=1000 end
det 30 0 0 30 0 2 30 0 4 30 0 6 30 0 8 30 0 10 30 0 15 30 0 20
128.7 0 0 128.7 0 5 128.7 0 10 128.7 0 15 128.7 0 20 128.7 0 25 128.7 0 30
128.7 0 35 end
sxy 1 -5.4 5.4 -5.4 5.4 0 10 100 100 100 100 end
gend
shielding problem
0 0 0 0
rcc 0 0 -5.64 0 0 15.11 5.40
sph 0 0 -3.74 5.72
rcc 0 0 -5.64 0 0 16.71 6.795
sph 0 0 -3.74 7.12
rcc 0 0 -5.64 0 0 16.71 10
rcc 0 0 -10.86 0 0 21.93 6.875
rcc 0 0 -18.25 0 0 7.39 6.875
rcc 0 0 -18.25 0 0 20.32 7.52
rcc 0 0 2.07 0 0 9 8.74
rcc 0 0 -18.25 0 0 36.79 13.97
rcc 0 0 -20.79 0 0 41.87 13.97
rcc 0 0 -30.35 0 0 60.81 13.97
rcc 0 0 -30.35 0 0 60.81 15.24
rcc 0 0 -48.69 0 0 99.13 28.58
rcc 0 0 -48.84 0 0 99.43 28.73
sph 0 0 0 300
rcc 0 0 -2.936 0 0 5.872 4.032
rcc 0 0 -2.936 0 0 5.872 4.445
end
src +1
src +2 -3
tbl +3 -1
tbl +4 -2 -5
vod +6 -5 -4 or 6 5 8 -3
wod +7 -6
```

```

cop +8 -7 -6
vod +9 -3
wod +10 -9 -8
alu +11 -10
wod +12 -11
alu +13 -12
wod +14 -13
drm +15 -14
vod +16 -15
exv -16
end
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1 1 2 2 1000 1000 6 1000 1000 4 3 4 3 5 1000 0
0

```

End

Code Listing 5-3 SAS4 Input Stream for NCT Reduced-Density Smearred Cylinder Source (radial side neutron)

```

=shell
[copy ORIGEN-S ft71f001 output file previously saved to file named ft30f001]
end
'Input generated by Espn 5.1 Compiled on 8-07-2006
=sas4      parm=size=1000000
pat-1 pu large cyl 3d case
27n-18couple infhommedium
pu 1 den=0.818 1 300 end
redwood 3 den=0.36 1 300 end
aluminum 4 den=2.6989 1 300 end
ss304 5 den=7.9 1 300 end
copper 6 den=8.94 1 300 end
mgconcrete 7 1 300 end
arbmph13-8mo 7.5 5 0 0 0 24000 12.75 28000 8 13000 1.125 42000 2.25
26000 75.875 2 1 300 end
end comp
ity=1 irf=9029 izm=6 mhw=2 frd=5.4 end
5.4 6.8 13.97 15.24 28.58 28.73 end
1 2 0 4 3 5 end
xend
ran=000003600621 tim=1200 nst=4000 nmt=12000 nit=200 nco=4 ist=0 ipr=0
iso=0 nod=16 sfa=1.95e+6 igo=4 inb=0 ine=0 mfu=2 isp=7 ipf=0 isd=4
nda=1000 end
det 30 0 0 30 0 2 30 0 4 30 0 6 30 0 8 30 0 10 30 0 15 30 0 20
128.7 0 0 128.7 0 5 128.7 0 10 128.7 0 15 128.7 0 20 128.7 0 25 128.7 0 30
128.7 0 35 end
sxy 1 -5.4 5.4 -5.4 5.4 0 10 100 100 100 100 end
gend
shielding problem
0 0 0 0
rcc 0 0 -5.64 0 0 15.11 5.40
sph 0 0 -3.74 5.72
rcc 0 0 -5.64 0 0 16.71 6.795
sph 0 0 -3.74 7.12
rcc 0 0 -5.64 0 0 16.71 10
rcc 0 0 -10.86 0 0 21.93 6.875
rcc 0 0 -18.25 0 0 7.39 6.875
rcc 0 0 -18.25 0 0 20.32 7.52
rcc 0 0 2.07 0 0 9 8.74
rcc 0 0 -18.25 0 0 36.79 13.97
rcc 0 0 -20.79 0 0 41.87 13.97

```

```

rcc 0 0 -30.35 0 0 60.81 13.97
rcc 0 0 -30.35 0 0 60.81 15.24
rcc 0 0 -48.69 0 0 99.13 28.58
rcc 0 0 -48.84 0 0 99.43 28.73
sph 0 0 0 300
rcc 0 0 -2.936 0 0 5.872 4.032
rcc 0 0 -2.936 0 0 5.872 4.445
  end
src +1
src +2 -3
tbl +3 -1
tbl +4 -2 -5
vod +6 -5 -4 or 6 5 8 -3
wod +7 -6
cop +8 -7 -6
vod +9 -3
wod +10 -9 -8
alu +11 -10
wod +12 -11
alu +13 -12
wod +14 -13
drm +15 -14
vod +16 -15
exv -16
  end
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1 1 2 2 1000 1000 6 1000 1000 4 3 4 3 5 1000 0
0

```

End

Code Listing 5-4 SAS4 Input Stream for NCT Reduced-Density Smearred Cylinder Source (axial top neutron)

```

=shell
[copy ORIGEN-S ft71f001 output file previously saved to file named ft30f001]
end
'Input generated by Espn 5.1 Compiled on 8-07-2006
=sas4      parm=size=1000000
pat-1 pu large cyl top 3d case
27n-18couple infhommedium
pu 1 den=0.818 1 300 end
redwood 3 den=0.36 1 300 end
aluminum 4 den=2.6989 1 300 end
ss304 5 den=7.9 1 300 end
copper 6 den=8.94 1 300 end
mgconcrete 7 1 300 end
arbmph13-8mo 7.5 5 0 0 0 24000 12.75 28000 8 13000 1.125 42000 2.25
26000 75.875 2 1 300 end
end comp
idr=2 ity=1 irf=9029 izm=6 mhw=2 frd=5.4 end
9.46 11.06 18.54 21.08 50.44 50.59 end
0 0 0 0 0 0 end
xend
ran=000003600621 tim=1200 nst=4000 nmt=12000 nit=1000 nco=4 ist=0 ipr=0
iso=0 nod=7 sfa=1.95e+6 igo=4 inb=0 ine=0 mfu=2 isp=7 ipf=0 isd=4
nda=1000 end
det 0 0 52 2 0 52 4 0 52 6 0 52
0 0 150.59 5 0 150.59 10 0 150.59 end
sxy 1 -5.4 5.4 -5.4 5.4 0 10 100 100 100 100 end
gend

```

```

shielding problem
0 0 0 0
rcc 0 0 -5.64 0 0 15.11 5.40
sph 0 0 -3.74 5.72
rcc 0 0 -5.64 0 0 16.71 6.795
sph 0 0 -3.74 7.12
rcc 0 0 -5.64 0 0 16.71 10
rcc 0 0 -10.86 0 0 21.93 6.875
rcc 0 0 -18.25 0 0 7.39 6.875
rcc 0 0 -18.25 0 0 20.32 7.52
rcc 0 0 2.07 0 0 9 8.74
rcc 0 0 -18.25 0 0 36.79 13.97
rcc 0 0 -20.79 0 0 41.87 13.97
rcc 0 0 -30.35 0 0 60.81 13.97
rcc 0 0 -30.35 0 0 60.81 15.24
rcc 0 0 -48.69 0 0 99.13 28.58
rcc 0 0 -48.84 0 0 99.43 28.73
sph 0 0 0 300
rcc 0 0 -2.936 0 0 5.872 4.032
rcc 0 0 -2.936 0 0 5.872 4.445
end
src +1
src +2 -3
tbl +3 -1
tbl +4 -2 -5
vod +6 -5 -4 or 6 5 8 -3
wod +7 -6
cop +8 -7 -6
vod +9 -3
wod +10 -9 -8
alu +11 -10
wod +12 -11
alu +13 -12
wod +14 -13
drm +15 -14
vod +16 -15
exv -16
end
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1 1 2 2 1000 1000 6 1000 1000 4 3 4 3 5 1000 0
0

end

```

Code Listing 5-5 SAS4 Input Stream for HAC Reduced-Density Smearred Cylinder Source (radial gamma)

```

=shell
[copy ORIGEN-S ft71f001 output file previously saved to file named ft30f001]
end
'Input generated by Espn 5.1 Compiled on 8-07-2006
=sas4      parm=size=1000000
pat-1 pu large cyl 3d case
27n-18couple infhommedium
pu 1 den=0.818 1 300 end
redwood 3 den=0.36 1 300 end
aluminum 4 den=2.6989 1 300 end
ss304 5 den=7.9 1 300 end
copper 6 den=8.94 1 300 end
mgconcrete 7 1 300 end
arbmph13-8mo 7.5 5 0 0 0 24000 12.75 28000 8 13000 1.125 42000 2.25

```

```

26000 75.875 2 1 300 end
end comp
izm=6 mhw=2 frd=5.4 end
5.4 6.8 13.97 15.24 28.58 28.73 end
1 2 0 0 0 0 end
xend
ran=000003600621 tim=1200 nst=4000 nmt=12000 nit=900 nco=4 ist=0 ipr=0
iso=0 nod=10 sfa=9.517e+12 igo=4 inb=0 ine=0 mfu=2 isp=6 ipf=0 isd=4
nda=1000 end
det 106.8 0 0 106.8 0 5 106.8 0 10 106.8 0 15 106.8 0 20 106.8 0 25 106.8 0 30
106.8 0 35 0 0 -110.98 0 0 111.06 end
sxy 1 -5.4 5.4 -5.4 5.4 0 10 100 100 100 100 end
gend
shielding problem
0 0 0 0
rcc 0 0 -5.64 0 0 15.11 5.40
sph 0 0 -3.74 5.72
rcc 0 0 -5.64 0 0 16.71 6.795
sph 0 0 -3.74 7.12
rcc 0 0 -5.64 0 0 16.71 10
rcc 0 0 -10.86 0 0 21.93 6.875
rcc 0 0 -18.25 0 0 7.39 6.875
rcc 0 0 -18.25 0 0 20.32 7.52
rcc 0 0 2.07 0 0 9 8.74
rcc 0 0 -18.25 0 0 36.79 13.97
rcc 0 0 -20.79 0 0 41.87 13.97
rcc 0 0 -30.35 0 0 60.81 13.97
rcc 0 0 -30.35 0 0 60.81 15.24
rcc 0 0 -48.69 0 0 99.13 28.58
rcc 0 0 -48.84 0 0 99.43 28.73
sph 0 0 0 300
rcc 0 0 -2.936 0 0 5.872 4.032
rcc 0 0 -2.936 0 0 5.872 4.445
end
src +1
src +2 -3
tbl +3 -1
tbl +4 -2 -5
vod +6 -5 -4 or 6 5 8 -3
wod +7 -6
cop +8 -7 -6
vod +9 -3
wod +10 -9 -8
alu +11 -10
wod +12 -11
alu +13 -12
wod +14 -13
drm +15 -14
vod +16 -15
exv -16
end
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1 1 2 2 1000 1000 1000 1000 1000 1000 1000 1000 1000 1000 1000 0
0
end

```

The Shielding Analysis Sequence #1 (SAS1) code reads the shielding problem definitions from a single input stream, then proceeds to automatically execute the BONAMI, NITAWL, XSDRNPM, and XSDOSE computer codes in sequence. The SCALE driver software reads the single input stream and prepares individual inputs for each of the above codes, automatically

executes each code, and then collects all output into a common output file. The (α ,n) source description written by the SOURCES4C code with the input stream shown in Code Listing 5-6 is entered by hand into the SAS1 input stream.

Code Listing 5-6 SAS1 Input Stream for Pu/Be spherical source with full density alpha-Pu metal

```
=sas1  parm=nitawl
pube neutron source alpha phase - no void
27n-18couple infhommedium
plutoniumalp 1 1.0 293 end
end comp
end
last
neutron case
spherical
1 1.34 1 -1 0 0 3304 0
end zone
2.90211e-1 4.11765e-1 2.26912e-1 1.91999e-2 2.54550e-2
2.39615e-2 2.58964e-3 8.56173e-5 3.16844e-6 4.29906e-8
17z 18z
ndetec=2
read xsdose
23.33 123.33
end
```

The SOURCES4C code is designed to predict the (α ,n) source generation for homogenous and interface problems. This analysis uses the interface option to determine the (α ,n) source per unit area of contact between the α generator and a target nucleus. In this case, the α generator is plutonium metal and the target material is Be. The code can output the neutron source in any group structure; in this case, the 27-group structure used in SCALE is specified and the source spectrum from SOURCES4C is used directly in the SAS1 case shown above.

Code Listing 5-7 SOURCES4C Input Stream for Pu-Be Interface Source Problem

```
WPu-Be Interface Problem
2 2 1
2 0 6.50 0.0000001
 94 0.99
 95 0.01
100
5
 942380 0.0005
 942390 0.9238
 942400 0.0648
 942420 0.0010
 952410 0.0099
target is composed of Be
1 0
 4 1.0
-27 20.0 1e-11
20 6.43 3 1.85 1.4 0.9 0.4 0.1 0.017 0.003 0.00055
1e-4 3e-5 1e-5 3.05e-6 1.77e-6 1.3e-6 1.13e-6 1e-6
8e-7 4e-7 3.25e-7 2.25e-7 1e-7 5e-8 3e-8 1e-8
1 4000
 40090 1.0
```

This page intentionally left blank