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Scoping Thermal Response Calculations of RNS Waste During Transport to and Disposal at the WIPP

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ABSTRACT

Sandia National Laboratories (SNL) was contracted by the United States Department of Energy Environmental Management (DOE-EM), Los Alamos Field Office to perform mechanical and thermal scoping calculations as part of a study seeking to understand the ignitability risk of the Remediated Nitrate Salts (RNS) waste drums during transportation from the Waste Control Specialists (WCS) facility to Waste Isolation Pilot Plant (WIPP) and permanent disposal of the waste at WIPP. The scoping thermal simulations described in this report pertain to thermal calculations performed with a packaging system consisting of one Standard Waste Box (SWB) loaded with drums placed inside a Standard Large Box 2 (SLB2). During transportation, the SLB2 is inside Transuranic Package Transporter Model III (TRUPACT-III), which provides the third layer of the packaging. Once at the WIPP, it is assumed the SLB2 is extracted from the TRUPACT-III and maintained above ground, and then subsequently placed underground for permanent disposal. In these proposed configurations, the space between the SLB2 and the SWB is always filled by a layer of insulation consisting of air-filled glass microbubbles except for the bottom which rests directly on the SLB2.

The thermal scoping calculations described in this report specifically address whether the introduction of external heat inputs, combined with the contributions from the internally generated radiolytic decay heat and chemical reactions, lead to an unstable thermal state during the time of its movement and placement in the permanent disposal location. The external heat inputs are of two forms: 1) ambient thermal irradiation (e.g., solar and ambient storage/disposal temperatures) and 2) accident-induced fire. Three scoping calculation scenarios were derived as representative, conservative scenarios: 1A) TRUPACT-III transient transportation, 1B) SLB2 48-hour outdoor storage with solar radiation, and 2) fully-engulfing fire during SLB2 handling or emplacement following a steady-state analysis in a 38 °C environment. All the simulated scenarios are conservative relative to the operational conditions expected for handling the waste package during transportation and placement in the WIPP underground disposal unit.

The predictions obtained from simulating the three exposure scenarios revealed that adding the SLB2 and the air-filled glass microbubbles to the transport and storage/disposal configurations provides additional thermal protection of the drums beyond what the SWB provides alone, both during long-term above ground insolation and underground during a fire accident. Under the current transportation/storage/disposal concepts, the degree of protection provided by the packaging concept is sufficient to prevent the waste from being ignitable.

The simulation results demonstrate that there is adequate margin to safely transport and place the RNS waste from WCS to the WIPP under the current operational concept.

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ACRONYMS AND TERMS

Acronym/Term	Definition
CFR	Code of Federal Regulations
DOE	Department of Energy
EM	Environmental Management
IAEA	International Atomic Energy Agency
NCT	Normal Conditions of Transportation
RNS	Remediated Nitrate Salt
SARP	Safety Analysis Report for Packaging
SNL	Sandia National Laboratories
SLB2	Standard Large Box 2
SWB	Standard Waste Box
TAT	Technical Assessment Team
TRU	Transuranic
TRUPACT-II	Transuranic Package Transporter Model II
TRUPACT-III	Transuranic Package Transporter Model III
WCS	Waste Control Specialists
WIPP	Waste Isolation Pilot Plant

1. INTRODUCTION

The United States Department of Energy (DOE) is required to remove Standard Waste Boxes (SWBs) containing Remediated Nitrate Salt (RNS) waste drums from the Waste Control Specialists (WCS) facility in Andrews, Texas. The Waste Isolation Pilot Plant (WIPP) near Carlsbad, New Mexico is the DOE's preferred destination. The RNS waste drums in question are from the same waste stream that resulted in an incident at WIPP on February 14, 2014, and other waste streams that contain RNS waste [1].

A Technical Assessment Team (TAT) assembled by DOE to investigate the incident concluded that the cause of the breach was incompatible waste. Experiments conducted as part of that investigation showed that various combinations of nitrate salt, Swheat Scoop®, nitric acid, and oxalate self-heat at temperatures below 100°C. The team concluded that this heat generation in the days leading up to the incident, coupled with obstruction of the vent system, resulted in a thermal runaway that caused the drum to over pressurize and breach [1]. Continued temperature monitoring of the SWBs at WCS since the incident suggests the temperature of the drums is decreasing indicating that the waste is becoming more stable. Testing performed by LANL [2] identified that venting and maintaining the drum contents below 60°C were key to prevent thermal runaway, suggesting a pathway to demonstrate the safe transport of the drums.

Sandia National Laboratories (SNL) was contracted by DOE Environmental Management (EM), Los Alamos Field Office to perform mechanical and thermal scoping calculations as part of a study seeking to understand the ignitability risk of the RNS waste drums during transportation from the WCS facility to WIPP and disposal of the waste at WIPP. The thermal scoping calculations described in this report specifically address the questions posed above, namely, can the introduction of external heat inputs, combined with the contributions from the internally-generated radiolytic decay heat and chemical reactions, lead to an unstable thermal state during the time of its movement and placement in the permanent disposal location. Two general classes of external heat exposure were considered: 1) ambient thermal irradiation (e.g., solar and ambient storage) and 2) accident-induced fire. For all the scenarios considered within these two classes of exposure, the packaging system consists of one SWB loaded with drums, inside a Standard Large Box 2 (SLB2). Enhanced thermal protection of the drums is achieved through the inclusion of an insulating layer of air-filled glass micro-bubbles in the space between the SLB2 and SWB, except for the bottom, which is in direct contact. This proposed configuration provides one additional layer of thermal protection of the drums during transportation within a TRUPACT-III, during long-term insolation exposure of a SLB2, and during a potential fire accident.

2. SCOPING CALCULATION SCENARIOS

Three scoping calculation scenarios were derived as notionally representative, conservative scenarios to serve as a basis for assessing risk of transporting RNS waste from WCS to WIPP and storage or permanent disposal. Two of the scenarios fall within the first general class of exposure, and the third scenario falls into the second class of general exposures. Table 1 lists the details of those scenarios.

Table 1. Scoping calculation analysis scenarios

Scenario	Name	Description
1A	TRUPACT-III Transient NCT	TRUPACT-III transient Normal Conditions of Transport (NCT) from WCS to WIPP for a period of 24 hours
1B	SLB2 Transient NCT	SLB2 above ground in the sun for 48 hours
2	SLB2 Fire	SLB2 5-minute, constant temperature, fully-engulfing fire with 5-minute ramp-up and 5-minute ramp-down

Note that a 10 CFR Part 71.73(c)(4) thermal event during transportation was not considered because the current TRUPACT-III SARP covers this case.

2.1. Scenario 1A: TRUPACT-III Transient NCT

This scenario begins with a three-layer packaging system consisting of one SWB loaded with drums, inside an SLB2. During transportation the SLB2 is inside a TRU Package Transporter Model III (TRUPACT-III), which provides the third layer of the packaging. During transportation, the TRUPACT-III is exposed to ambient temperatures and insolation. The transient NCT scenario includes a 24-hour road transport period in case the truck stalls on the side of the road en-route to WIPP and needs repair time, or an alternate truck is sent to pick up the TRUPACT-III trailer to continue the route to WIPP. The 24-hour transient is significantly longer than the likely transport duration of ~1.3 hours. Operational plans for the handling of RNS waste include immediately backing the TRUPACT-III into the Waste Handling Building air lock when it arrives at WIPP, so there will be no extended period of exposure to solar insolation.

2.2. Scenario 1B: SLB2 Transient NCT

Under this scenario, the drums in transportation configuration arrive at WIPP and the SLB2 is extracted from the TRUPACT-III at the Waste Handling Building. The SLB2 then is placed above ground and exposed to solar insolation for 48 hours with two 12-hour periods on insolation followed by two 12-hour periods without. While operations at the WPP never leave waste packages outdoors, this scenario was simulated to provide information on the thermal response of the SLB2 when exposed to more severe heating than takes place while it is transported within the TRUPACT-III.

2.3. Scenario 2: SLB2 Fire

In this scenario, the SLB2 is moved underground for disposal. Because fires have occurred underground at WIPP (the last one occurred February 5, 2014 (see Ref. [3]), just days before the drum breach) the SLB2 is exposed to a fully-engulfing, constant temperature fire for five minutes.

The scenario also includes five-minute temperature ramps accounting for the initial rise to maximum temperature and final decline back to ambient non-fire state. The total thermal load applied in this scenario is equivalent to a 10-minute, constant temperature, fully-engulfing fire. For this simulated calculation, the steady-state initial temperature distribution inside the SLB2 in an underground facility is obtained before the start of the fire. Note that this scenario also covers the case where the SLB2 is stored inside a facility away from the sun (i.e., above ground or underground with no insolation).

Because of underground fuel loading restrictions at WIPP, fire risk analysis indicates an expected maximum fire duration of five minutes [4]. A transportation fire is not included in the scoping calculations because the TRUPACT-III provides sufficient insulation to protect the drums in case of a road accident based on the thermal analyses performed as part of the TRUPACT-III Safety Analysis Report for Packaging (SARP).

3. GEOMETRY USED FOR TRUPACT III, SLB2, SWB, AND RNS DRUMS

Figure 1 shows a three-dimensional, two-plane symmetry, cutaway model of the TRUPACT-III used for the transient NCT scenario. Note that only a quarter of the TRUPACT-III is modeled, as shown in the figure. There are minor differences between the front and back side of the TRUPACT-III, but for the purpose of these simulations, these differences were disregarded. To minimize complexity, features like bolts, bolt holes, small plates, groves, etc., were removed, and only the major features of the package were retained. One exception is the large volume between the inner and outer walls of the container of the TRUPACT-III occupied by air and corrugated sheets. These volumes occupy a significant portion of the packaging system but were excluded from the geometry because their combined thermal effect is available via effective thermophysical properties obtained from Ref. [5]. Additionally, the volume between the inner wall of the SLB2 and the SWB is filled with the glass micro-bubble material, except for the bottom where the SWB rests directly on the SLB2. The SLB2 is not credited in the transient NCT calculations. Since the SLB2 is a thin-walled box, the thin walls are assumed to contribute minimally to the thermal response of the three-layer packaging system.

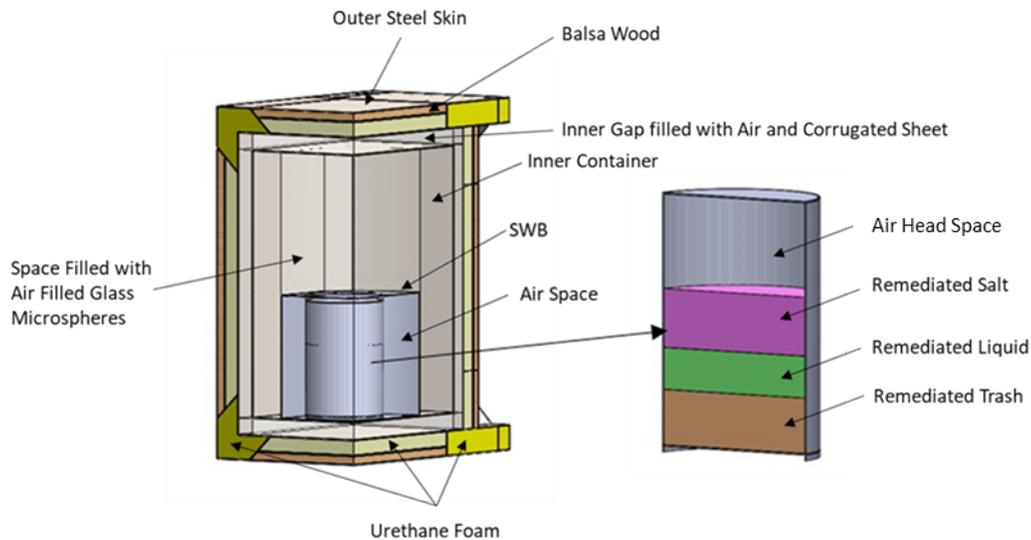


Figure 1. Cutaway of TRUPACT-III used as a model for transient NCT.

The TRUPACT-III was assumed to contain four RNS waste drums, one in each quadrant of the quarter symmetry model. This will result in slightly conservative predictions of drum temperature since none of the SWBs at WCS contain more than three RNS waste drums with the possibility of generating heat from chemical reactions. Further, the maximum decay heat for any loaded SWB at WCS is used in the analysis. The drum included contains the RNS waste with both decay heat and temperature-dependent chemical heat generation. The quarter symmetry model forces the temperature distribution in all four drums to be the same.

Figure 2 shows the SLB2 geometry with the SWB and the drums inside used for the 48-hour NCT scenario and the SLB2 Fire scenario. The top and side of the SLB2, the lid of the SWB, and the sides of one of the drums have been removed to show the internals. In this case the 4th drum (which may be empty or may contain non-RNS waste) is neglected. The glass micro-bubble and air volumes are transparent. The SWB and drum geometries are the same as shown in Figure 1. As with the transient NCT model, features assumed not to contribute significantly to the overall response of

the two-layer packaging system were removed. The SLB2 outer skin was again neglected in the model formulation.

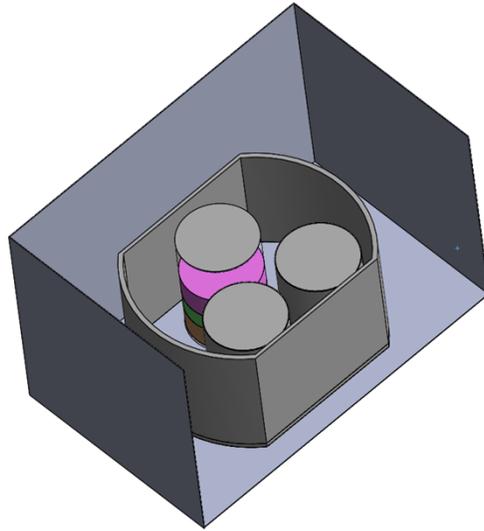


Figure 2. Internal view of SLB2/SWB/Drum model used for 48-hour NCT and SLB2 Fire.

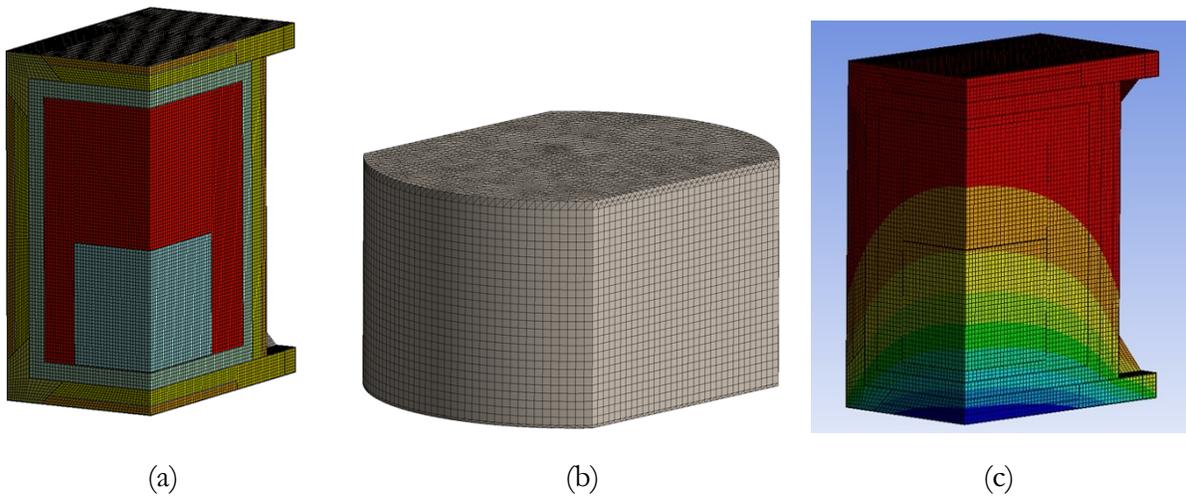


Figure 3. (a) Transient NCT mesh, (b) 48-hour NCT and SLB2 Fire mesh, and (c) boundary condition results.

The dimensions for each of these components were obtained from TRUPACT-III, SLB2, and SWB SARP drawings. The mesh for the TRUPACT-III and SLB2 were approximately 500,000 and 400,000 elements in size, respectively (see Figure 3(a) and (b)). The relatively higher density mesh for the SLB2 is required to produce accurate results for the higher heat flux ramp used in the transient fire scenario. Prior to conducting the runs, mesh convergence studies and model symmetry implementation checks were performed (Figure 3(c)).

4. MATERIALS USED FOR TRUPACT III, SLB2, SWB, AND RNS DRUMS

Figure 1 and Figure 2 also differentiate the constituent materials employed in the model by color. In these figures, the steel components are shown in gray, and the volume of glass micro-bubbles and air are shown transparent. The RNS waste with sorbed liquid is modeled as a salt layer and a liquid layer. The remediated salt and liquid are shown in magenta and green, respectively, and the drum trash is the brown volume. In Figure 1, the yellow volumes correspond to various density urethane foam components, and the tan volume corresponds to balsa wood.

Table 2 through Table 8 show the material properties used for the models. In these tables the density, specific heat, and thermal conductivity are given in units of kg/m^3 , J/kg-C , and W/m-C , respectively. Except for the air-filled glass (soda-lime, borosilicate) micro-bubbles [6], all material properties were obtained from the SARP [5], and corroborated with the literature where possible. Structural steel (UNSS31803) was used for both the SWB, SLB2, drum walls, and for all metal plates in the TRUPACT-III.

Table 2. Thermophysical properties of steel (UNSS31803) components in the TRUPACT-III, SLB2, and SWB

Temperature (°C)	Density	Specific Heat (Cp)	Thermal Conductivity (k)
20	7890	492	14
100		518	15
200		538	17

Table 3. Thermophysical properties of balsa wood in TRUPACT-III

Temperature (°C)	Density	Specific Heat (Cp)	Thermal Conductivity (k)
20	120	1800	0.04
100		14000	0.17
200		1800	0.04

Table 4. Thermophysical properties of 100 kg/m^3 polyurethane foam in TRUPACT-III

Temperature (°C)	Density	Specific Heat (Cp)	Thermal Conductivity (k)
20	100	1477	0.03
100	100		0.03
200	90		0.05

Table 5. Thermophysical properties of 160 kg/m³ polyurethane foam in TRUPACT-III

Temperature (°C)	Density	Specific Heat (Cp)	Thermal Conductivity (k)
20	160	1477	0.03
100	160		0.03
200	145		0.05

Table 6. Thermophysical properties of 290 kg/m³ polyurethane foam in TRUPACT-III

Temperature (°C)	Density	Specific Heat (Cp)	Thermal Conductivity (k)
20	290	1477	0.05
100	290		0.05
200	262		0.07

Table 7. Thermophysical properties of 480 kg/m³ polyurethane foam in TRUPACT-III

Temperature (°C)	Density	Specific Heat (Cp)	Thermal Conductivity (k)
20	480	1477	0.07
100	480		0.07
200	433		0.09

Table 8. Thermophysical properties of air/corrugated sheets in inner container of TRUPACT-III

Temperature (°C)	Density	Specific Heat (Cp)	Thermal Conductivity		
			kxx	kyy	kzz
20	1130	492	0.7	2.4	1.6
100		517	0.9	2.5	1.7
200		538	1.2	2.8	1.9

Table 9. Effective properties of microbubbles and air filling the space between SLB2 and SWB

Temperature (°C)	Density	Specific Heat (Cp)	Thermal Conductivity (k)
20	90	998	0.043
800		1160	0.1

Various density foams are used for the TRUPACT-III but all are made from polyurethane. Note that the specific heat and thermal conductivity of this foam varies very little with density. The thermal conductivity of the air/corrugated sheets varies with direction due to the orientation shift

on each side of the TRUPACT-III walls. The model accounts for orthonormal thermal conductivity by adding different coordinate systems to each of the elements in the geometry making up these walls.

For the first class of exposures (ambient irradiation), material properties up to 200 °C suffice to properly model the thermal response of the package. The material properties for the glass micro-bubbles for these cases near room temperature were obtained from 3M™ [6]. The effective thermal properties for the micro-bubble after accounting for air space inside the bubbles are: $\rho = 150 \text{ kg}/\text{m}^3$, $k = 0.055 \text{ W}/\text{m} \text{ }^\circ\text{C}$, and $C_p = 994 \frac{\text{J}}{\text{kg}}^\circ\text{C}$. The effective values for the conductivity are obtained by using the fraction of the diameter of the micro-bubble occupied by air and by glass. The density and thermal conductivity are based on 6.7% glass and 93.3% air by volume and is provided by 3M™. Thus, for example, the specific heat and density are calculated from the values for glass and air by adjusting according to their relative percentages (e.g., $C_p = 0.933 \times 1005 + 0.067 \times 840 = 994 \text{ J}/\text{kg}\text{-C}$). Afterwards, the effective thermal properties for the material in the space between the SLB2 and SWB are calculated by including the air (40% by volume) surrounding the micro-bubble (60% by volume), which results in the properties shown in Table 9. Since the outer skin of the SLB2 is neglected in the model, the only material that reaches temperatures above 200 °C in the fire scenario is the glass micro-bubbles.

5. BOUNDARY CONDITIONS

As described in Section 0, three scenarios were analyzed. First, a 24-hour transient NCT was conducted of the TRUPACT-III to cover the transport phase of the packaging. This was followed by a 48-hour transient NCT, which covers the scenario where the SLB2 is in temporary storage above ground. In both these NCT cases, insolation values are consistent with those used in the transient NCT and change every 12 hours from insolation to no insolation. The last scenario is a 5-minute constant temperature SLB2 Fire. The SLB2 Fire scenario assumes a five-minute ramp up to the constant temperature and a five-minute ramp down back to ambient temperature. The following sections describe the boundary conditions in more detail for each of these scenarios.

5.1. Drum Heat Decay and Chemical Heat Generation

In all scenarios, the decay heat was assumed to be 21.5 W/m^3 per drum, which is the maximum decay heat in any of the drums in the inventory at WCS. Additional heat generation was added to the drums' decay heat to account for the incompatible waste chemical reactions. The heat generation rate is based on an Arrhenius reaction model:

$$\dot{Q} = h_r V_{waste} \cdot A e^{-E/RT},$$

where h_r is the energy produced by the waste during chemical reaction per unit volume ($528 \times 10^6 \text{ J/kmol} \cdot 4.07 \text{ kmol/m}^3$), V_{waste} is the volume of the remediated waste in the drum (0.054 m^3), A is the reaction constant ($1.586 \times 10^{15} / \text{s}$), E is the activation energy of the reaction, R is the universal gas constant, and T is the absolute temperature at which the reaction takes place. The values for these variables were obtained from the waste model reported in Ref [7]. The heat generation has the exponential form shown in Figure 4.

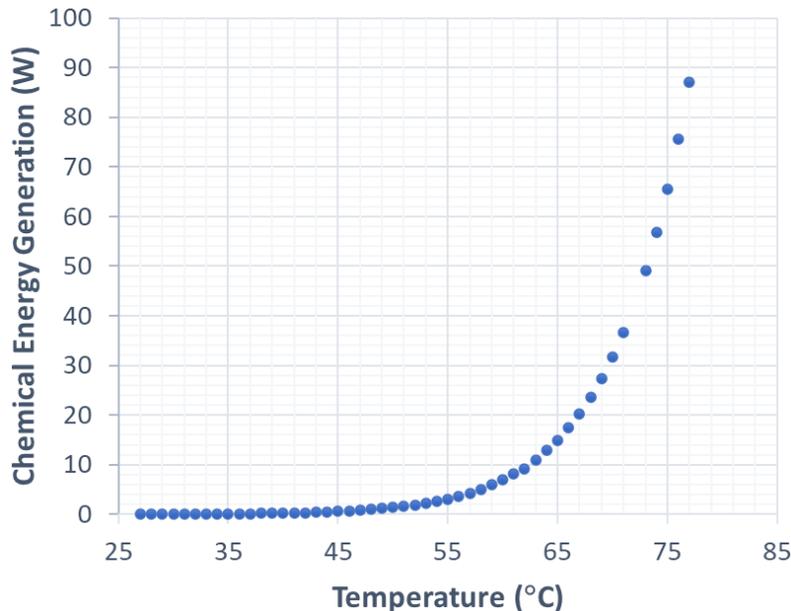


Figure 4. Chemical energy generated by the waste.

5.2. TRUPACT-III Transient NCT

The TRUPACT-III is assumed to be outdoors on a trailer. The drums are assumed to be standing on the bottom of the SWB, which is in turn standing on the bottom of an SLB2. The total time the packaging is in this configuration is 24 hours. Insolation (i.e., sun irradiation) is imposed for the first 12 hours, followed by 12 hours of no insolation. The insolation values,

Table 10, were assembled from information found in 10CFR 71.71 and IAEA Regulations for the Safe Transport of Radioactive Material, Section IV, Par. 657. For the initial 12 hours, the insolation value applied to the TRUPACT-III was 800 W/m² on the top flat surface and 200 W/m² on the vertical flat sides. No insolation heat flux was applied to the bottom (downward facing) surface of the TRUPACT-III, since it will not receive any direct solar exposure during this scenario.

Table 10. Scenario 1 insolation values (W/m²)

Surface Configuration	TRUPACT-III Transient NCT
Flat Surfaces Transported Horizontally – Upward Facing	800 daytime 0 nighttime
Flat Surfaces Transported Horizontally – Downward Facing	0
Flat Surfaces Not Transported Horizontally	200 daytime 0 nighttime

All outer surfaces of the TRUPACT-III were exposed to an ambient temperature of 38 °C. Ambient radiation and ambient convective heat transfer were applied on all outer surfaces of the TRUPACT-III using the ambient temperature as a reference temperature, except for the bottom surface, which only has ambient radiation. Note that the surface temperature of the package is expected to be hotter than the ambient temperature due to insolation. Although TRUPACT-III packages are painted white, an emissivity value of 0.25 was used, which corresponds to the value for non-oxidized steel surfaces. Typical white paint emissivity is much greater than 0.25, so using this smaller value results in bigger emitted heat flux from the outer surface of this packaging during NCT (and consequently higher predicted content temperature). All surfaces were assumed gray and diffusive (emissivity equals absorptivity), which is common for rough metallic surfaces.

For convection, the values applied to the outer surfaces varied between 2 and 6 W/m², depending on the orientation of the surface. This value assumes free flow around the package. During transport, these values will be higher due to forced flow conditions, but since the outer surface of the package is expected to be hotter, the effect of this forced convection is to cool the package. Therefore, free convection values are used, which again is conservative.

Internally, since the gaps between surfaces are small or non-existent, no convection is assumed between internal surfaces and the gas gaps. In this scenario, the internal temperatures are expected to be < 200 °C; therefore, radiation is not expected to be a major contributor to internal heat transfer (less than 10%). As a result, no credit is taken for radiation heat transfer between the inner

wall of the SWB and the outer wall of the drums. All surfaces are assumed to be in perfect contact. This assumption increases the heat transfer from the top and sides of the package to the inside of the package, compensating for radiation and convection heat transfer not included in the model. Note that the drum rim on the bottom portion of the drum provides an air gap between the bottom of the drum and the floor of the SWB, creating an insulated layer; therefore, the configuration just described maximizes heat input to the drums.

It was assumed the initial temperature of the TRUPACT-III and contents was 22 °C and that it and all the components of the packaging systems were brought inside a temperature-controlled facility (the Perma-Con® building at WCS) prior to loading. This initial temperature is based on estimated temperature of the Perma-Con® building at WCS where the SWBs are stored prior to loading into the SLB-2 and TRUPACT-III.

5.3. SLB2 Transient NCT

For the SLB2 transient NCT scenario, the model is comprised of the SLB2 with the SWB and drums inside. The SLB2 is assumed to be on the ground with the drums at the bottom of the SWB, which is in contact with the bottom of the SLB2. The boundary conditions applied to the outer surface of the SLB2 were the same as those for the TRUPACT-III transient NCT, except in this case the run lasts 48 hours instead of 24 hours (see

Table 10). Although the SLB2s are typically painted white, the emissivity of the outer skin was also conservatively assumed to be 0.25. Again, all surfaces are assumed gray and diffusive.

5.4. SLB2 Fire

The SLB2 Fire includes the glass micro-bubble insulation with the SWB with three drums inside. The SLB2 is assumed to be on the ground of the underground facility with the drums at the bottom of the package.

The SLB2 Fire scenario starts with in-shade conditions, i.e., the package is exposed to steady-state ambient temperature of 38 °C and no insolation. The results from this initialization run provide the initial temperature conditions for the SLB2 Fire.

During the fire portion of the SLB2 Fire simulation, the top and side external surfaces of the SLB2 were exposed to a five-minute ramp from 38 °C to 800 °C, a five-minute constant 800 °C, and a five-minute ramp down from 800 °C to 38 °C thermal radiant heat environment with a “sooty fire” characteristic emissivity of 0.9 (based upon fire testing experience at Sandia). The bottom of the package was assumed to be insulated by the ground. The internal boundary surfaces are the same as those applied in the transient NCT, except thermal radiation between internal surfaces was included in addition to assuming perfect contact between mating surfaces. Thermal radiation boundary conditions were applied over the internal surfaces of the SWB, the external surfaces of the drums, the internal surfaces making up the head space of the drum, and the top surface of the remediated salt. The emissivity of the internal SWB steel surfaces was assumed to be fixed at 0.8, and the emissivities of the drum and remediated salt surfaces were assumed to be 0.8. The drum walls are typically coated with gray or black paint, which typically have an emissivity of at least 0.8. The remediated waste surfaces were assumed to also have this value, as is common for most nonmetal surfaces. Considering interaction between these surfaces results in four radiation enclosures.

An initial five-minute temperature rise was employed to minimize solution errors. The same length of time was used for the temperature decay back to in-shade conditions (i.e., down to cool-down

conditions). During the subsequent cool-down transient, the external boundary conditions of the SLB2 are returned to their initial in-shade conditions, except for external surface emissivity, which is assumed to have risen to the emissivity of oxidized steel, 0.6, during the fire. In total, the SLB2 Fire lasts 15 minutes. The additional 10-minute transient time is equivalent to an additional 5 minutes of 800 °C heat input to the package. The total liquid fuel (diesel) required to maintain such a fire is around 500 gallons. Recall that an underground fire is not expected to be fully engulfed or last more than 5 minutes given the limited amount of fuel available in the underground at WIPP. The 20-ton diesel fork-lifts used to transport the SLB2s have a capacity of 50 gallons of diesel fuel and 64 gallons of hydraulic fluid [8], so the 500 gallons necessary to achieve the analyzed fire is very conservative.

6. SIMULATION RESULTS

The results presented in this section show temperature contour plots of the interior of the package and the drums. Some of the contour plots for the transient runs represent peak temperatures observed. Where necessary, time series plots of key areas in the drum are shown to clarify results. All the simulations were performed using the ANSYS Mechanical 2023 package.

6.1. TRUPACT-III Transient NCT

Figure 5 shows a contour plot of the cross section of the TRUPACT-III after 12 and 24 hours. As observed in Figure 5(a), maximum temperatures on the package occur on the outer top skin after 12 hours, when the transition to no insolation begins (i.e., start of nighttime exposure). The maximum predicted temperature on the top of the package is 147 °C. Over the next 12 hours the heat absorbed during the initial 12 hours continues to transfer inward, as shown in Figure 5(b). After 24 hours, the maximum temperatures are just below the skin of the package, and far from where the closest drum is located. The highest temperatures on the perimeter of the package affecting the drums occur closer to the bottom of the package, near the axial ends of the package, because the bottom section of the TRUPACT-III octagonal ends (see lower right corner of each image) are flat and assumed to be exposed to insolation during the initial 12 hours. Although the temperatures in this region are considerably less than on the top, the distance from this region to the bottom of the drum is less.

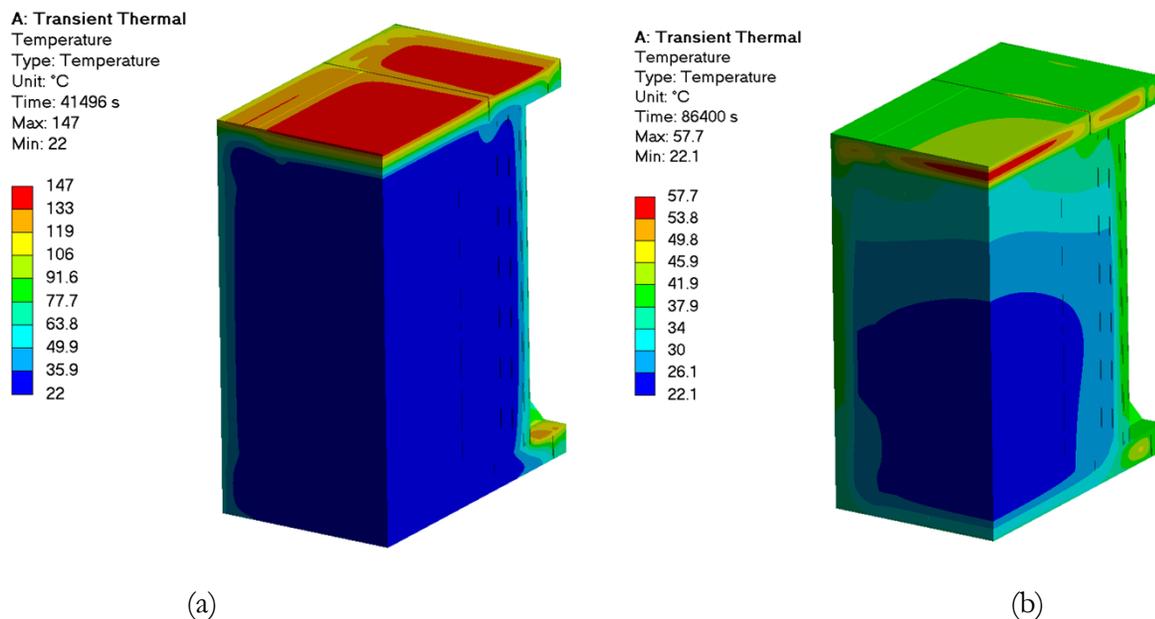


Figure 5. Contour plots of TRUPACT-III transient NCT: (a) 12 hours and (b) 24 hours.

Figure 6 shows the minimum, maximum, and average temperatures in the RNS waste. Consistent with the above description, the highest temperatures in the drum (24.3 °C) were observed near the bottom perimeter of the waste, while the lowest were found on the top center of the waste. Figure 6 shows that the drum reached peak temperatures at the end of the 24 hours (86,400 seconds). The overall increase in temperature of the waste is very small, the maximum temperature being less than 2.5 degrees greater than the initial temperature of 22 °C.

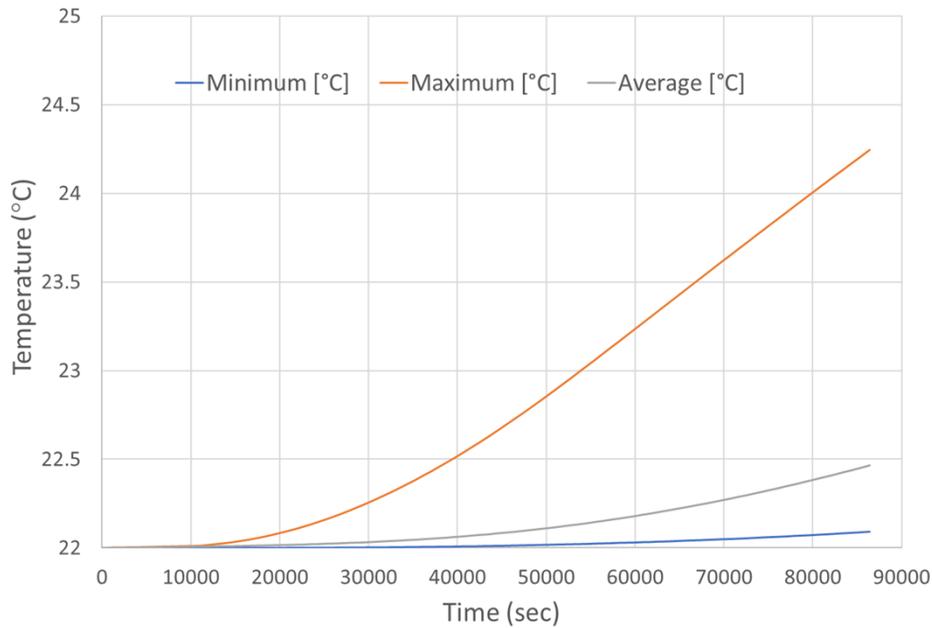


Figure 6. Predicted minimum, maximum, and average temperature of waste in the drum in the transient TRUPACT-III NCT

6.2. SLB2 Transient NCT during Above Ground Storage

Figure 7 shows the contour plot for the 48-hour transient NCT at the end of the second period of insolation (36 hours, or 1.2628 E+5 seconds). The peak temperatures in the skin are higher than the TRUPACT-III transient NCT because in this case the solar insolation is impinging directly on the SLB2, resulting in more heat absorption into the package. The highest temperatures in the SLB2 are on the top and around the sides, as expected because these are the areas affected by insolation.

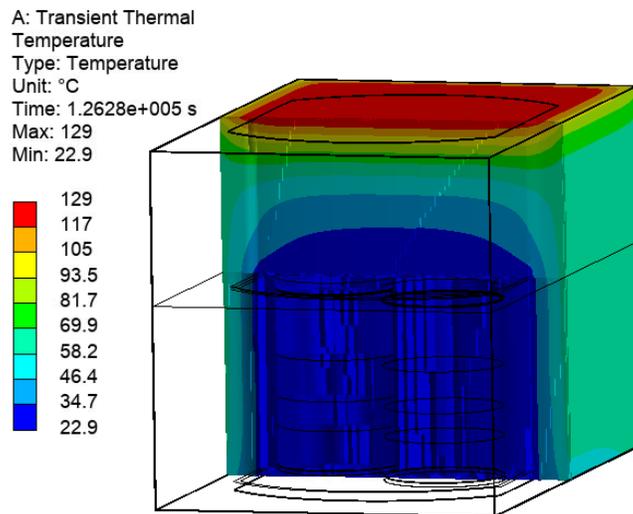


Figure 7. Contour plots of SLB2 after 36 hours of transient NCT.

Figure 8 shows a contour of temperatures in the drum waste at the end of the 48-hour transient, which does not include the head space above the waste. Peak temperatures are just below 30 °C on

the bottom of the waste. Note that at these temperatures the contribution of chemical heat generation is negligible.

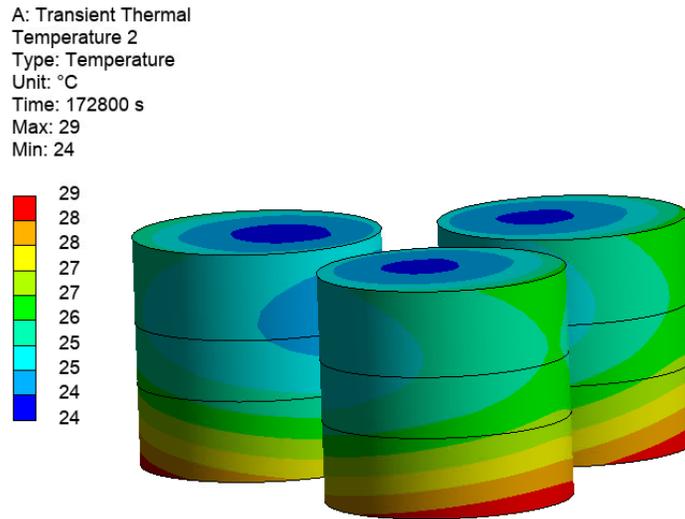


Figure 8. Temperature contours on waste sections of the drum for the 48-hour transient NCT.

6.3. Initial Conditions for SLB2 Fire

The contour plots shown in Figure 9 correspond to steady-state storage conditions of the SLB2 with no insolation. Maximum temperatures are just five degrees above the ambient temperature (38 °C), since at these low temperatures only the 21.5W/m³ of decay heat spread over the volume of the remediated waste contributes to heating of the drums; the chemical heat generation is still negligible, as noted in Figure 4.

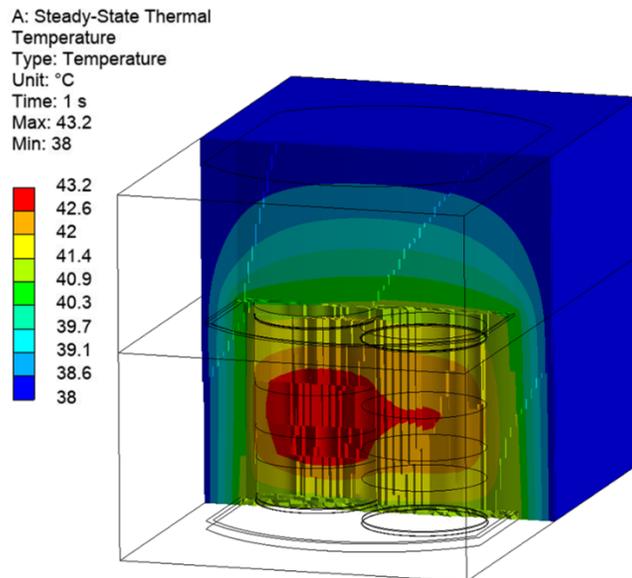


Figure 9. Contour plots of SLB2 under steady-state in-shade conditions

6.4. SLB2 Fire

Figure 10 shows contour plots of the SLB2; the top figure shows when the SLB2 has reached peak temperature on its external surface (at the start of the ramp-down to ambient temperature), and the bottom figure shows temperatures just when the fire is out (i.e., air temperature is back to 38°C ambient temperature). Both figures show there are very high gradients all along the perimeter of the SLB2 (peak temperature of 800 °C on the outer surface at the end of the 800 °C fire and 408 °C just inside the upper corners of the SLB2 at the end of the fire ramp-down) but not near the SWB due to the very low thermal conductivity of the glass micro-bubbles. Figure 11 shows the maximum temperatures in the SLB2 and within the waste during the cooldown. The highest temperature in the drums converge with the maximum temperatures slightly below 44 °C. This temperature is less than 1 degree above the maximum initial temperature shown in Figure 9, suggesting the waste never truly feels the fire effects. Again, at this peak drum temperature the chemical heat generation is negligible. These results show that the drum temperatures are significantly below the temperature (60 °C) defined to preclude thermal runaway [2].

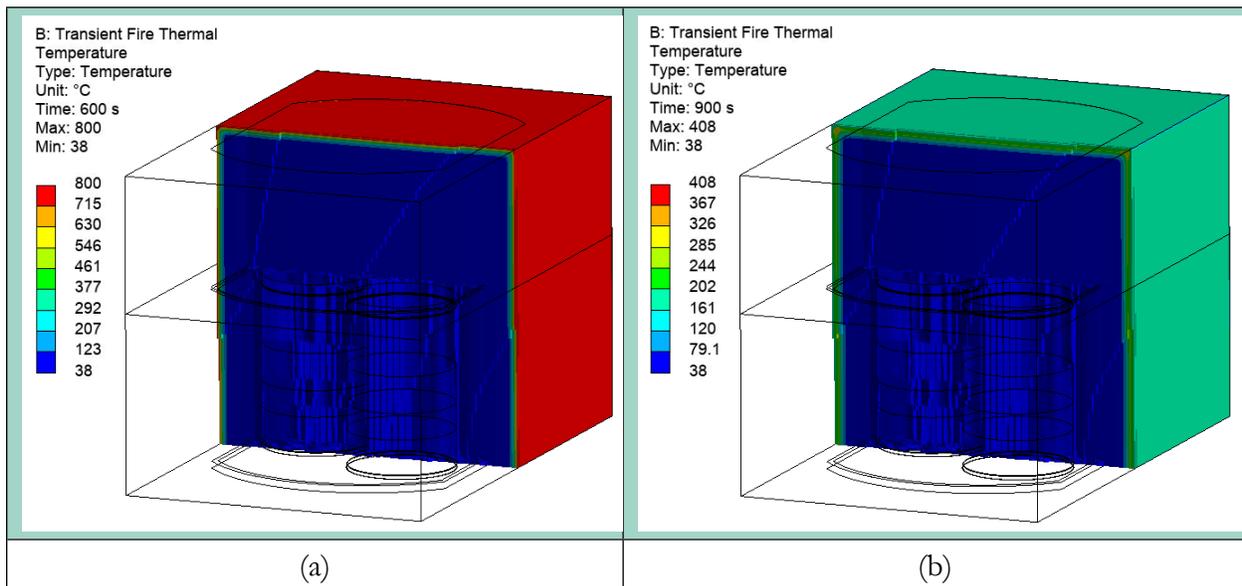


Figure 10. Contour plots of SLB2 under (a) SLB2 Fire peak and (b) SLB2 Fire end.

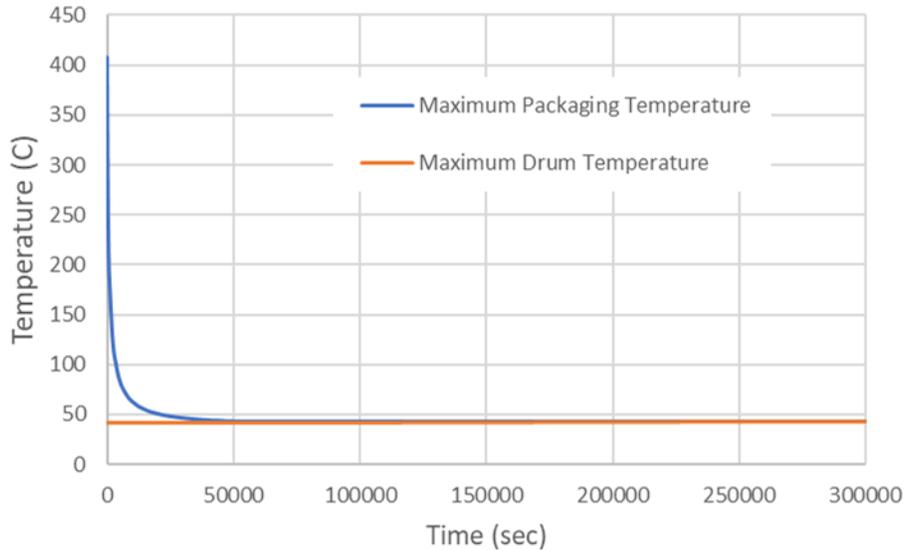


Figure 11. Maximum temperatures on the packaging and the drums

6.5. Discussion of Results

The scenarios explored here considered consequences to the drums while inside a transportation package or in a storage/disposal configuration. The configurations analyzed in this report are based on a design proposed by DOE EM/LA using information learned from previous analysis (i.e., SWB inside a TRUPACT-II during transportation and SWB in storage). At the start of this effort, it was believed that a three-layer configuration (SWB inside an SLB2 inside a TRUPACT-III) during transportation and the two-layer configuration (SWB inside an SLB2) during storage, with additional insulation provided by glass micro-bubbles between the SWB and SLB2 in both configurations, would provide thermal protection of the RNS waste and mitigate risk of thermal runaway reaction.

The initial temperatures inside the drum were assumed to be either 22 °C (transient NCT) or 38 °C (SLB2 Fire). The 22 °C used in the NCT runs is based on estimated temperature of the Perma-Con® building at WCS where the SWB is stored prior to loading it into the SLB-2 and TRUPACT-III. These temperatures would effectively bound the expected operational temperatures over most of the year. The initial temperature (38 °C) used in the fire run is based on an upper bound of temperatures recorded in WIPP. All the scenarios explored assumed there are no other external heat sources nearby in storage or transportation, such as other waste packaging or equipment operating at a higher temperature than these initial temperatures.

Under all the configurations and conditions analyzed, the results demonstrate the combination of the SLB2-SWB packaging with air-filled glass micro-bubbles prevents the drums from exceeding a temperature (60 °C) which precludes chemical heat generation runaway [2]. It is not expected that the SLB2 will be exposed to insolation for more than 24 hours and it would take many additional days for this configuration to reach a steady-state temperature.

For the underground fire, the inner drum temperatures remained near the imposed ambient temperatures before the fire started. It would take significantly more energy to have an impact on the interior temperature of the drum. Note that during the cool-down most of the energy absorbed in the outer perimeter of the packaging is expected to diffuse back to the surface because of the higher internal thermal resistance rather than to continue penetrating the package.

For the fire, it was assumed that the package is fully engulfed for a period of 5 minutes with 5-minute ramp-up and ramp-down periods. In terms of energy input, the initial and final 5-minute burn time are equivalent to an additional 5-minute burn time at 800 °C (total of 10 minutes of equivalent full engulfment). The amount of fuel (e.g., diesel) required to produce this 15-minute burn is approximately 500 gallons. Underground the most fuel available is from the 20-ton diesel powered forklifts used to transport waste, which are reported in Ref [8] to contain at most 114 gallons of diesel fuel plus hydraulic fluid, which is less than one fourth the amount of fuel used for the fire calculation. While there are other sources of fuel underground, administrative controls assure this fuel would not be collocated with SLB2 and forklift during transport. Further discussion in this reference suggests that it would be highly unlikely to have a fully engulfing fire that's longer than 5-minutes at WIPP. Thus, based on information available, it is believed the fire duration used for this analysis is very conservative. Moreover, underground pool fires at WIPP are typically modeled, according to DOE-STD-5506-2007, as short duration events lasting approximately 70 seconds, which is much shorter than the temperature profile used in these calculations.

A key assumption in the underground fire is that the SLB2 is on the ground where it's impossible for flames to affect the underside of this packaging. It is believed that a 5-minute fire with flames impinging on the underside of the SLB2 poses the greatest threat to a thermal runaway under the proposed configuration because there is very little insulation between the outer bottom surface of the SLB2 and the drum. Fires sufficiently large to fully engulf the SLB2 usually have an oxygen starved dome, where gases are relatively cool compared to flame temperatures. Typical flame temperatures on the lower portion of the SLB2 are less than that postulated in these runs. To mitigate this risk, it is recommended that the SLB2 be transported in storage as low to the ground as possible and stored on the ground to prevent flame from impinging the bottom of the SLB2.

7. SUMMARY

Three thermal exposure scenarios were postulated to explore the feasibility of transporting the RNS waste from WCS to the WIPP site and emplacing it within the mine. The scenarios span exposure conditions that are conservative with respect to actual operational conditions. In all cases, it is assumed the SLB2 contains an SWB containing RNS waste drums, each with radioactive decay heat no greater than 21.5 W/m^3 and including the possibility of energy being released from exothermic chemical reactions via an Arrhenius model. Additionally, the space between the SLB2 and the SWB was filled by a layer of insulation consisting of air-filled glass micro-bubbles. This arrangement provides one additional insulation barrier.

The predictions obtained from simulating the three exposure scenarios revealed that adding the SLB2 and the air-filled glass micro-bubbles to the transport and storage configuration provides additional thermal protection of the drums beyond what the SWB provides alone, both during long-term above ground insulation and underground during a fire accident. All the simulated scenarios indicated drum temperatures below the temperature ($60 \text{ }^\circ\text{C}$) defined to preclude thermal runaway [2].

Based on the simulation predictions, it is asserted that there is adequate margin to safely transport and place the RNS waste from WCS to the WIPP. Under the current transportation/storage/disposal concepts, the degree of protection provided by the packaging concept is sufficient to prevent the waste from being ignitable.

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