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Book of Abstracts
November 2-5, 1998

Kellie Ann Beall, Editor

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A MIXED LAYER MODEL FOR PYROLYSIS OF BUBBLING THERMOPLASTIC MATERIALS

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Introduction For many thermoplastic materials exposed to a strong heat flux from above, a layer of bubbles forms in the melted region near the upper surface. The action of these bubbles is observed to range from slow growth and bursting to vigorous boiling behavior. Although the bubbles appear to have a significant effect on the macroscopic thermal and mechanical properties of the material,[1] the mechanisms by which a bubbling layer affects heat and mass transfer are not well understood. Since the thermal conductivity of a gas is much lower than the thermal conductivity of a liquid, we might expect the transport of heat to be slowed considerably in the presence of bubbles. Alternatively, vigorous boiling behavior could be mixing the upper layer of melted thermoplastic material, resulting in a nearly uniform temperature throughout the bubbling layer. How would these seemingly contradictory mechanisms affect heat and mass transfer, and which dominates behavior during pyrolysis?

Several models have considered the effects of in-depth gasification on the temperature profiles and mass loss rate of pyrolyzing materials.[2,3] The physical effects of bubbles are generally neglected by assuming that gases escape on a timescale short compared to the phenomena of interest, although an effective thermal conductivity based on the local volume fraction of gas has been introduced as a simple way to investigate the insulating properties of trapped gas.[4] A literature on mixed layer effects on heat transfer may be found in oceanography, where such models have been used to understand diurnal and seasonal variations in the temperature profile of the upper ocean.[5] Although the driving forces in ocean models are very different, a similar approach can be used to study the limiting case of a perfectly mixed bubble layer. This is the model described in this abstract.

Model The geometry of this model is shown in Figure 1. At time $t = 0$, a solid slab of thermoplastic material of thickness L is exposed on its upper surface to a constant heat flux. The lower surface, located at $z = 0$, is perfectly insulated. The solid material heats up through conduction until the upper surface reaches the melt temperature, at which time a phase change takes place. The location $z = l_s(t)$ of the moving interface between solid and liquid layers, where the temperature is equal to the melt temperature, is one of the variables in this problem. The heat consumed during the phase change is included in the heat flux balance across this interface.

As the temperature in the melt continues to increase, gasification begins through a chemical reaction described by an Arrhenius expression. This causes turbulence that stirs the uppermost region of melt and forms a mixed layer of uniform temperature. The mixed layer thickness $h(t)$ increases through entrainment of the quiescent melt beneath the mixed layer. Over the thin entrainment layer (whose thickness goes to 0 in the analysis), the temperature varies linearly in space from the temperature at the top of the quiescent melt to the higher temperature of the mixed layer. Although gasification occurs over the entire sample according to temperature, turbulence is limited to the mixed (bubble) layer. The timescale of mass transport of the gases is assumed to be much smaller than the timescale over which the quantities of interest are evolving, so that gases escape instantly as they are generated. Mass transport is of interest in this problem only in that it results in thorough mixing of the uppermost layer of liquid.

To incorporate turbulent mixing into the model equations, Reynolds averaging is used. The existence of a timescale long enough to adequately average horizontal and vertical disturbances in the mixed layer but short enough to follow the evolution of the averaged quantities of interest is assumed. The problem is homogeneous horizontally, so that Reynolds-averaged quantities are functions of z and t only. Each field variable is then decomposed into the sum of a Reynolds averaged part and a deviation from the mean, and equations are derived for both mean and turbulent parts. At the upper surface, the incident heat flux transforms into a turbulent heat flux that is uniform within the mixed layer. The final model equations necessary to solve for temperatures and thicknesses in the solid, melt, and mixed layers are obtained by relating the transport of turbulent heat flux and turbulent kinetic energy to gasification and the mixed layer thickness.

Results The mixed layer model can be compared to a model of a heated thermoplastic sample subject to melting and in-depth gasification but without a turbulent mixed layer. Figure 2 displays the temperature profiles near the upper surface from both models after the same time has elapsed. At this point mass losses have begun (the initial thickness of the sample was 2 cm) and the mixed layer has begun to grow. The mass loss rate is found to be slightly higher for the mixed layer model. At the upper surface, the temperature of the mixed layer exceeds the melt temperature of the in-depth model. However, the presence of the mixed layer actually decreases the temperature in the interior of the sample. This is an interesting result, since a reduction in interior temperature would also be expected for a model that takes the lower thermal conductivity of the bubbles into account.

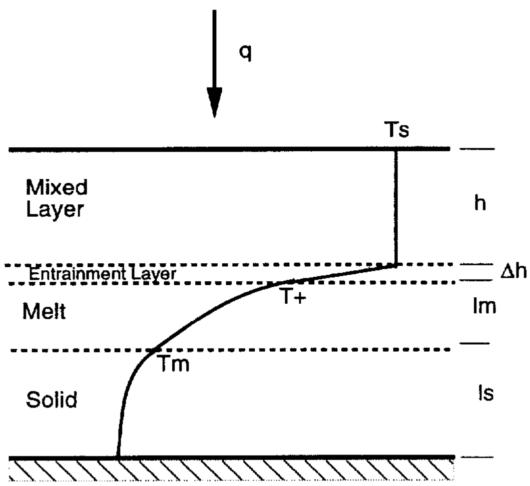

FIGURE 1: Mixed layer model

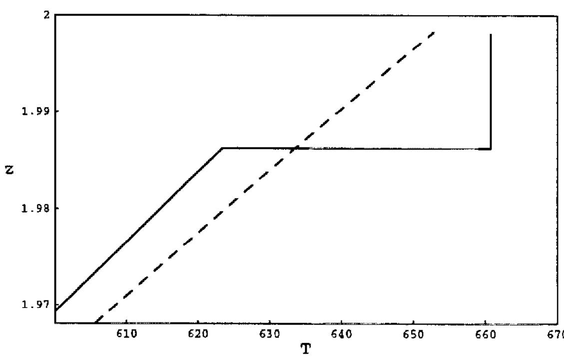

FIGURE 2: Comparison of temperature profiles near the upper surface for in-depth gasification model with (solid) and without (dashed) a turbulent mixed layer. Distance z is measured in centimeters and temperature T in degrees Kelvin.

Conclusions A model representing the bubbling behavior of a pyrolyzing thermoplastic material as a mixed layer of uniform temperature has been developed. Initial results indicate that the formation of a mixed layer tends to increase the mass loss rate and decrease the temperature in the quiescent melt and solid layers beneath.

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