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Heat Transfer and Pressurization with Dynamic Radiation Enclosures for Thermally Decomposing PMDI Polyurethane Foam in a Sealed Container

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Abstract

Polymer foam encapsulants provide mechanical, electrical, and thermal isolation in engineered systems. In fire environments, gas pressure generation due to pyrolysis of polymers in fire environments can cause mechanical failure of sealed systems. In this work, dynamically changing radiation enclosures are added to an already existing decomposing PMDI-based polyurethane foam model. This addition to the model allows the foam to decompose and create a gas region based on a decomposition temperature. This new model is then compared to a baseline model and to experimental results in order to understand the effect of adding enclosure radiation.

Keywords

Pyrolysis, Heat Transfer, Polyurethane Foam, Radiation

Nomenclature

T	Temperature (K)

1 Introduction

Polymers and other organic materials have a long history of use in mechanical systems to provide mechanical, electrical, and thermal isolation. Accurately modeling organic materials in thermal environments can be challenging due to complex physics, uncertain thermal properties, and the relatively low decomposition temperatures. When polymers are exposed to a source of heat, such as fire, they undergo both physical and chemical changes [1]. The chemical breakdown, or decomposition, of the polymer causes large molecules to fragment, forming a variety of smaller molecules. These smaller fragments can vary greatly in size and properties and can undergo further decomposition. The chemical subspecies have differing equilibrium vapor pressures and those subspecies with the highest vapor pressures will quickly vaporize and in a sealed system can cause the container to pressurize. The subspecies that do not vaporize are left in either a liquid or solid form. While it is possible for a polymer to decompose completely into vapor, it is unlikely. Typically, solid residue is left behind and, in a material that chars, this layer can be porous. Due to the wide range of mechanical systems where polyurethane foam is used (e.g. automobiles, airplanes), it is prohibitively expensive to test all of these systems in multiple configurations to understand the foam's behavior in each case. Therefore, it is desirable to have a physics based computational model of the foam that can be used to examine multiple heating scenarios and physical configurations.

This work presents a discussion of experimental results as well as a comparison to experiments of a computational model for thermally decomposing polymeric methylene diisocyanate (PMDI)-polyether-polyol based closed cell polyurethane foam. The computational model, described in Erickson et al. [2]-[4], simulates organic material decomposition, heat transfer, and pressurization. This model has been validated against several sets of experimental data [5][6][7] and in these works it had been noted that the model would benefit from additional physics.

The prior model uses the radiation-diffusion approximation to model radiative heat transport through the pores of the foam by adding an effective conductivity contribu-

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tion to the heat conduction term of the equations. This approximation is based on the assumption of an optically thick medium. This assumption works well for the virgin foam material, and for certain foams that leave behind a stable char after the decomposition process [4]. However there is experimental evidence that PMDI does not leave behind a stable char, and validation work on the prior model suggests that this violation of the optically thick assumption causes significant model form error in some cases [5][7].

This current work is a first step at including additional physics into the model. While the radiation-diffusion approximation is still used to model radiative heat transfer through the virgin foam, enclosure radiation is used to model radiation through the gas. The enclosure is dynamically built as the foam reaches its decomposition temperature and the foam front regresses. The results from this form of the model are compared to the previous model as well as experimental results in order to assess the effect of adding the radiation enclosure.

2 Experiment and Simulation Design

The experimental data that is used for comparison is referred to as foam in a can (FIC). The experimental configuration consists of a stainless steel cylindrical container filled with foam along with an embedded metal object (Fig. 1). In this work, only experiments performed in the inverted orientations will be discussed (Fig. 2).

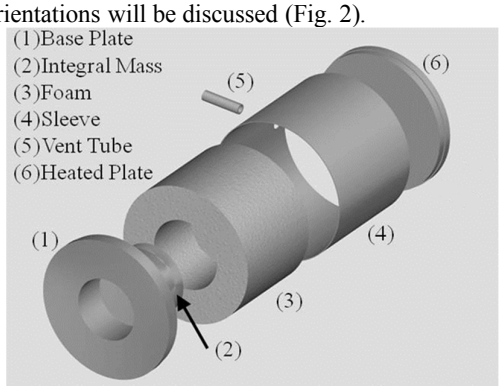

Fig. 1 Exploded view of the FIC geometry

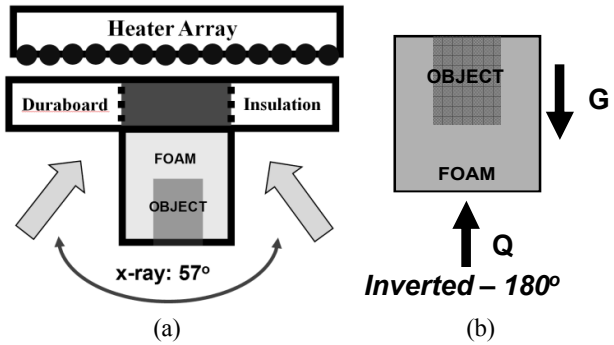

Fig. 2 (a) Experimental setup for the foam in a can experiment and (b) description of inverted heating

The sidewall of the container is seamless tubing, 8.89 cm (3.5 in) outside diameter and 1.60 mm (0.063 in) wall thickness. The heated plate was machined from SS304L, 10.8 mm (0.425 in) thick. The base plate was a similar thickness but included an embedded mass. The encapsulated SS304L mass was 4.45 cm (1.75 in) in diameter and consisted of a solid and a hollow end. The exterior surfaces of the can were painted with PyromarkTM 2500 series flat black paint to ensure consistent, uniform radiative properties. Foam samples are cast oversized and then machined to a snug fit in the container and around the encapsulated mass. The foam samples were polymeric methylene diisocyanate (PMDI)-polyether-polyol based polyurethane foam (PUF) with a density of approximately 320 kg/m3 (20 lb/ft3). Mass of the individual foam samples was documented and the range was 60 to 65g [5],[6].

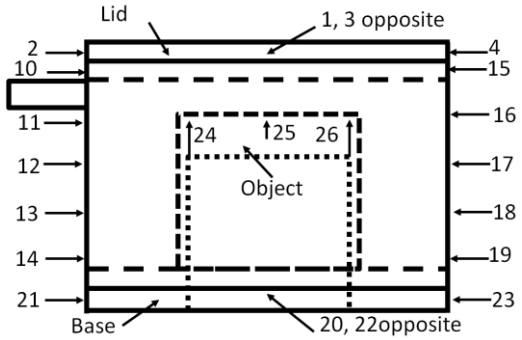

Fig. 3 Experimental setup of the foam in a can experiments, (b) the location of thermocouples

The can is heated by radiant heat flux from an array of silicon rod heaters directed at the lid of the can. The power to the silicon rod heaters is controlled to supply a specified ramp rate (50 K/min) to hold temperature of 1073K. Temperatures were measured during the experiment using K-type thermocouples (TC) mounted on the exterior of the can and by embedded thermocouples in the object, lid, and base (Fig. 3). A pressure transducer (Omegadyne pressure gauges model PX309) was used to measure pressure re-

sponse during the experiment. Measurement error on thermocouples and transducer was ± 2%. X-rays were also used to observe physical changes of the foam as a function of time throughout the experiment. This experimental test series yielded eight experiments, four each in the upright and inverted orientation. The experiment ended when the can breached due to pressurization of the can. Test to test variability was very small; as a result, only one of the experiments was selected for discussion in this paper.

A 3-D finite element model composed of tetrahedral elements was evaluated in the Sierra Thermal/Fluids [8] radiation-conduction code to computationally simulate the FIC experimental configuration. All parameter values used to model the reactions were determined from independent laboratory-scale experiments. These experiments were discussed in detail previously [2][3][4], [9][10][11]. Values for the foam specific heat and foam bulk thermal conductivity were obtained from published reports. Convective and radiative boundary conditions were applied to all sides with the exception of the heated surface, which has direct view of the heating rods and thermal radiation is the dominant mechanism for coupling of the heated surface to the energy source. The silicon rod heater radiation source is idealized as a uniform far field radiation source of time-varying temperature.

3 Computational Model

The computational model used in this work builds on prior foam decomposition models [2][3][4] by incorporating interface tracking and enclosure radiation to better model radiative heat transfer through regions where the foam has fully decomposed and not left a stable char behind. As in the prior work time dependent heat transfer through the foam is calculated by solving an energy conservation equation including storage, conduction, and heat of reaction terms. The decomposition kinetics are modeled using a multi-step Arrhenius rate reaction mechanism and ODEs for the amount of generated gas are solved throughout the domain. A user-defined subroutine calculates the pressure in the domain based on the amount of gas produced and temperature distribution. Further details of the reaction model and pressure calculation can be found in [2][3][4][5].

The novel contribution to the model in this work is the addition of an interface tracking method to divide the foam volume into two regions; one containing virgin foam, and one containing decomposed foam. In the virgin foam region we continue to use the radiation-diffusion approximation. In the decomposed foam region we assume that it is optically transparent and use a viewfactor based enclosure radiation calculation to model radiative heat transport between the exposed surfaces of the surrounding pressure vessel and the decomposing foam interface. The rest of the model remains the same between the virgin and decomposed regions.

In order to track the foam decomposition front we use the conformal decomposition finite element method (CDFEM) [12], [13] implemented in the Sierra Thermal/Fluids radiation-conduction code. In the CDFEM an isosurface of a nodal field is used to define the position of the interface, and the finite element mesh is locally refined to create faces that conform to that interface. A simple example of this refinement process is depicted in Fig. 4. The most physically justifiable interface definition for this problem would be to choose a threshold based on extent of the decomposition reaction. Unfortunately the model implementation solves the reaction ODEs at the integration points of the finite elements, and as a result there is no nodal field to use for the interface definition. Instead this work defines the interface based on the temperature field as the isosurface where $T = T_{decomp}$. The threshold temperature is used as a fitting parameter. Future work will use an extent of reaction based interface definition.

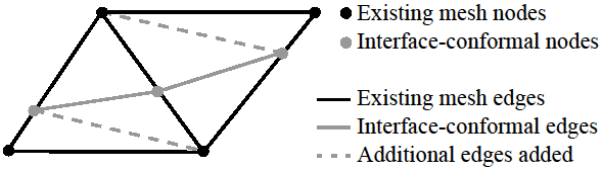

Fig. 4. Example decomposition of two linear triangle elements using CDFEM. Additional nodes are added at the interface location on the existing mesh edges. Interface edges are then added to connect the new nodes and create a surface that boundary conditions may be applied to. Finally, edges are added to divide any quadrahedra back into triangles.

4 Results and Discussion

The computational model, using a foam decomposition temperature of 600 K, is compared to the experimental results in Fig 5 through Fig 7. As seen in Fig 5, along the sides of the can, the model over predicts the experiment closest to the heated surface. There are several possible reasons for this. First, there is no contact resistance anywhere in the model. Second, the convective coefficient is constant for the entire side of the can, whereas in reality it varies with temperature. Finally, in the x-ray images it can be seen that there is a significant amount of pooling of liquid decomposition products as well as motion of gases. This would alter the heat transfer from the radiation-conduction model that was used and disproportionally affect the temperature nearer the heated surface.

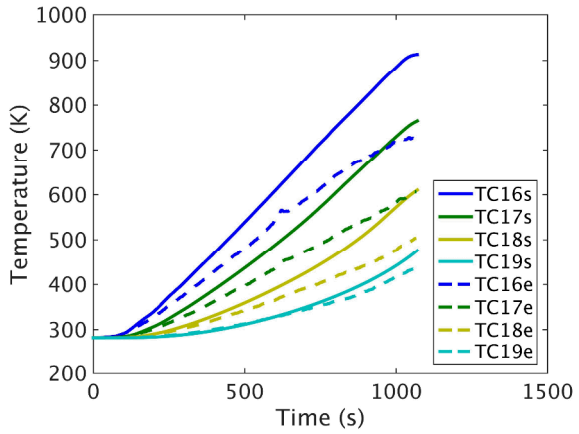

Fig 5 Comparison of simulations (s) and experiment (e) for one set of thermocouples on the side of the can.

Fig 6 compares temperatures on the embedded object between the experiment and simulation. The model predicts the temperature of the embedded object well, however it does not capture the slope changes at approximately 800 and 900 seconds. These slope changes are most likely due to unmodeled physics, such as the liquid decomposition products and gas phase motion.

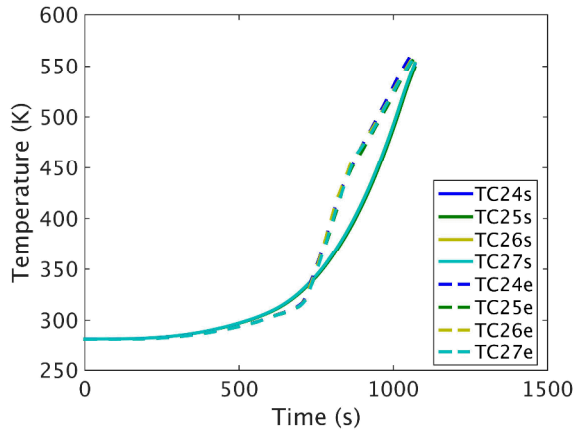

Fig 6 Comparison of simulations (s) and experiment (e) for the thermocouples on the embedded object.

The pressure response for the experiment and simulation are shown in Fig 7. Similar to the embedded object, the model predicts the pressure response relatively accurately. However, again, the model is not predicting slope changes, such the one seen at approximately 800 seconds.

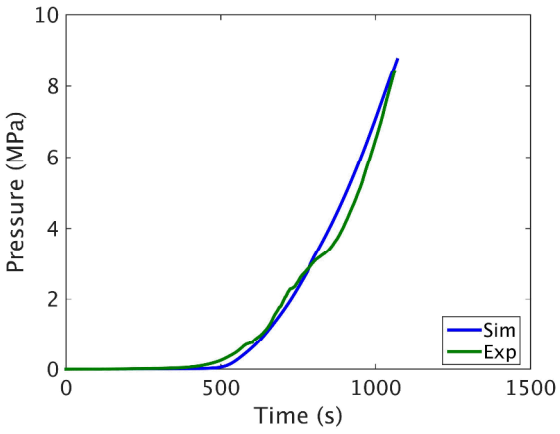

Fig 7 Comparison of pressure for simulation and experiment

Since the exact decomposition temperature of the foam is unknown, simulations with the decomposition temperature set at 550 K and 650 K were also run in order to understand the effect this would have on the result. Fig 8 through Fig 11 show the results of the three decomposition temperatures, the previous, baseline model (labeled NoCDFEM), and the experiment.

Fig 8 and Fig 9, which show thermocouples along the side of the can, show that the decomposition temperature does not have a large effect on the temperature response. However, including the enclosure radiation has a large response when compared to the baseline model. In the case of TC 16 (which is closest to the heated surface) the addition of the radiation enclosure causes the model to over predict temperature even more than it did with the baseline model. Fig 9 shows the inclusion of the radiation enclosure for thermocouple 19 (furthest from the heated surface) is an improvement over the baseline model, even though it over-predicts.

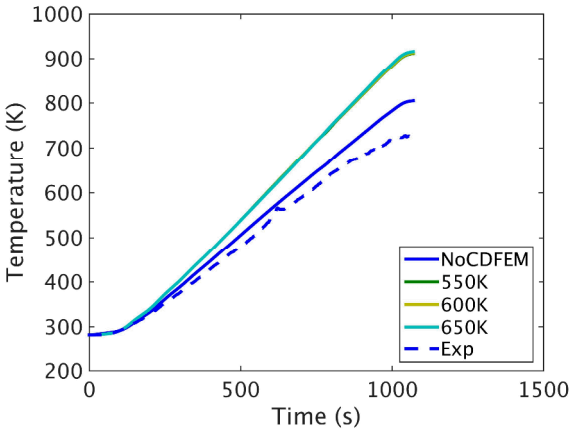

Fig 8 Comparison of three CDFEM decomposition temperatures (550K, 600K, 650K), the simulation without CDFEM, and the experiment for TC 16.

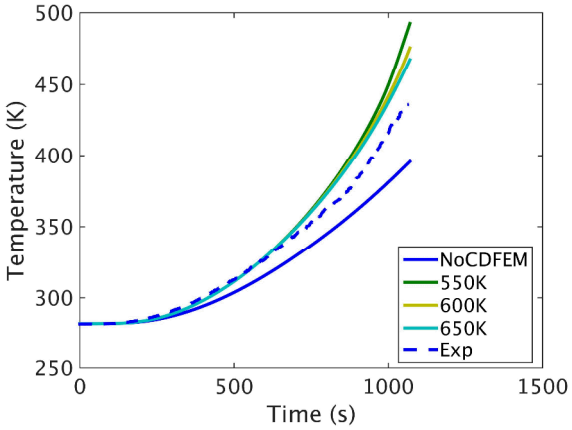

Fig 9 Comparison of three CDFEM decomposition temperatures (550K, 600K, 650K), the simulation without CDFEM, and the experiment for TC 19.

Fig 10 shows the temperature response for a thermocouple on the embedded object. Decomposition temperature has a stronger effect on this response than the thermocouples on the sides of the can. This is most likely because radiative heat transfer has a stronger effect than conduction for this location. Therefore when the embedded object is exposed to the radiation enclosure earlier (as occurs when the decomposition temperature is lowered), this location heats more over the course of the experiment.

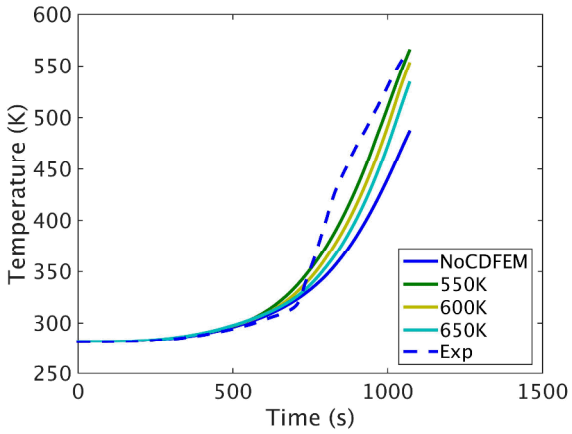

Fig 10 Comparison of three CDFEM decomposition temperatures (550K, 600K, 650K), the simulation without CDFEM, and the experiment for TC 24.

Pressure showed the largest response to altering the decomposition temperature, as shown in Fig 11. As the decomposition temperature increases, so does the pressure response for a given point in time. This is because as the decomposition temperature is raised, the amount of foam that is decomposed (and therefore the volume of the gas) is less. The ideal gas law therefore states that the pressure of this gas will be higher for the same temperature.

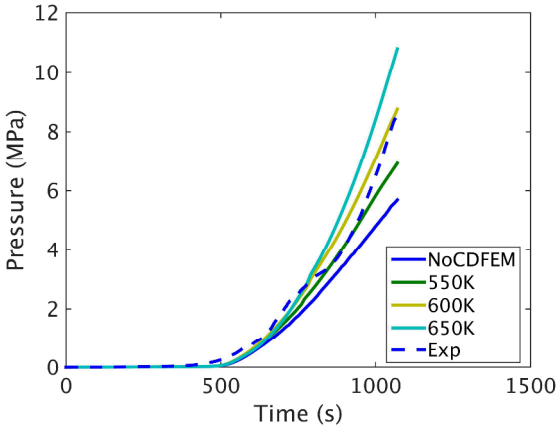

Fig 11 Comparison of three CDFEM decomposition temperatures (550K, 600K, 650K), the simulation without CDFEM, and the experiment for pressure.

5 Conclusion

Pressure and temperature responses from an enhanced computational model and experimental dataset were examined for the foam in a can apparatus. These responses were then compared to both the base line model and to experimental results.

Based on the inconsistencies between the model and the experiment discussed throughout this paper, a model with additional physics beyond the decomposition front tracking is needed. Future efforts are focusing on developing models that include fluid motion and convective heat transfer involving both gas-vapor and liquid phases, Specifically, incorporating porous media transport, liquefaction and flow, and liquid-vapor equilibrium models will allow for better agreement with experimental data.

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