

# NUMERICAL SIMULATION OF FIRE SPREAD ON POLYURETHANE FOAM SLABS

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## ABSTRACT

Computational Fluid Dynamics (CFD) models are used extensively by fire protection engineers for performance based design and forensic analysis. The equations of motion describing the gas phase are relatively well known and the approximations in the various gas phase sub-models have been extensively studied. However, coupling of the gas phase and the condensed phase to describe flame spread over a burning solid, has proven to be difficult to model. This is due to a lack of understanding of the underlying physical phenomena that take place during the decomposition of the solid as well as poor characterization of the fundamental material properties that control the burning process.

The overall goal of this project is to improve the capability of the fire models to predict flame spread over materials that typically burn in a compartment fire. In this paper, we attempt to simulate fire growth and spread on 10 cm thick slabs of polyurethane foam. A multi-layered, multi-material model was developed to simulate flame spread, and material properties were obtained from various small scale experiments. Model predictions were compared with large scale experiments on polyurethane foam slabs, ignited on one edge. Results indicate that the model is capable of qualitatively predicting the observed trends in heat release rate, flame spread rate and heat fluxes measured in the experiments. This report will describe the progress that has been made to date on modeling fire growth and spread on polyurethane foam slabs and the comparison of these results with experimental data.

## INTRODUCTION

U.S. residential fire statistics [1] indicate that thermoplastic objects such as upholstered chairs and mattresses (common household items) are most relevant to the goal of reducing fire losses. Flexible polyurethane foam (PUF) is often found as the soft cushioning in upholstered chairs and in mattresses. The foam that is found in these objects is a low density sponge-like material and is usually covered with a face cloth. Modeling fire growth and spread on such objects is difficult since the polyurethane foam decomposes to yield a melt layer, when burning under realistic fire conditions. This is usually accompanied by a dramatic reduction in the thickness of the foam (sometime referred to as foam collapse). A detailed fire growth model also requires input on thermo-physical properties, kinetics of degradation and gasification of the individual components that make up the burning object. The material properties of these objects are often poorly characterized and are not readily available for modeling. The long term objective of this study is to quantitatively understand fire growth and spread on real objects, although the focus of this paper is limited to modeling flame spread on polyurethane foam slabs, by

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performing numerical simulations using the Fire Dynamics Simulator (FDS) and comparing model predictions with available experimental data.

## **MATERIAL PROPERTY ESTIMATION FROM SMALL SCALE EXPERIMENTS**

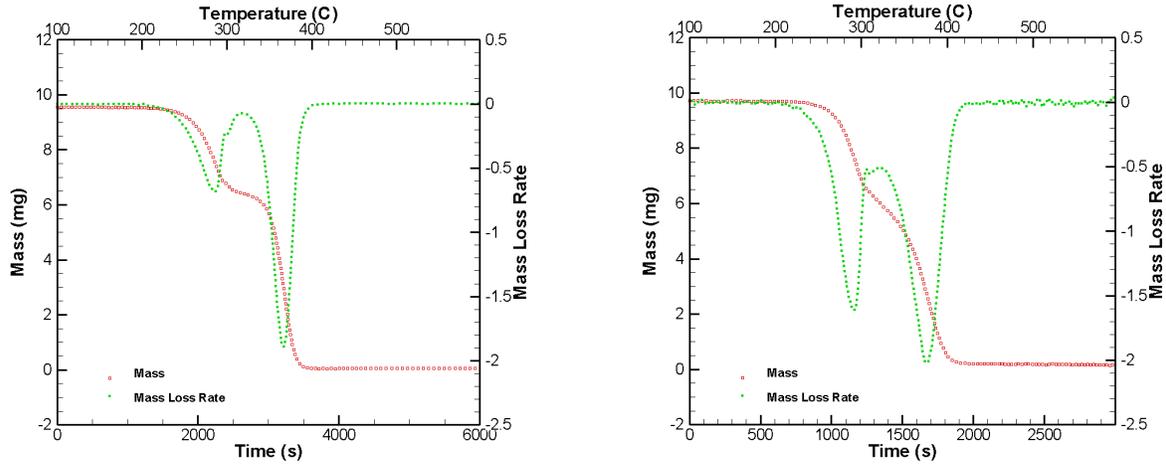
In order to capture the various physical and chemical processes occurring during the decomposition of polyurethane foam and subsequently use that information in flame spread models, it is critical to understand how polyurethane is created. Polyurethane foam is formed out of a reaction of an isocyanate (typically, toluene diisocyanate or TDI) with a polyol [2]. The isocyanate and the polyol form the major components of all polyurethane foam. Commercial foam may contain eight different ingredients, including these two plus catalysts, blowing agents, surfactants and fire retardants. The physical properties can be widely varied by adjusting the nature and proportions of these many ingredients. All of these in turn affect the details of the fire behavior of polyurethane foams. Thermal stability of the various materials that make up the foam can have an important effect on their ignition and flammability. The foam used for the small scale laboratory tests, as well as the large scale experiments with which the numerical simulations will be compared in the current paper, can best be described as a commercially available flexible poly-ether polyurethane foam similar to, but not exactly like the special reference material GM 21 [3]. For comparison purposes only, a summary of the chemical and physical information for material GM 21 can be found in [3].

Thermal decomposition and decomposition kinetics of different polyurethane foams and elastomers have been studied extensively in the literature for many years [4,5,6,7]. Since foam formulations can vary significantly, thermal decomposition analysis was performed on the specific foam samples used in the flame spread experiments (as discussed later in the modeling section) with a Pyris-1 thermogravimetry (TG) apparatus. A constant sample mass of ~10 mg (powder) was used in all experiments (three replicates at three different heating rates). The TG tests were performed in a transient environment with nitrogen at a flow rate of 30 ml/min. The TG curves for polyether-polyurethane foam (used in the current study) under the heating rate of 5 °C/min (left) and 10 °C/min (right) in nitrogen are shown in Figure 1. Results indicate that there are two distinct stages of decomposition for PUF in a nitrogen environment. In the first stage, approximately 34.5 % of the sample mass was lost in a temperature range of 250 °C to 310 °C, while in the second stage, 65.5 % of mass was lost at higher temperature from 340 °C to 380 °C. The mass loss rate curve peaks at 280 °C and 362 °C for the first and second stages respectively. As the heating rate increases, the peak value of the mass loss rate increases significantly for the first stage and to a small extent for the second stage. Mass loss rate peaks shift to higher temperatures as the heating rate increases.

TG measurement, when combined with observations of the physical structure of the foam [4] during the decomposition process (as obtained from a rheometer test [4]), can provide an important input for numerical modeling and simulation of flame spread on large foam slabs. Rheometer tests indicate that the onset of physical collapse of the foam is closely related to the first weight loss peak, and that this is essentially the temperature at which the foam appears to melt. The foam is a cross-linked polymer and the polymer bonds must be broken for any melting / collapse to occur. Understanding the decomposition of PUF can be difficult because the type of bonds and their number can vary with foam formulation. Ravey and Pearce [5] have explained that decomposition of PUF involves breaking of biuret and allophanate bonds at temperatures below 200 °C, however these bonds do not exist in significant proportions in most PUF. The urethane and urea bonds break above 200 °C and regenerate toluene diisocyanate (TDI) along with the original polyol. Depolymerization chemistry [5-7] indicates that the TDI boils at about 250 °C, while the polyol is left behind and forms a melt pool. Polyol itself degrades at much higher temperatures of 320-350 °C. The first peak in the mass loss rate curve is thus attributed to the release of TDI (escaping in the form of toluene diamine), while the second peak is associated with the decomposition of polyol. Note that foams are typically formed out of a reaction between TDI and polyol and that most formulations

contain approximately 33 % by mass of TDI, 66 % by mass of polyol and 1 % of other additives. This again is consistent with TG data, where the mass lost during the first and second stage were 34.5 % and 65.5 % respectively.

Figure 1. TG and DTG curves of polyurethane foam in nitrogen environment at heating rates of 5 °C/min (left) and 10 °C/min (right).



Kinetic parameters governing the thermal degradation of PUF required for the subsequent numerical modeling were obtained using TG data and genetic algorithms [8]. TG tests were performed in an air environment as well, but only the data from tests performed in nitrogen (Figure 1) were used in the subsequent analysis. Since the goal is to model flame spread on large foam slabs, it is expected that the ambient oxygen is consumed in the flame and will not be available for oxidative decomposition. As a result only thermal decomposition of the foam is considered in this study and TG tests performed in a nitrogen environment are suitable for this purpose. Arrhenius type reaction rate parameters were fitted using the GPYRO software [8, 9] for the two step mechanism (the first involving breaking of the polyurethane bond and vaporization of TDI, while the second involves decomposition of the liquid polyol) as suggested by TG data, as listed in Table 1. The parameters can be used to obtain the rate of decomposition using the expression,

$$\frac{d(m/m_0)}{dt} = A \exp\left(-\frac{E}{RT}\right)(m/m_0)^n$$

where,  $m$  is the instantaneous mass of the sample,  $m_0$  is the original mass,  $A$  is the pre-exponential factor,  $E$  is the activation energy and  $n$  is the reaction order. See Equation 3.87 in [10] for more details on the reaction rate expression where the Arrhenius parameters are used.

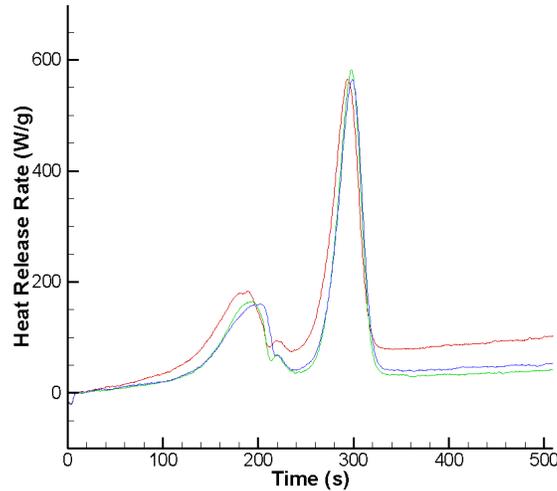
Table 1. Kinetic parameters for thermal decomposition of PUF derived from TG data

	Pre-exponential factor A (1/s)	Activation Energy E (kJ/kmole)	Temperature Exponent n
Reaction 1	1.686E8	135000	1.00
Reaction 2	8.746E9	175000	1.16

The microcalorimetric measurements were performed on a pyrolysis combustion flow calorimeter (PCFC) to obtain heat release rates for the first and second stage reactions. Tests were performed in triplicate on ~1 mg sample at a heating rate of 20 °C/s. The raw data as shown in Figure 2 shows the heat release rate (Watts per gram of virgin material) plotted as a function of time. The two stage behavior

consistent with TG data was again observed in the microcalorimeter measurements. After a baseline shift correction, the area under the curve was integrated to obtain an average heat release of 9,600 kJ/kg and 17,500 kJ/kg for the first and second stage respectively, with a total heat release of 27,100 kJ/kg (per kg of original foam). The TG mass loss data can be combined with microcalorimeter data to obtain heat release rates per kg of gases released.

Figure 2. Microcalorimeter raw data (three replicates) indicating the two stage behavior as seen in the heat release rate vs. time profile for polyurethane foam samples.



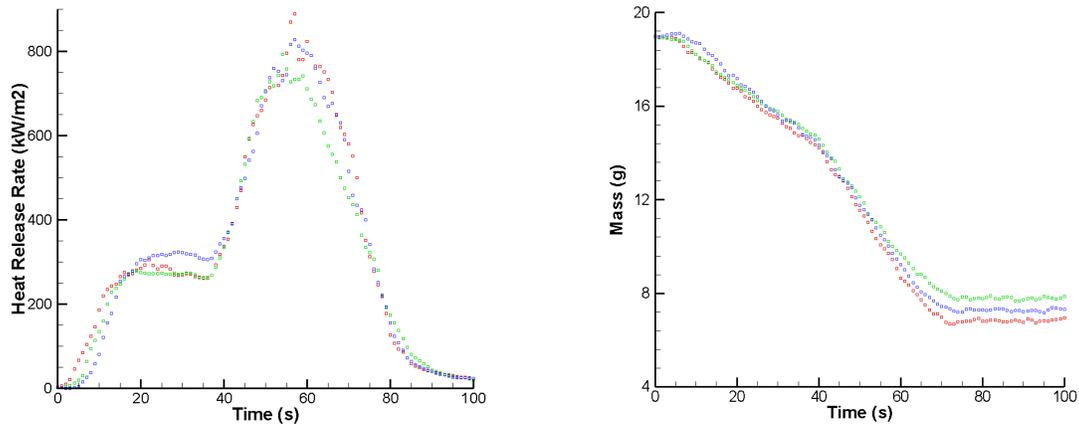
Cone calorimeter experiments were conducted using the original prototype of the cone calorimeter, on 100 mm square polyurethane foam samples at flux levels ranging from 20 kW/m<sup>2</sup>-50 kW/m<sup>2</sup>. The test protocol detailed in ASTM E 1354 was used in the experiments. The primary result of a cone calorimeter test was a measurement of the heat release rate (derived from oxygen consumption calorimetry) as a function of time. The mass loss of the burning specimen was also recorded in the cone calorimeter test.

Figure 3 shows the heat release rate (kW/m<sup>2</sup>) and sample mass plotted as a function of time for an external heat flux of 45 kW/m<sup>2</sup>. Data indicates that the pyrolysis process and burning of the foam slab is a two stage process as previously noted. The first stage lasts for approximately 40 seconds, during which the heat release rate goes from zero to a peak value of 300 kW/m<sup>2</sup>. During this stage the mass of the sample decreases gradually, and approximately one third of the mass is lost. Video observations of the test sample indicate that the foam has collapsed at the end of the first stage and a liquid melt layer is left at the bottom of the pan. During the second stage, the heat release rate increases dramatically to over 800 kW/m<sup>2</sup> followed by a decay phase. From the heat release rate and mass loss rate, the effective heat of combustion (heat release per unit mass) was calculated and was found to compare favorably with the microcalorimeter data. The heat of gasification was also derived from the cone data using the methods proposed by Dillon et al. [12] and Janssen et al. [13]. Since the external flux in the cone experiments is comparable to that measured in the flame spread experiments, the heat release rate measured in the cone calorimeter experiments can be used directly in the models as discussed in the next section.

Thermo-physical properties of foam (density, thermal conductivity and specific heat) are needed to model the burning process. The density of foam was measured to be 23.5 kg/m<sup>3</sup>. However, no direct measurements were made for temperature dependent thermal conductivity and specific heat for the foam used in the current study. Instead, temperature independent values for a generic foam formulation were obtained from literature [14, 15]. Thermo-physical properties of polyether polyol (obtained during the melt phase) were not directly measured, instead properties of VORANOL 235-056 were obtained [16] and used in the flame spread modeling. Radiation is the dominant mode of heat transfer in the gas phase

and optical properties such as emissivity and absorption coefficient for both foam and polyol were estimated from published literature [17]. Properties used in the flame spread simulations are listed in Table 2.

Figure 3. Cone calorimetry data (three replicates) for a 10 x 10 cm sample of polyurethane foam subjected to a heat flux of 45 kW/m<sup>2</sup> (non piloted case). Heat release rate (left) and mass loss (right) are plotted as a function of time (with three replicates), indicating the two stage behavior.



## NUMERICAL MODELING OF PYROLYSIS ON POLYURETHANE FOAM SLABS

Simulations of flame spread on polyurethane foam slabs have been performed using the NIST Fire Dynamics Simulator (FDS). FDS is a low Mach number CFD (computational fluid dynamics) software suitable for modeling fires, that has been used extensively by fire protection engineers for fire modeling and forensic analysis. Over a period of six months, hundreds of FDS simulations were performed with models of various levels of complexity. Simulations included one-dimensional models which are computationally inexpensive, as well as two and three-dimensional models running on multiple processors. Various strategies were developed to model the solid phase and compare predicted results with observed flame spread rate and heat release measured in the experiments. Sensitivity to input parameters was determined and the effect of initial conditions, burner configuration, boundary conditions and grid resolution was ascertained. In the following section, we will describe how the modeling of polyurethane foam slabs has evolved over the past few months.

### Pyrolysis Model #1

The first attempt at modeling flame spread on large slabs of PUF assumed that the heat release rate history of a solid element was identical to that measured from the cone calorimeter or other small scale tests. This approach is one that is used commonly by the fire protection engineers [18]. In this model, the burning rate of the polyurethane foam (modeled as a homogenous material) was controlled by specifying the heat release rate per unit area obtained directly from the cone calorimeter tests. An ignition temperature can be specified to delay burning until this specified temperature is reached in the solid. The mass flux at the foam surface is computed by dividing the heat release by the heat of combustion. The advantage of this approach is that the user does not need to specify parameters associated with the decomposition kinetics, and that the cone data can be directly used in the simulations. The computed burning rates however are independent of the external flux on the surface, which can lead to significant errors, if the object is part of a building fire. Since during the cone tests, heat release rate and mass loss

rate vary with the intensity of the external flux, it is difficult to determine, a priori, which heat release rate curve (from the cone data) should be used in the flame spread simulations.

### **Pyrolysis Model #2**

A more complete predictive capability is needed, where the burning rate would be computed in the simulation, instead of being dialed in from the cone calorimeter data as in Pyrolysis Model #1. The parameters for solid phase reaction are specified to model the burning rate of PUF decomposition. In this model, the foam is again modeled as a homogeneous material and a single solid phase decomposition reaction controls the burning rate. A heat of reaction value accounts for the energy that is used to vaporize the fuel. When foam decomposes, fuel gases are produced, which in turn undergo gas phase combustion to form products. In this approach, a multi-layered model was used the foam slab resting on a 1" thick gypsum board slab, modeled as an inert layer of material. This model does not have the capability to predict the two step process (observed in the TG data as well as the cone experiments) where the foam collapses and melts releasing TDI during the first stage and the polyol decomposes during the second stage).

### **Pyrolysis Model #3**

In order to capture the two stage behavior that was observed in the experiments, the approach (described in Pyrolysis Model #2) was modified such that the foam decomposition was modeled as a two step process. In the first step, foam decomposes to release TDI gases and liquid polyol, while during the second step, polyol vaporizes into fuel gases, which in-turn undergoes exothermic gas phase combustion. This multi-material model can capture the two step process that is observed in the TG data and the cone tests, but requires additional Arrhenius kinetic parameters, heats of gasification and heat of combustion for the two step reaction. Implementation of this model within FDS version 5.2 is difficult due to the large differences in the densities of foam and polyol (23.5 and 1012.0 kg/m<sup>3</sup> respectively). Visual observations during the tests reveal that during the melting/collapse phase, tiny beads of polyol were formed on the surface of the foam. The surface area occupied by these tiny beads of polyol is small compared to that of the foam (due to the very high density ratio between polyol and foam) and as a result the foam continues to melt and collapse, while releasing TDI. At some point, all the TDI has been release and the foam collapses resulting in a polyol melt layer whose thickness is much smaller than that of the foam. The current FDS version does not have the capability to model this multiphase behavior (i.e. the polyol is distributed uniformly, not beaded) and it moreover, assumes a one-dimensional solid phase model. This limitation in modeling capability results in the conversion of the cells consisting of foam into polyol. The cells containing polyol are now directly heated by the fire. As a result, in the model, the cells containing polyol decompose and vaporize before all the TDI has been released. This approach is therefore not suitable since it would contradict the observations made from the TG test data, rheometer tests and video observations during a cone test.

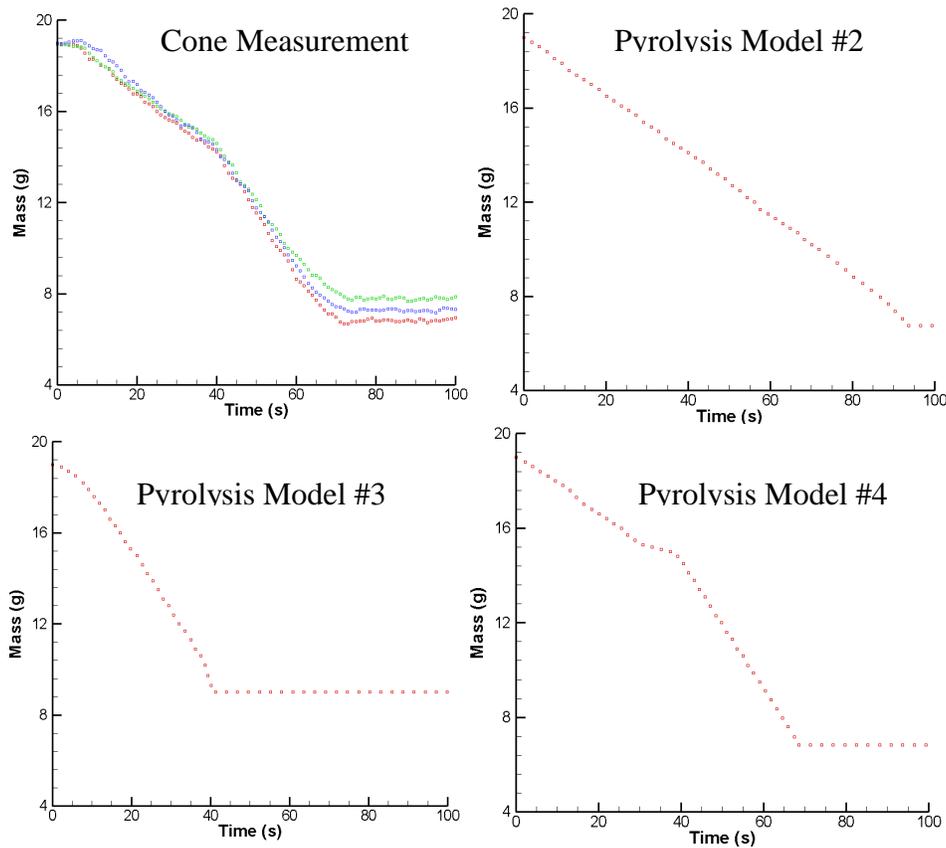
### **Pyrolysis Model #4**

The flame spread model for polyurethane foam slabs was modified again to overcome some of the problems that were identified with the previous approach (Pyrolysis Model #3). Cone calorimeter data as well as TG data indicates that approximately one-third of the foam decomposes and releases TDI, while the remaining foam collapses and forms liquid polyol. The cone tests further indicate that the polyol mainly burns after the TDI has been released. These two important observations along with the fact that the numerical tools are currently unable to model collapse of the foam led to the development of the new model. In this model, the foam slab resting on a gypsum board is modeled with three layers. The top most layer is assumed to release TDI only. Based on TG data, TDI forms approximately one-third of the mass of the foam, and as a result the thickness of this layer was one-third the thickness of the foam slab used in

the experiments. The layer has thermal properties of foam and has a reference temperature corresponding to the first peak of the chemical reaction in the TG tests. The second layer has properties of liquid polyol. The thickness of this layer accounts for the density differences between the foam and the polyol and the fact that only two thirds of the foam produces liquid polyol. Both the foam layers and the polyol layers are assigned a heat of combustion value, obtained from microcalorimeter data and cone tests. The kinetic parameters were obtained from TG data. The bottom most layer consists of a non-reacting 2.5 cm thick slab of gypsum board. As the foam (top layer) is heated, the foam will decompose and release TDI. When all the foam is consumed, the liquid polyol will heat up and undergo decomposition.

Pyrolysis model #2, 3 and 4 were used to simulate a cone experiment using a 1-D model. Figure 4 shows the results of the cone simulations for model #2 (top right sub-figure), model #3 (bottom left sub-figure) and model #4 (bottom right sub-figure). Since the 1-D simulations did not include a gas phase, an external flux value of  $85 \text{ kW/m}^2$  was used. Note that the cone data used an external flux value of  $45 \text{ kW/m}^2$ , but an additional  $40 \text{ kW/m}^2$  was applied to simulate the flux from the flame (as observed in the flame spread experiments). Performing cone simulations in a nitrogen environment would be very helpful in comparing the various models, since it would remove the complexity associated with burning in the gas phase. A qualitative comparison of the results with cone data (Figure 4 top left sub-figure) indicates that only pyrolysis model #4 can replicate the two stage behavior. As a result the flame spread simulations (discussed in the next section) were performed with pyrolysis model #4.

Figure 4. Comparison of mass vs. time plots measure in a cone experiment (top left sub-figure), with 1-D simulations performed using pyrolysis model #2 (top right sub-figure), model #3 (bottom left sub-figure) and model #4 (bottom right sub-figure).



## Comparison of Numerical Predictions with Experimental Measurements on Flame Spread

Numerical simulations were performed using the NIST Fire Dynamics Simulator (FDS) software to study flame spread on large slabs of 10 cm thick polyurethane foam [10, 19]. Material property data was derived from the laboratory scale experiments (Table 1 and Table 2) and the approach for modeling the condensed phase was as discussed in the previous section. The degree of complexity in the simulations has evolved gradually over a period of six months. Initially very simple 1-D simulations were performed to simulate a cone experiment performed in a nitrogen environment. This removes the complexity associated with combustion in the gas phase and the heat flux back to the solid surface, instead the sample was radiated with a constant specified external heat flux from a radiant heater. The goal of these preliminary calculations was to understand the condensed phase mechanisms and the role of the various condensed phase parameters. The 1-D simulations are attractive since they are computationally inexpensive (CPU costs is of the order of a few minutes). 2-D numerical simulations of flame spread were conducted to understand the role of gas phase parameters and grid resolution on flame spread. The CPU time for these simulations is of the order of one day. Sensitivity studies were conducted with these models to identify the relative importance of various input parameters. Further refinements to the model were made during the course of 3-D simulations of the cone calorimeter experiments to simulate the burning of PUF in air. Heat release rate and burning rates were compared with experimental data. Although the results of these simulations and comparison with experimental data has not been reported in this paper (results will be reported elsewhere due to lack of space), these simulations were critical in the development of the 3-D models that were eventually used for simulating flame spread on large polyurethane foam slabs.

Table 2. Property values for foam and polyol used in the flame spread simulations

Property	Polyurethane Foam		Polyol	
	Value	Source	Value	Source
Density	23 kg/m <sup>3</sup>	Flame spread experiment	1012 kg/m <sup>3</sup>	Ref. [16]
Heat Capacity	1 kJ/kg/K	Ref. [14, 15]	2 kJ/kg/K	Ref. [16]
Thermal Conductivity	0.05 W/m/K	Ref. [14, 15]	0.15 W/m/K	Ref. [4]
Heat of Reaction	1960 kJ/kg	Ref. [3] , DSC	1960 kJ/kg	Ref [3] , DSC
Heat of Combustion	9600 kJ/kg	Micro-calorimeter	17500 kJ/kg	Micro-calorimeter
Thickness	3.4 cm	TGA	0.16 cm	TGA
Absorption Coefficient	50000 1/m	Default	50000 1/m	Default
Emissivity	0.9	Default	0.9	Default

The base of the computational domain used for 3-D simulations of flame spread on 10 cm thick slabs of PUF was 1.2 m x 1.2 m square ( covering the entire slab) and extended 1 m above the surface of the foam. Four multiple meshes were used to grid the computational domain above the foam slab. Each mesh was uniformly spaced in the horizontal direction and the grid size in the horizontal direction was 1 mm. Mesh stretching was used in the vertical direction with very fine mesh close to the surface (minimum grid size was 1 mm). Open boundary conditions were used on all faces except the bottom face which represents the PUF slab. In the simulations the slab was ignited with a line burner along one entire edge of the slab, supplying energy at the rate of 1000 kW/m<sup>2</sup>.

Simulation results were compared with experiments on 10 cm thick slabs conducted at NIST's Large Fire Laboratory (20). Figure 5 shows three photographs taken during a flame spread experiment on a 10 cm thick slab of PUF. During each experiment (conducted on a 1.2 m square slab) heat release rate, flame spread rate, heat flux and thermocouple temperature measurements were made to create a database to

validate numerical models. The PUF used in the large scale tests was identical (same batch) to that used in the small scale laboratory tests such as TG, microcalorimeter and cone experiments, and these data have been reported earlier. The photographs show the ignition stage (left sub-figure), the flame spread stage (middle) and the final burning stage (right sub-figure) of the foam. Smokeview visualizations (heat release rate per unit volume) of the flame spread simulation on PUF slabs are shown in Figure 6. The smokeview images also show an ignition stage (left sub-figure), a flame spread stage (middle) and full burning stage (right sub-figure), and these pictures qualitatively compare with the photographs of the flame spread experiments. During the initial ignition stage, the flame profile was parallel to the edge that was ignited, but it gradually transitions into a parabolic profile (middle sub-figure). Flame spread rate was fastest in the centre (due to higher radiative flux from the flames to the foam slab) and relatively slower at the edges of the slab. Note that the early stages of the experiment can be approximated as a 2-D phenomena, if the parabolic flame spread profile or the 3-D pool burning do not have to be captured in the simulations. During the flame spread stage, the foam collapses and releases the TDI, while the polyol is left behind as a pool on top of the gypsum board. The last sub-figure indicates burning of the polyol which is accompanied by very intense heat release rates and tall flames.

Figure 5. Ignition, flame spread and burning of a 10 cm thick slab of polyurethane foam.

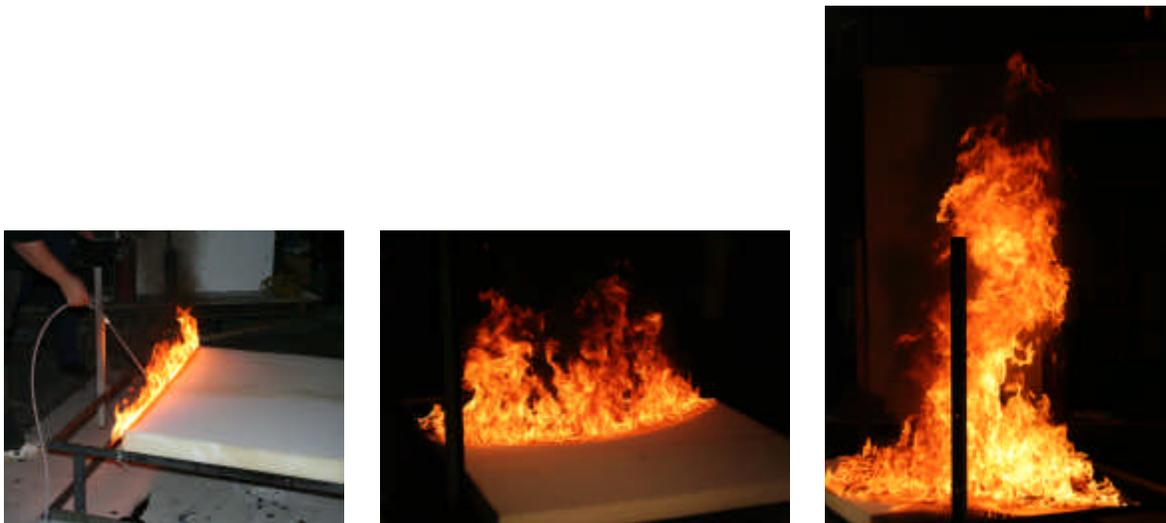


Figure 6. 3-D Smokeview visualization of the flame spread on a 4" thick slab of polyurethane foam.

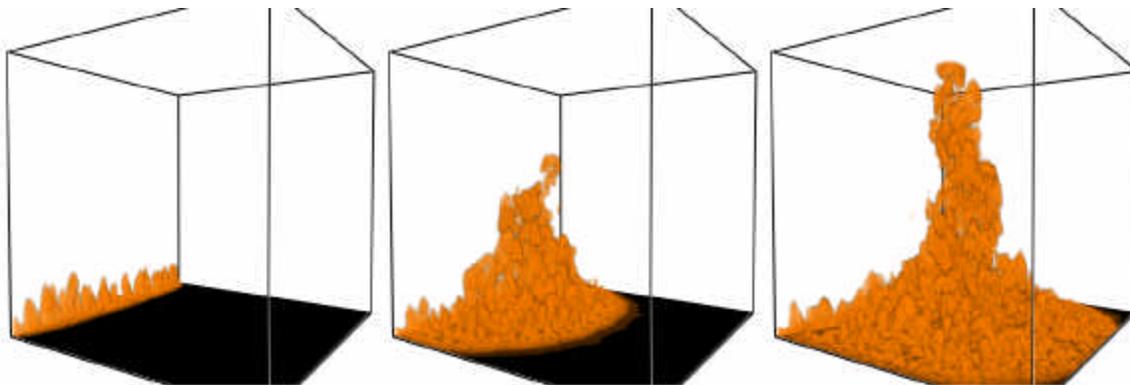


Figure 7 shows a comparison of heat release rate (kW) plotted as a function of time for the experiments (left sub-figure, measured using oxygen consumption calorimetry) and the model predictions (right sub-figure). Model predictions indicate that the heat release rate increases gradually during the first 70 s and

reaches a plateau at about 200 kW. Beyond that point, the increase in heat release rate was more rapid and a peak value of 650 kW was obtained at 150 s. The heat release rate curve died down, once the foam slab was completely consumed. The experiments indicate a similar behavior of slow gradual increase in the heat release rate curve followed by a more intense burning regime and a subsequent decay phase. Numerical simulations indicate that the flame spread rate was at least twice as fast as observed in the experiments, although the peak heat release rate values compared favorably.

Figure 7. Comparison of experimentally measured (left sub-figure, showing a set of five tests) and numerical predicted (right sub-figure) heat release rate (kW) plotted as a function of time for a 10 cm thick polyurethane foam slab.

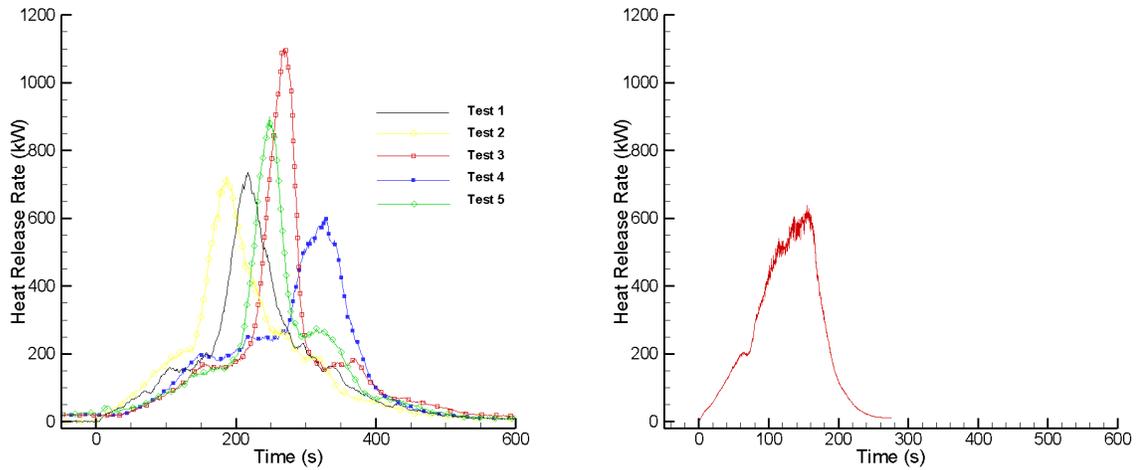
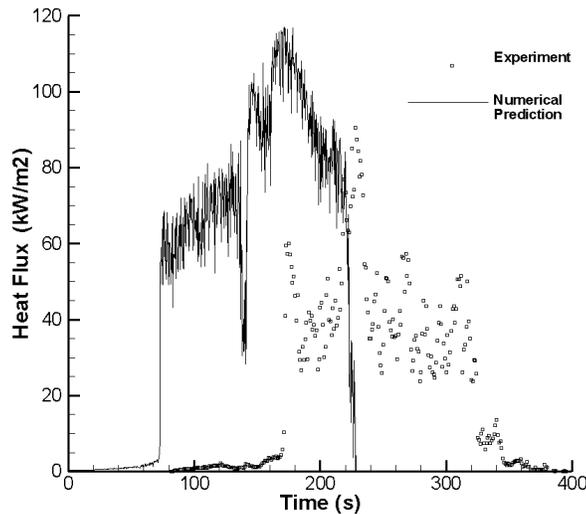


Figure 8. Comparison of experimentally measured and numerical predicted heat flux plotted as a function of time. The flux was measured by a heat flux gauge located at 0.9 m from the ignited edge.



The experimentally measured heat flux ( $\text{kW/m}^2$ ) plotted as a function of time was compared with model predictions as shown in Figure 8. The heat flux was measured by a heat flux gauge located on the center line and at a distance of 91 cm from the edge that was ignited by the heaters. Results indicate that the measured flux was approximately zero until the flames reached the gauge. The heat flux then jumps abruptly to a value of 50-60  $\text{kW/m}^2$ . Peak value of 95  $\text{kW/m}^2$  was measured, and the sample was completely consumed in 400 s. Model predictions show qualitatively similar behavior, even though the

flame spread rates are significantly higher. Model predictions also indicate that the heat flux ranges between 60-120 kW/m<sup>2</sup>, but that the sample is completely consumed in 200 s. The higher heat flux might be responsible for the higher flame spread rates as predicted in the simulations.

## **CONCLUSIONS AND FUTURE WORK**

Modeling the flame spread on polyurethane foam slabs is difficult due to the highly complex process occurring during its decomposition (phase change, shape change, charring, bubbling etc.). A simple model has been developed to approximately model this very difficult problem. Detailed understanding of the various physical and chemical processes that occur during the burning of polyurethane foam slabs derived from small scale tests (TG, Cone Tests, Microcalorimeter) has been used to estimate material property data. Simulations results for flame spread behavior and heat release rates were found to compare qualitatively with measured experimental data.

Attempts are underway to further improve the material property input data that is used in the models as well as the approach for representing the condensed phase. Differential scanning calorimetry (DSC) and simultaneous TGA/DSC (SDT) tests are currently being performed on PUF to better estimate the heat of reaction for each stage. The flame spread rates were found to be very sensitive to the heat of reaction and it is believed that incorporating the new test data will significantly increase the accuracy of the predictions. Simulations are also being performed on 2.5 cm, 5.1 cm and 20.3 cm thick slab samples and these results will be compared with experimental data. Further studies have been planned to investigate the effect of radial flame spread on foam slabs with pre-heating [21], impact of covering the foam with polypropylene or rayon face cloth, use of brominated foam samples (fire retardants) and orientation of the foam slabs on predicted flame spread rates.

## **ACKNOWLEDGEMENT**

The authors would like to thank Michael Smith for performing the cone calorimeter experiments; Matt Bundy for providing technical support in the Large Fire Laboratory; Jeff Gillman, Kevin McGrattan and Anthony Hamins for their continued support of this internally funded study at NIST; and Lucas Bustamante, Simo Hostikka, Chris Lautenberger and Guillermo Rein for useful discussions.

## REFERENCES

1. "Extended Abstracts and Presentations from the Workshop on Fire Growth and Spread on Objects," <http://www.fire.nist.gov/bfrlpubs/flamespread/>, March 4-6, 2002.
2. "Polyurethane handbook: chemistry, raw materials, processing, application, properties," Oertel, Gunter, Hanser Publishers, New York, 1985.
3. "Materials Bank Compendium of Fire Property Data," Products Research Committee, February 1980.
4. "Aspects of the Fire Behavior of Thermoplastic Materials," Ohlemiller, T. J., Shields, J. R., NIST Technical Note 1493, 2008.
5. "Flexible Polyurethane Foam 1. Thermal Decomposition of a Polyether-based, Water-Blown Commercial Type of Flexible Polyurethane Foam," Ravey, M. and Pearce, E., J. Appl. Poly. Sci. 63, (1997) p.47
6. "Studies on the Thermal Behavior of Polyurethanes," Shufen, Li, Zhi Jiang, Kaijun Yuan, Shuqin Yu, Chow, W. K., Polymer-Plastics Technology and Engineering, 45: 95-108, 2006.
7. "On Heat Release and Pool Fires of Flexible Polyurethane Foams, Part I – Experimental," Kramer, R. H., Zammarano, M., Gedde, U. W., Gilman, J. W., submitted, J. of Polymer Science, 2008.
8. "Application of Genetic Algorithms and Thermogravimetry to Determine the Kinetics of Polyurethane Foam in Smoldering Combustion," Rein, G., Lautenberger, C., Fernandez-Pello, C., Torero, J., Urban, D., University of California Postprints, Paper 1154, 2006.
9. "A Generalized Pyrolysis Model for Combustible Solids," Chris Lautenberger, PhD. Thesis, University of California, Berkeley, 2007.
10. "Fire Dynamics Simulator (Version 5) Technical Reference Guide," Kevin McGrattan, Simo Hostikka, Jason Floyd, Howard Baum, Ronald Rehm, Randall McDermott, NIST Special Publication 1018-5, 2008.
11. "Material Property Estimation Method using a Thermoplastic Pyrolysis Model," Seung Han Lee, Thesis Worcester Polytechnic Institute, 2006.
12. "Determination of Properties and the Prediction of the Energy Release Rate of Materials in the ISO 9705 Room-Corner Test," Dillon, S. E., Kim, W. H. and Quintiere, J. G., National Institute of Standards and Technology, Gaithersburg, MD NIST-GCR-98-753, 1998.
13. "Computer Tools to Determine Material Properties for Fire Growth Modeling From Cone Calorimeter Data," Janssens, M. L., Kimble, J., Murphy, D., Proceedings of Fire and Materials, 2003, pp 377-387, 2003.
14. "Thermal characteristics of polyurethane foams incorporated with phase change materials," Sarier, N., Onder, E., Thermochemica Acta 454 (2007) 90-98.
15. "Thermal Conductivity of Selected Foams and Systems from 100 to 300 K," Sparks, Larry, L., U.S. Dept of Commerce, NBSIR 88-3086, 1988.
16. VORANOL 235-056, Dow Plastics Product Information, The Dow Chemical Company, 2001
17. "Polymer surface reflectance-absorptance characteristics," Hallman, J. R., Ph. D., Dissertation, University of Oklahoma, 1971.
18. "Using cone calorimeter data for the prediction of fire hazard," Tsai, K. C. and Drysdale, D., D., Fire Safety Journal, 27:697-706 (2002).
19. "Fire Dynamics Simulator (Version 5) User's Guide," Kevin McGrattan, Bryan Klein, Simo Hostikka, Jason Floyd, NIST Special Publication 1019-5, 2008.
20. William Pitts, Private communication, 2008.
21. "A Study of Transient Horizontal Fire Spread Over Cellular Plastics," Tan, Seng, Chuan, Ph.D. Dissertation, Harvard University, 1983.