

Modeling Smolder Combustion and Transition to Flaming

Amanda B. Dodd^{1,2}, Chris Lautenberger², Carlos Fernandez-Pello²,

¹Sandia National Laboratories, Albuquerque, NM 87185

²Department of Mechanical Engineering,
University of California at Berkeley, Berkeley, CA 94720

1 Introduction

An important aspect of smoldering combustion is its potential to transition to flaming. The transition to flaming process is a fire safety concern because smoldering can occur for a long time before erupting into flames, and when it happens the fire can spread very quickly. The transition from smoldering to flaming is a complex process where the smolder reaction acts both as a source of heat to pyrolyze the fuel and ignite the resulting flammable gaseous mixture. Many researchers have studied smoldering combustion which involves heterogeneous reactions including both thermal and oxidative pyrolysis. Experimentally, the transition to flaming from forward smoldering has been studied [1, 2], but very little computational work has been expended [3]. Tse *et al.* [1] and Putzeys *et al.* [2] found that a highly exothermic reaction, the secondary char oxidation reaction, is the precursor to transition to flaming. The current body of work incorporates the ideas formulated by Tse *et al.* [1] and Putzeys *et al.* [2] and extends the work presented in Dodd *et al.* [4], who developed a reduced reaction mechanism for two-dimensional smolder in polyurethane foam. The current work extends this reaction model [4] by adding a homogeneous gas phase reaction and incorporates a two-temperature thermal nonequilibrium approach to simulate transition from smoldering to flaming. The present approach is the first attempt to use a two-temperature model with a global gas phase reaction to simulate transition to flaming in polyurethane foam. The approach is introduced, a base case model is presented, and detailed profiles are examined. The experiments of Putzeys *et al.* [2] are simulated. The model reproduces the phenomena observed by Putzeys *et al.* [2].

2 Computational Model

The computational model used in this body of work is Gpyro [6], a generalized pyrolysis model for decomposing solid materials; it contains the effects of heat transfer, mass transfer, momentum transfer, and heterogeneous and homogeneous chemical reactions. The model was originally developed by Lautenberger [5] and was recently expanded to include two-dimensional effects. Details of the computational model can be found in Lautenberger [6]. The governing equations are not presented here for brevity, but they are two-dimensional and transient [6]. Gpyro solves seven governing equations: condensed phase mass conservation, condensed phase species conservation, gas phase mass conservation, gas phase species conservation, pressure evolution equation, condensed phase energy conservation, and gas phase energy conservation. The pressure evolution equation is derived from the

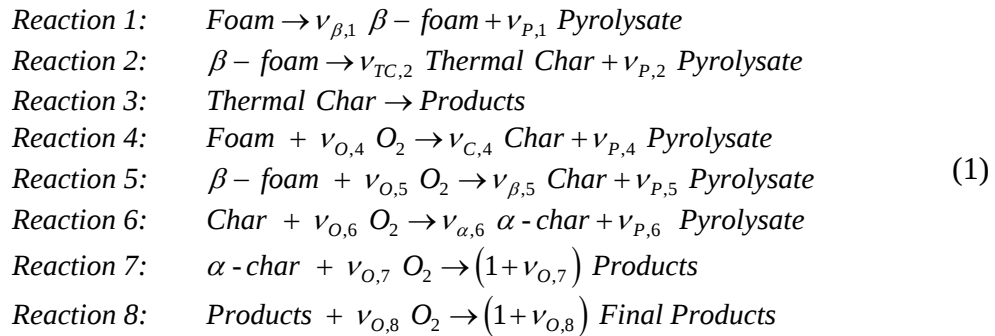
Correspondence to: abdodd@me.berkeley.edu

1

a Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

gas-phase mass conservation equation using Darcy's law, where the gravity term is included in the z-direction mass flux. The gas and solid phase energy equations are coupled using a volumetric heat transfer coefficient, which is modeled through a Nusselt number correlation.

The decomposition model for polyurethane foam implemented is the same as that presented in Dodd *et al.* [4], but with an additional gas phase reaction to simulate the shift from the dominance of condensed phase reactions during smoldering combustion to the gas phase reactions during flaming combustion. Also, there were small changes to the heats of reaction to be able to predict both forward and opposed flow smolder, the secondary char oxidation reaction kinetic constants, and to the gas phase products. The reaction scheme is shown below.



3 Simulation Results

The small scale polyurethane foam experiments performed by Putzeys *et al.* [2] were selected for simulation. The two dimensional planar computational representation of the three dimensional experiments is shown in Figure 1. The igniter is modeled as a time dependent temperature history at $z=0$ cm. A small forced internal flow was applied $z=0$ cm. Heat losses are modeled through a heat transfer coefficient at $z=12.5$ cm. The boundary at $x=0$ cm is set at a constant temperature to simulate the guard heaters in the experimental set-up. A radiant heat flux is applied at $x=5$ cm to simulate the radiant heaters in the experiment. The duct flow is modeled via heat and mass transfer coefficients applied as boundary conditions (the external boundary layer flow is not explicitly simulated). The ambient duct and forced flow oxygen concentrations are initially set at 0.21 oxygen mole fraction. At a given time, the oxygen concentration is changed to 0.35 mole fraction, following the experimental procedure.

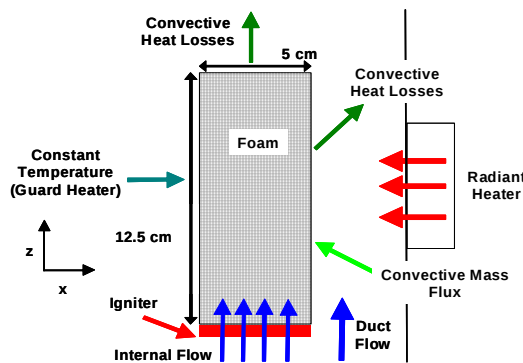


Figure 1. (left) Model representation of small transition to flaming experimental apparatus.

Typical results from a simulated transition to flaming case are shown in Figures 2, 3 and 4. The three figures, through the gas temperature profiles, show progression of the smolder front (Fig. 2), the secondary char oxidation reaction front (Fig. 3), and transition to flaming (Fig. 4). The three figures are separated to emphasize the different time and gas temperature scales associated with the smolder and transition to flaming processes. In comparing Figures 2, 3, and 4, it is important to note the

differences in peak temperature (450°C, 550°C, and 1000°C, respectively) and time lines (~500 s, ~17 s, and 1 s, respectively). The timescales of forward smolder, secondary char oxidation reaction, and gas phase reaction are each separated by one order of magnitude. Thermal nonequilibrium allows for a divergence of the solid and gas temperature. During forward smolder, the difference between the gas and solid temperature is less than 10°C. During the secondary char oxidation reaction propagation, the solid temperature is hotter than the gas by 30- 40°C. During the transition, the gas temperature exceeds the solid temperature by up to 300°C.

Figure 2 illustrates the progression of the forward smolder front. Figure 2a shows the temperature profile just prior to smolder ignition. The igniter has heated up the bottom of the foam and the radiant heater has heated the right side of the domain. Figure 2b shows the smolder front formation at the bottom of the domain. Figures 2c and 2d show the evolution of the smolder front as it moves upwards. The main contributing reactions to the forward smolder processes shown in Figure 2 are the first six reactions in Eq. 1.

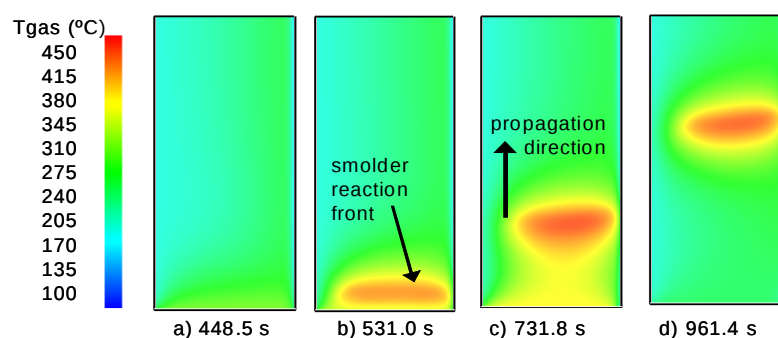


Figure 2. Gas temperature profiles during forward smolder from 448.5 to 961.4 seconds. (Scale from 100-450°C)

The oxygen concentration of the internal and duct flows was changed from 0.21 to 0.35 oxygen mole fraction at 962 seconds. Figure 3a shows the smolder front at 961.4 seconds just before the oxygen concentration is changed. As pointed out before, it is important to note that Figure 2d and 3a are at the same time step, but on different temperature scales, i.e. the maximum temperature in Figure 2 is 450°C and in Figure 3 it is 550°C. At 967.5 seconds (Fig. 3b), a region of hotter temperature can be seen. Additional oxygen due to the increased oxygen concentration in the flow field has reached the smolder front and is being consumed by the secondary char oxidation reaction (Reaction 7). To further explain, prior to the 962 seconds, all of the available oxygen was consumed at the smolder front. The additional oxygen provided by the increase in oxygen concentration is available for use by Reactions 7 and 8. Reaction 7 requires both heat and oxygen to progress, so it begins at the smolder front where heat is being generated. Then, the secondary char oxidation reaction propagates downwards towards available oxygen, in the direction opposite that of the forward smolder front. The change in direction is shown in Figure 3 (c, d, e, and f). The secondary char oxidation reaction is highly exothermic and creates a large region of high temperature (Fig. 3e and f). The downward propagation of the secondary char oxidation reaction and its high exothermicity has been reported in experimental observations by Putzeys *et al.* [2].

Figure 4 illustrates the growth of the gas phase reaction rate. As was done with Figure 2d and 3a, Figure 4a is at the same time step as Figure 3f, but the temperature scale is different. The temperature scale has increased from a maximum of 550°C in Figure 3 to a maximum of 1000°C in Figure 4. The gas phase reaction begins to increase and generate heat substantially at 979.55 seconds. When examining the reaction rates, the gas phase reaction rate spikes in a small area as shown by the red temperature area in Figure 4b and the reaction rate of the secondary char oxidation reaction (Reaction 7) is negligible in that area but high in the surrounding areas. This indicates that the fuel gases being produced by the secondary char oxidation reaction are being trapped and consumed by Reaction 8 as opposed to being convected away.

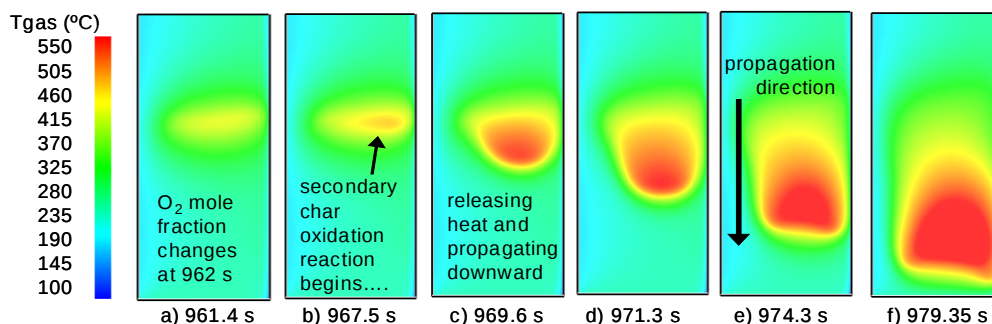


Figure 3. Gas temperature profiles from 961.4 to 979.35.2 seconds. (Scale from 100-550°C)

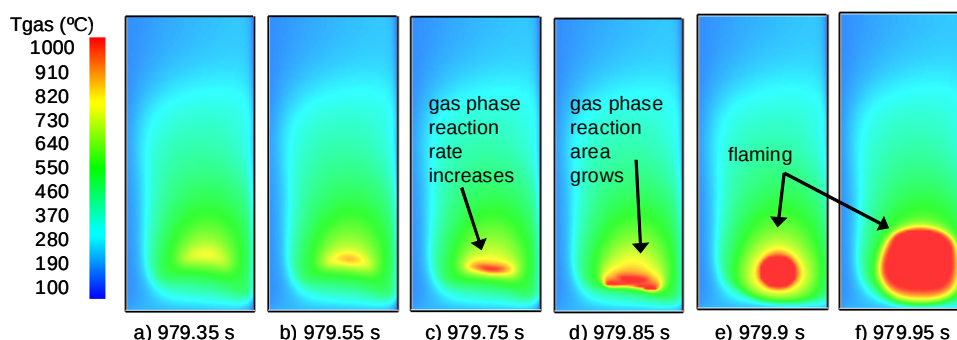


Figure 4. Gas temperature profiles from 978.35 to 979.95 seconds. (Scale from 100-1000°C)

4 Concluding Remarks

The findings presented in this abstract are only a fraction of the information that is available from these calculations. Other parameters such as the evolution of the reaction rates, oxygen concentration, porosity and concentration profiles provide additional information about the transition to flaming process. Further examination of these parameters will aid in understanding the key contributors to the transition to flaming process, as well as aid in more accurately predicting experimental results. The ideas presented here can be expanded upon for different materials and applications.

References

- [1] Tse, S. D., Fernandez-Pello, A. C., and Miyasaka, K., (1996). Controlling mechanisms in the transition from smoldering to flaming of flexible polyurethane foam, *Proc. Combust. Inst.* 26:1505.
- [2] Putzeys, O. Amnon Bar-Ilan, A. Rein, G., Fernandez-Pello, A. C., Urban, D. L., (2007). The role of secondary char oxidation in the transition of smoldering to flaming, *Proc. Combust. Inst.* 31:2669.
- [3] Aldushin, A.P., Bayliss, A., and Matkowsky, B.J. (2007). On the mechanism of triggering the Transition from Smoldering to Flaming, *Proc. Combust. Inst.* 31: 2661.
- [4] Dodd, A. B., Lautenberger, C. Fernandez-Pello, A. C. (2009). Numerical Examination of Two-Dimensional Smolder Structure in Polyurethane Foam, *Proc. Combust. Inst.* 32: 2497.
- [5] Lautenberger, C., (2007). A Generalized Pyrolysis Model for Combustible Solids, PhD thesis, University of California at Berkeley, Berkeley, CA.
- [6] Lautenberger, C., (2008) "Gpyro-A Generalized Pyrolysis Model for Combustible Solids: Technical Reference", <http://code.google.com/p/gpyro/>, Version 6.57.