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IMPROVED MODELS FOR FOAM DEGRADATION DURING THERMAL HYPOTHETICAL ACCIDENT CONDITIONS

Sarah Suffield
Pacific Northwest National Laboratory,
Richland, WA, USA

James A. Fort
Pacific Northwest National Laboratory,
Richland, WA, USA

ABSTRACT

Current practice in Safety Analysis Report for Packaging (SARP) thermal analysis for hypothetical accident conditions (HAC) of packages is to not explicitly model the consequence to the foam impact limiting material, but instead to make conservative estimates of those consequences and begin calculations from that point. This approach is typically used for the foam regression distance, which is the thickness of the degraded foam layer after the 30-minute fire event. Estimates for regression distance can come directly from package burn test results or from correlations based on one-dimensional testing by the foam manufacturer. In either case this is a subjective process and, although it can be used to produce a conservative result, it is a significant approximation in the analysis.

This paper describes testing and refinement of a simplified foam regression model. Comparisons are made against available data from laboratory experiments. Model refinements were tested until satisfactory agreement was achieved. The final modeling approach was then compared with post-test inspection results from HAC burn test data. A new model with an effective thermal conductivity based on foam to char density variation was shown successful in representing laboratory scale foam thermal degradation experiments and full-scale burn tests of a current package. This model offers a technically defensible and predictive approach for modeling thermal degradation of rigid polyurethane insulation in transport packages.

INTRODUCTION

It would be beneficial to move toward a more predictive modeling strategy for foam property change under HAC thermal conditions to provide a more accurate and defensible analysis result. A detailed investigation of rigid polyurethane foam behavior in fire conditions was conducted by Sandia National Laboratories (SNL) from 1995 to 2000. This work was documented in a series of reports and conference papers, culminating with a summary journal article which discussed select experimental measurements and a comparison with model predictions (Hobbs, Erickson, and Chu, 2000). Laboratory tests included foam recession in a simple one-dimensional experiment consisting of a cylindrical foam test sample that was subjected to a heat flux at one end representative of fire conditions (Chu et al. 1995). In subsequent experiments, a stainless-steel dummy component was embedded in the same foam geometry (Chu et al. 1999). SNL developed detailed numerical models that were validated against the laboratory experiments. While these models accurately represented measured temperatures and rate of foam regression in the SNL experiments, the models are complex and not practical for Safety Analysis Report for Packaging (SARP) calculations.

For SARP purposes, a less-detailed modeling approach is desired that still provides reasonable predictive accuracy for the foam-char boundary. Initial results from a simplified model of the 9977 burn test (SRNL 2006) suggest that acceptable results may not require such detail. Model results gave a reasonable match with foam regression observed in 9977 post-test inspections. However, the modeling approach needed further evaluation to determine its applicability to other packages.

This paper describes testing and refinement of a simplified foam regression model. Comparisons are made against available data from the SNL experiments. Model refinements were tested until satisfactory agreement was achieved. The final modeling approach was then compared with post-test inspection results from the 9977 burn test data.

ANSYS FOAM DEGRADATION MODEL – SNL EXPERIMENT #1

An ANSYS APDL model was constructed to simulate the first in the series of SNL experiments investigating the degradation of rigid polyurethane foam when exposed to a fire (Chu et al. 1995). The experiment placed a foam sample in a cylindrical test vessel and exposed it to a simulated fire condition by heating the bottom of the test vessel to 1283 K (1850°F) using a radiant heat source (Figure 1). Provision was also made in this test to pressurize the system, but only the ambient pressure data is of interest here. General Plastics Last-A-Foam FR3706 was used for the foam sample. This foam has a density of 6 lb/ft^3 (96 kg/m^3). Thermocouples embedded in the foam sample captured the thermal response of the foam. The number associated with each temperature curve in the plot is the thermocouple location (in mm) relative to the surface of the foam sample.

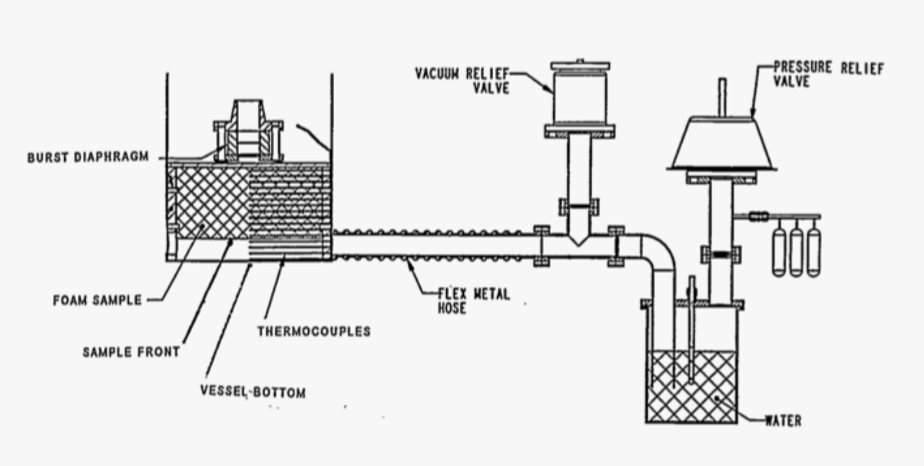

Figure 1. Experimental configuration used in Chu et al. 1995 (this is Fig. 1 in that reference)

Initial Model

The model geometry was constructed using the commercial CAD program SolidWorks, and then imported into the utility ANSYS Mesh. A discretized form of each solid region and each interior gas space was generated. A conformal interface was established across all internal boundaries between parts, which constitute shared nodes along any part-to-part boundary. The left side of Figure 2 shows a cross-sectional view of the CAD geometry. The foam is shown in green, the stainless-steel canister is shown in gray, and the gap region between the foam and canister base is shown in yellow. The gap region is filled with air. The right side of Figure 2 shows a cross-sectional view of the mesh. The mesh contains hexahedral and wedge elements.

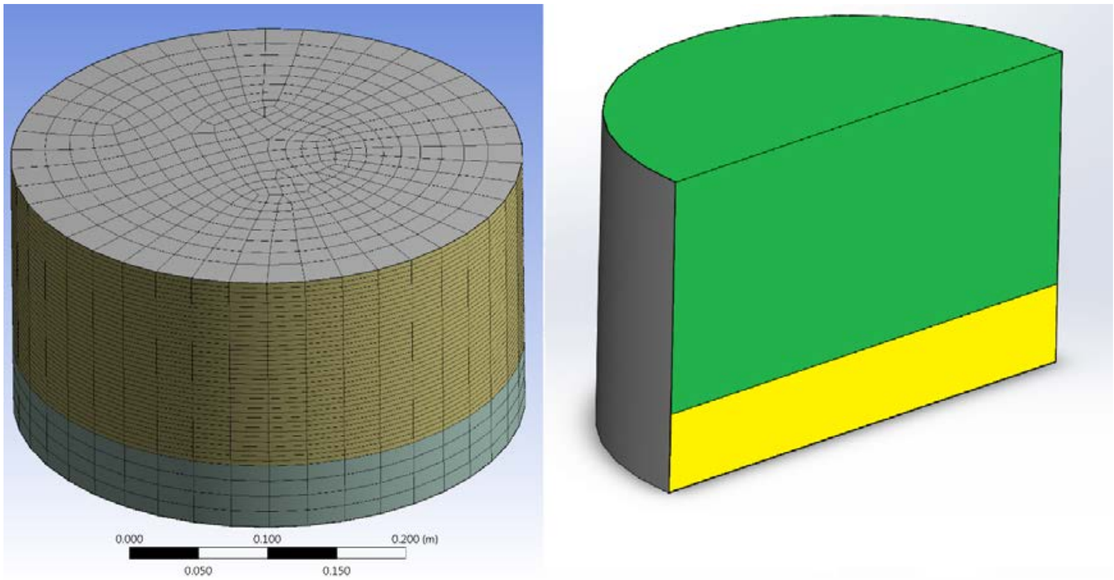

Figure 2. Overall and cross-sectional view of the canister assembly mesh

Free convection to ambient air from external surfaces of the canister and foam was calculated using natural convection correlations from the *Handbook of Applied Thermal Design* (Guyer, 1989) for the following surface geometries:

- Vertical cylinder (cylindrical sides of canister outer shell).
- Horizontal surface upward facing (top of canister, top of foam).

Thermal radiation between the environment and canister was also included in the model. An ambient temperature of 60 °F (15.6 °C) was applied at all exterior environment nodes. Internal surface-to-surface radiation was included for the air cavity region within the model using radiation matrices with view factors created by ray-tracing. The emissivity values were applied along the exposed surfaces within the air region.

A transient analysis was run treating the foam region as a simple solid material with no thermal degradation. At the start of the analysis an 1850 °F (1283 K) temperature boundary was applied along the bottom surface of the canister. This was to simulate the radiant heat source applied along the base of the canister. The heating phase of the experiment lasted for 1320 seconds (22 minutes). After 1320 seconds the temperature boundary along the base of the canister was changed to a natural convection boundary with thermal radiation to the surroundings and the transient analysis was continued out to 2000 seconds to capture the cooldown of the experiment.

The resulting predicted temperatures from the initial ANSYS model for the heated part of the transient are shown in Figure 3. The predicted temperatures are very different from the measurements, both in magnitude and rate of increase. Clearly, a more detailed model of the foam is required.

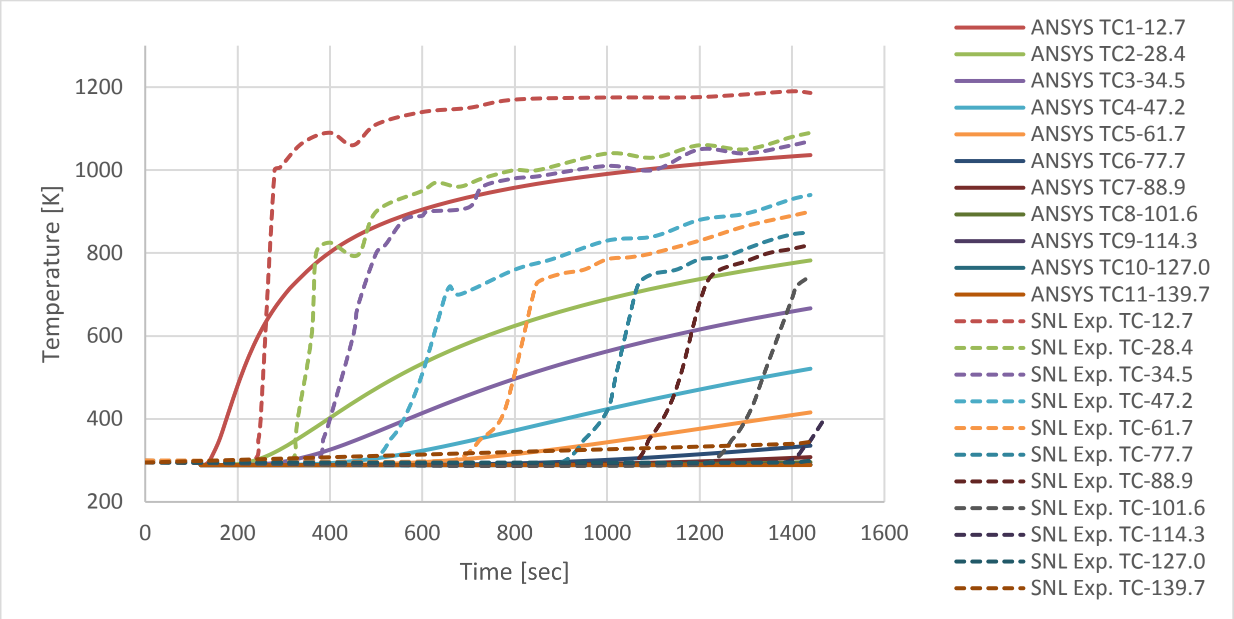

Figure 3. Thermocouple response compared to predicted temperatures – initial ANSYS model

Char Model with Default Parameters

For this case, the initial ANSYS model was modified to include conversion of the virgin foam to char as the foam heats up. The Last-A-Foam FR-3700 series foam was developed to form an intumescent char which prevents smoldering of the foam and provides a high level of thermal protection (General Plastics, 1991). The decomposition with temperature is represented in the thermogravimetric analysis results shown in Figure 5. The curve for a nitrogen environment is representative of the inert conditions inside a vented package. For the char model the foam elements are replaced with char once the elements reach a 600 °F temperature limit. At each timestep the model looks at the temperature for each element within the foam, and if the element temperature is greater than 600 °F (315 °C) the element material is changed to a char.

The material properties of char are based on a generalized pyrolysis model for combustible solids, including charring solids described by (Lautenberger & Fernandez-Pello, 2009). Their pyrolysis model uses the following equations for the bulk density, specific heat, and effective thermal conductivity of the condensed species:

Effective Density $\rho_{eff} = \rho_o \left(\frac{T}{T_r}\right)^{n_p}$ Eq. 1

Effective Specific Heat $c_{eff} = c_o \left(\frac{T}{T_r}\right)^{n_c}$ Eq. 2

Effective Thermal Conductivity $k_{eff} = k_o \left(\frac{T}{T_r}\right)^{n_k} + \gamma\sigma T^3$ Eq. 3

Where;

T = temperature
T_r = reference temperature (usually 300K)
σ = Stefan Boltzmann constant

The authors present coefficients for condensed phase species resulting from pyrolysis of an intumescent coating. The values for char are shown reproduced in Table 1. Using the values for char listed in Table 1 and equations 1 through 3, the effective char properties were calculated for the ANSYS model. The effective thermal conductivity was calculated using the average char element temperature.

Table 1. Condensed phase parameters for intumescent coating simulations, from (Lautenberger & Fernandez-Pello, 2009)

Char						
K_o [W/mK]	n_k	P_o [kg/m^3]	n_p	C_o [J/kgK]	n_c	ϒ [m]
0.041	0.441	17.4	0	1640	0	0.003

Results for the ANSYS "char" model are shown in Figure 4. Adding the foam degradation model improved the response of the foam at the two thermocouple locations nearest the heated surface, but temperatures at more deeply embedded thermocouple locations lag significantly behind the measured values.

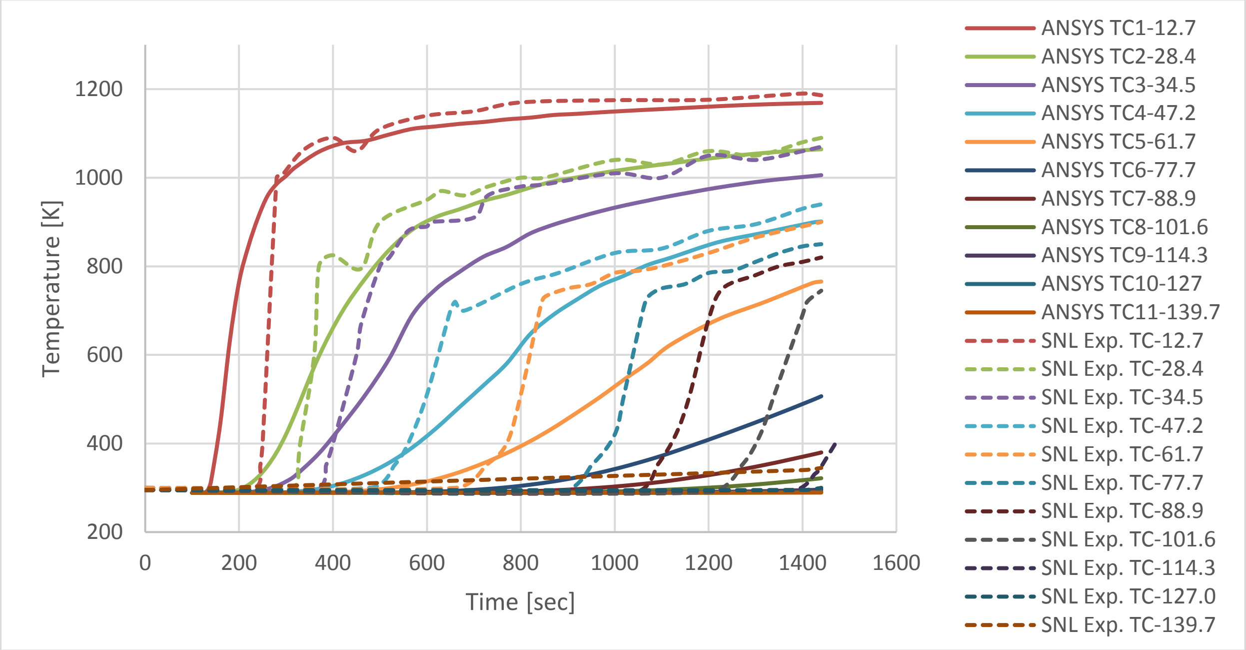

Figure 4. Thermocouple response – "char" ANSYS model

Char Model with Variable Gamma

In porous media at higher temperatures, one example being fiber insulation (Litovsky, et al., 2008), thermal radiation can become the dominant mode of heat transfer. This behavior should be expected for the char layer. The second term given in equation 3 (for effective thermal conductivity) accounts for radiation heat transfer across pores. The leading coefficient on that term, γ (gamma), is used by Lautenberger & Fernandez-Pello (2009) as a material dependent constant. To model the expected increase in thermal radiation through the pore space from a relatively dense virgin foam to a less dense char, a variable gamma formulation is proposed.

The ANSYS "char" model was modified to incorporate a variable γ term in equation 3 for the effective char thermal conductivity. The assumption made here is that γ should increase as the foam solid phase breaks down and the char becomes more porous, which should coincide with the decrease in material density. Figure 5 plots the change in weight percent of foam as a function of temperature.

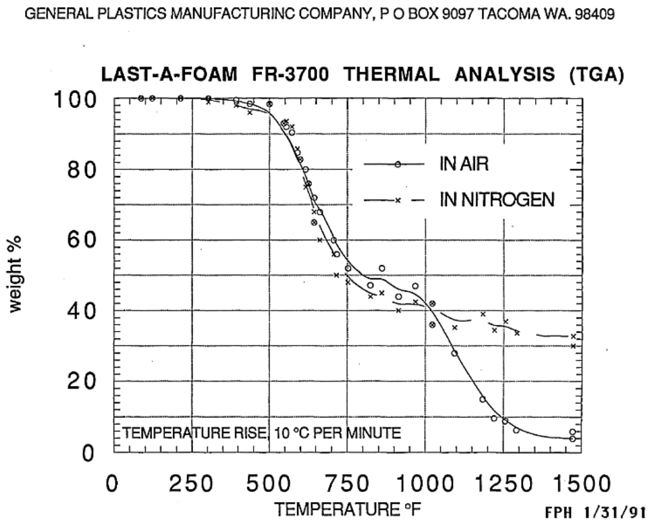

Figure 5. Last-A-Foam FR-3700 thermogravimetric analysis (General Plastics, 1991)

Using the "in air" data shown in Figure 5, the curve shown in Figure 6 was constructed by subtracting the weight fraction from 1 and scaling the resulting value to be consistent with the γ value listed in Table 1 (0.003). Subtracting the weight fraction of foam by 1 represents the fraction of void space within the foam, with a value of 1 representing no foam left. The void fraction curve was scaled to a γ value of 0.003 by dividing the void fraction by 100. This resulted in a value of 0.003 at 600 °F. Since the description of the TGA noted that at 600 °F the entire surface of each foam sample was covered with a continuous char (General Plastics, 1991), a value of 0.003 at 600 °F seems reasonable.

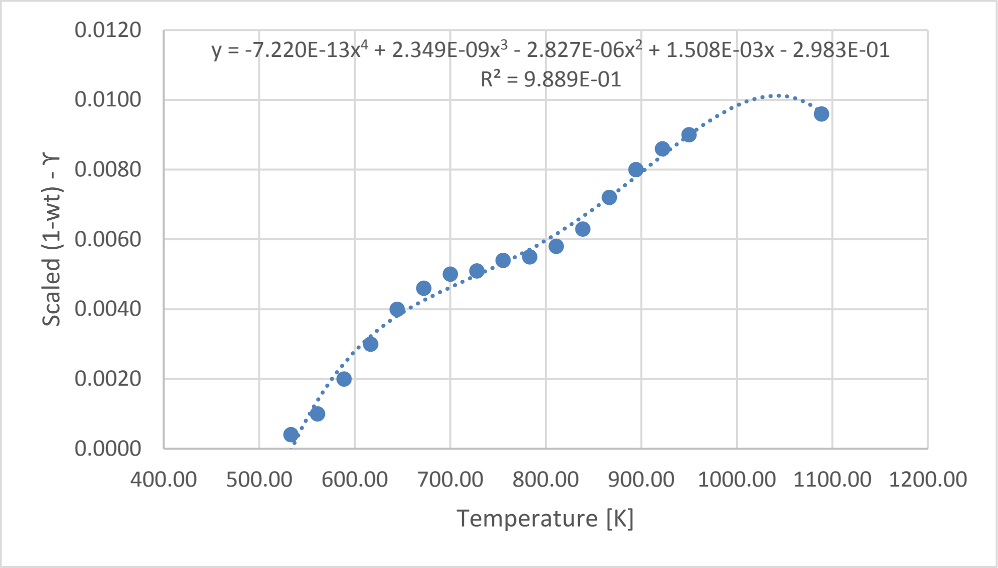

Figure 6. γ as a function of temperature

The equation listed in Figure 6 is a 4th order polynomial fit to the plotted gamma term and was used in the ANSYS simulation to calculate γ for the effective char thermal conductivity at each timestep. The value of γ and the resulting effective char thermal conductivity (Eq. 3) are both dependent on the temperature, which was calculated as the average temperature of the char elements. To avoid smearing an average effective thermal conductivity across all char elements, the char was split into three different layers within the ANSYS model. Ideally the effective thermal conductivity of the char would be calculated for each element based on the element temperature, but this would not be practical to implement because a unique material number would have to be created for each char element. A foam element was flagged as a char layer if the element temperature fell into one of the following temperature ranges:

- Char Layer 1: 600 °F (315 °C) < element temperature < 750 °F (400 °C).
- Char Layer 2: 750 °F (400 °C) < element temperature < 950 °F (510 °C).
- Char Layer 3: 950 °F (510 °C) < element temperature.

The temperature limits were chosen based on the three observed sections that make up the curve shown in Figure 5. The effective thermal conductivity for each char layer is calculated based on the average temperature for that layer. Results for the modified ANSYS "char with variable γ" model is shown in Figure 7.

The temperature results in Figure 7 compare reasonably well with the experiment results. Probes further away from the heat source (TC8-TC11) under-predicted the temperature compared to the measured results. However, it was noted that during the experiment the foam had moved downward during the test and was restrained by the thermocouple bundles. This downward movement would result in the thermocouples being closer to the heat source than in the model.

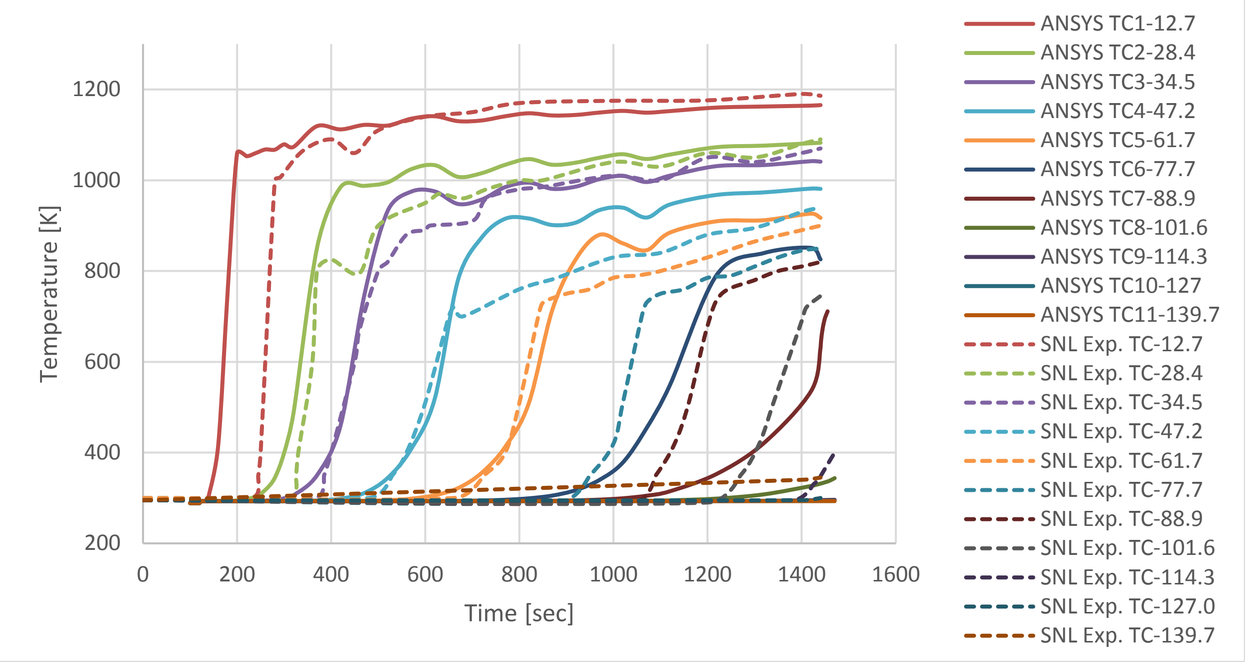

Figure 7. Thermocouple response – "char with variable γ" ANSYS model

CHAR MODEL APPLIED TO 9977 PACKAGE

The 9977 package was subjected to a series of burn tests to experimentally look at the thermal response of the package to a HAC fire (SRNL, 2006). The 9977 package is internally filled with a thick layer of Last-A-Foam FR-3716. Four test packages with FR-3716 foam were tested in the SRNL packaging burn test. A practice package with no Last-A-Foam was also burned during the experiment. The 9977 package geometry is shown in Figure 8, with the Last-A-Foam shown in blue.

During the burn tests, the package was equipped with temperature indicators at various locations within the package. Thermocouples were used to capture the flame temperature and the temperature at the outer surface of the package. Table 2 lists the recorded flame and package surface temperatures.

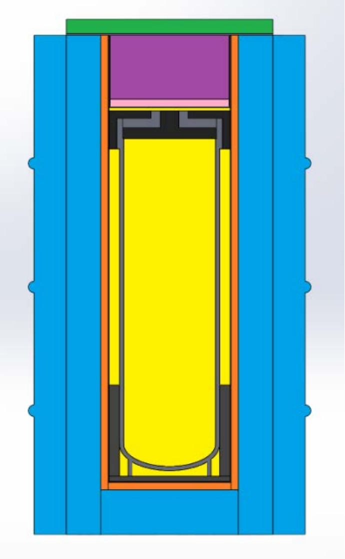

Figure 8. 9977 Package geometry – cross-sectional view through the center of the package

Table 2. SRNL packaging burn test – 30-minute temperature averages (SRNL, 2006)

Test	Package Number	Fire (°C)	Package (°C)
Practice	Practice Package	1014	889
Regulatory Test 1	SN-2	1023	968
Regulatory Test 2	SN-4	848	791
Regulatory Test 3	SN-5	866	995
Regulatory Test 4	SN-3	800	963

Both test packages SN-4 and SN-5 were tested in the vertical orientation with the bottom end of the package facing downward. An ANSYS APDL model of the 9977 package was constructed and subjected to a 30 minute fire in the same orientation as the test packages. The SN-4 package burn experienced fuel feed problems, but this was corrected for the SN-5 package burn test. Therefore, the ANSYS APDL model used the flame and ambient temperature from the SN-5 test to model the package burn experiment. Results from the ANSYS APDL model and comparisons with the measured data from SN-5 package are shown in Table 3. The resulting ANSYS APDL model temperatures compare reasonably well with the measured experiment temperatures.

Table 3. ANSYS APDL model temperature results compared with measured data for SN5

Temperature Indicator Location Description	**Temperature Indicator Label #**	**ANSYS Model**	**Measured Data**
		Tmax	**Tmax**
		[F]	**[F]**
Bottom of drum lid liner	1	390.29	420-435
Top of load distribution fixture	2	255.98	250-260
Side of drum lid liner	3	584.08	-
Bottom of cone seal plug	4	255.69	-
Top of cone seal nut	5	256.2	250-260

Inside CV - top of labels ~ even with bottom of cone seal plugs	6	255.31	< 250
Outside CV - top of labels ~ even with bottom of cone seal plug	7	255.28	< 250
Inside CV - center of labels at mid-point of CV length	8	220.39	< 250
Outside CV - center of labels at mid-point of CV length	9	220.5	< 250
Inside CV - center of labels at mid-point of load distribution fixture	10	224.41	< 250
Outside CV - center of labels at mid-point of load distribution fixture	11	224.94	< 250
Inside CV bottom	12	223.22	< 250
Inside bottom of drum liner	13	227.75	< 250
Inside drum liner - center of labels at mid-point of liner length	14	267.17	< 250
Outside CV - top	15 - Top	255.73	> 240
Outside CV - middle	15 - Middle	220.5	220-230
Outside CV - bottom	15 - Bottom	224.93	220-230

The SRNL experiment also did a post-fire examination of two of the packages, SN-2 and SN-3, to determine the amount of foam remaining after the HAC fire. The drum was opened, and all char was removed, leaving only the intact foam. It was determined that approximately 2.3-inches of foam remained around the drum liner and Fiberfrax after the HAC fire (SRNL, 2006). Figure 9 shows the foam remaining for the ANSYS APDL model after the HAC fire simulation. A ring of foam with a width of ~1.0 inches remains around the vertical sides of the thermal blanket for the model. There is no foam remaining on the underside of the thermal blanket. This indicates that the model predicted higher temperatures than the experiment and is a conservative representation of the foam degradation. One reason for this discrepancy between the model and experiment could be that in the experiment the package sat on a metal grill plate, which would have provided some shielding from the engulfing fire at the bottom of the package. This grate was not included in the ANSYS APDL model.

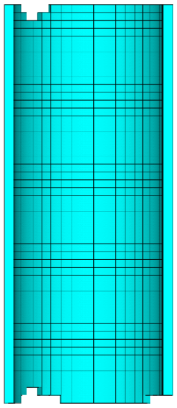

Figure 9. Remaining foam elements after the HAC fire and cooldown

CONCLUSIONS AND RECOMMENDATIONS

This study set out to find a predictive modeling strategy for rigid polyurethane foam material property changes under HAC thermal conditions, to provide accurate and defensible thermal analysis results. The major result and conclusion of this study are:

- A new model with an effective thermal conductivity based on foam to char density variation was shown successful in representing laboratory scale foam thermal degradation experiments and full-scale burn tests of a current package.

- This model offers a technically defensible and predictive approach for modeling thermal degradation of rigid polyurethane insulation of Office of Packaging and Transportation (OPT) transport packages.

It is recommended that comparisons with future package HAC thermal tests be conducted as these datasets become available. The DPP-3 is planned for a HAC furnace test in 2019 and this will be a good opportunity to compare model predictions with temperatures and foam degradation results.

ACKNOWLEDGMENTS

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