A MODEL OF MELTING AND DRIPPING THERMOPLASTIC OBJECTS IN FIRE

Kathryn M. Butler
National Institute of Standards and Technology, USA

ABSTRACT

A model of the melting and dripping behavior of thermoplastic materials in fire is being developed using the Particle Finite Element Method (PFEM), which is capable of tracking the large changes in shape inherent to this problem in addition to solving the equations of motion and energy. Experiments that approximate two-dimensional flow situations provide a basis for comparison for the model in its early stages of development. Reasonable agreement with experiment has been noted for the quasi-steady flow rate from an upright rectangular object that is heated on one face. The two-dimensional spread rate of the thermoplastic melt that has dripped onto a surface beneath the object has been measured experimentally for both horizontal and slightly tilted catch plates. The model agrees within 10% to experimental results when further degradation of the melt along the catch plate is taken into account.

INTRODUCTION

The melting and dripping of thermoplastic materials in fire has a substantial impact on flame spread. In fires involving objects with a large thermoplastic component, such as upholstered furniture, mattresses, and solid plastic assemblies, a polymer melt flows downward, forming a liquid pool at the base of the object. If this pool ignites, the burning surface area is increased, and the resulting pool fire typically interacts with the fire on the object to increase its burning rate, heat release rate (HRR), and rate of melt production. If the pool is not contained, the liquid melt may potentially spread the fire along the floor. The spread rate of the melt pool and its burning behavior (including whether it is even able to sustain ignition) are affected by the flooring material as well as by the properties of the melt.\(^1\) Melting behavior has been found to significantly affect upward flame spread\(^1,2\), adversely affect flammability properties,\(^3\) and play a significant role in upholstery fires when thermoplastic fabrics are involved.\(^4\)

A combined experimental and modeling effort by NIST and an international group of researchers has been undertaken to understand the behavior of thermoplastic materials in fire situations. The approach is to begin with a simple 2D geometry and add physical and chemical phenomena one step at a time, using experiments to assure that the model correctly simulates each new aspect of the problem. The initial modeling steps on this list are:

1) Steady heat flux with radiative and convective losses from free surface, with degradation represented by viscosity as a function of temperature
2) Gasification
3) In-depth absorption of heat
4) Melt pool spreading
5) Flaming, on both the object and the melt pool
6) 3-D capability
7) Foam structure
Other phenomena of interest for burning thermoplastic objects include ignition, bubbling, charring, and phenomena linked to nanoparticulate content. These further complications may be added in the future. Successful accomplishment of the above steps is intended to assemble the basic capabilities that will for the first time provide a basic modeling tool for evaluating the effects of real dripping thermoplastic objects on flame spread.

Up to now, little attempt has been made to explicitly incorporate melt flow in fire models. The large changes in shape of the burning material over time create a significant challenge for fire modeling, in addition to the difficulties normally encountered in modeling flame spread over solids. In the current effort, attempts to employ the Volume of Fluid (VOF) method with commercial finite element codes encountered difficulties with numerical instabilities and excessive runtimes. Progress on steps 1 through 4 was demonstrated using a finite volume method with time-varying grids, however, the addition of grid smoothing to combat instabilities resulted in questionable behavior of the free surface of the object as it evolved in time. The strongest potential for tackling this problem has been demonstrated by the Particle Finite Element Method, developed specifically to address problems with large changes in the free surface. The results from this method for steps 1 and 2 were found to compare well with experiment and theory, and a low resolution 3-D problem (step 6) has been successfully carried out with a reasonable runtime.

This paper reports on progress toward achieving step 4 – developing a model that accurately predicts the spread of a thermoplastic melt pool over a flat surface. This is an important aspect of the thermoplastic flame spread problem, since the growth in surface area increases the HRR and the location of the melt pool after it ignites determines where heat feeds back to the burning object above. In a study of different industrial flooring materials, Sherratt and Drysdale found that the thermal properties of the floor itself have a large impact on the burning rate. The next section describes the experimental setups for measuring flow from the heated thermoplastic object and for measuring the spread rate over the catch plate, as well as the computational approach. This is followed by illustrations of the numerical results and calculations of spread rate for horizontal and slightly tilted catch plates, which are found to be in good agreement with experimental results when continuing degradation of the polymer is taken into account.

APPROACH

Two-dimensional polymer melt flow experiment

The basic 2D problem that forms the basis of both experimental and modeling efforts is shown in Figure 1.
In this set-up, a solid rectangular thermoplastic sample is mounted vertically some height above a horizontal catch surface. The sample is exposed to a steady heat source along one side, which heats the material until chemical degradation and increased mobility of the polymer chains reduce the viscosity sufficiently to allow the material to flow. To maintain a constant heat flux on the sample surface, the polymer is mounted on a feeder assembly that moves the sample toward the radiant panel at a rate that keeps the irradiated face at the same distance from the heat source. The rear face of the sample is insulated, so the highest temperatures, and thus the region of flow, are within a narrow layer (2 mm-3 mm) along the heated surface. The sample is 5 cm thick by 10 cm high by 10 cm wide. Although some edge effects are observed, the insulation of side edges keeps the experiment reasonably two-dimensional. The polymer melt is captured by the catch surface below, and load cells monitor the mass of both the melt pool and the polymer remaining in the sample. The difference in mass between the sample and the melt pool indicates the amount of polymer that has gasified.

After the flow onto the catch plate begins, there is a time period during which the rate of mass loss from the thermoplastic object and the rate of mass accumulation on the catch plate are constant. This period continues until the free surface at the top of the object reaches the back wall. The quasi-steady state mass loss rate provides a basis for comparison between model and experiment. Figure 2 shows the values of mass loss rate as a function of incident heat flux from the experiment and from computational results. The difference of approximately 25% between experimental and computational values is due in part to the current neglect in the model of physics such as the melting of the crystalline fraction of the polymer.

The critical material parameter in the modeling of flow behavior is viscosity. As the temperature rises, the viscosity is decreased by both increased mobility of the polymer molecules and degradation of the polymer as bonds break and leave shorter polymer chains. This means that the viscosity is a strong function both of temperature and molecular weight. To avoid an unwieldy calculation of molecular weight distribution in the model, a technique was found to develop a relationship between viscosity and temperature alone. The technique requires rheometric measurements of the original polymer and of samples of the degraded melt from flow experiments run at various heat flux levels. In each case, the rheometer measures viscosity as a function of temperature until the material starts to gasify and bubble. To obtain a viscosity curve through the entire temperature range of interest, the curve for each degraded melt is extrapolated to the temperature at which the melt was generated (the surface temperature measured for that incident heat flux). The viscosity curve for the original polymer is then extrapolated through these points. This technique assumes that the history of the polymer during degradation can be
neglected, and that no further changes occur to the melt after removal from the experiment. Tests support this assumption by finding that doubling the residence time at a given temperature does not affect the melt viscosity.

Figure 3 shows three curves of viscosity vs. temperature for the polypropylene type PD702N, a low viscosity commercial injection molding resin formulation used in these experiments. The relationship used in the model, shown by the black line, connects the curve for the undegraded polymer to points A and B extrapolated from the viscosity curve for each melt sample to the temperature at which the sample was formed. The result is an empirical viscosity-temperature curve that implicitly accounts for molecular weight changes.

The idea for modeling is to treat the polymer melt as a fluid over all temperatures. For the upright object to behave as a solid at room temperature over the duration of the experiment, the viscosity at room temperature is set at $10^6$ Pa-s. Linear interpolation between 25 °C and 200 °C maintains the solidity of the sample at low temperatures. At temperatures above 415 °C, the viscosity is set to the value at point B.

For the melt pool on the catch plate, the temperature-dependent viscosity is that measured for the degraded melt. These viscosities will be much lower than for the original object.

**Two-dimensional melt spread experiment**

To support model development, a separate experiment was set up for investigating the flow of polymer melt on a horizontal or slightly inclined flat surface. The melt flow apparatus described above was used as a well-controlled source of polymer melt. From Figure 2, the quasi-steady state mass loss rate from this apparatus is limited to 0.1 to 0.2 g/s. For flow behavior that is nearly two-dimensional with a reasonable velocity, or spread rate, a 7 cm width was chosen for the catch plate. This results in a satisfactory melt flow about twenty times wider than it is thick, but presents a dimensional mismatch (10 cm wide heated thermoplastic object to 7 cm wide catch plate) that must be taken into account in calculations. Because surface tension causes the melt dripping from the sample to contract laterally and deposit onto the catch plate locally rather than uniformly across the width, a melt feeder device was designed to collect the drips into a slot across the catch plate width punctured along its bottom by five holes. The melt feeder is heated to a temperature high enough to keep the fluid moving but low enough to
minimize gasification and additional degradation. Streams of melt drop evenly through the holes onto the surface, coalescing into a single flow front. The side walls of the catch plate are insulated to minimize thermal effects, and nearly 2D behavior is achieved despite minor transverse viscous effects. In order to prevent the melt from freezing in place due to radiative and convective cooling, the catch plate also needs to be heated to a temperature high enough to sustain flow. This is accomplished by an aluminum heater plate below the catch plate.

A number of parameters needed to be adjusted to find conditions that provided results. In the final set-up, the incident heat flux to the thermoplastic object is 22 kW/m², providing a surface temperature of the flow layer on the sample measured at about 355 °C. The temperature of the spread device is set to 340 °C, and the bottom temperature of the catch plate is set to 235 °C, which gives the top surface a temperature of 207 °C ± 11 °C. The catch plate is a block of unfired alumina silicate ceramic (similar to mullite), 7 cm wide by 24.3 cm long by 1.27 cm thick, with a flat, machined surface. Tests are carried out for a horizontal configuration and for the catch plate tilted down from the melt feeder at 1.8° to the horizontal.

The apparatus is shown to the left in Figure 4. For comparison with the model, the spread velocity is measured by timing the passage of the melt front across lines drawn on the surface of the catch plate. The relationship of viscosity to temperature to describe the degraded polymer melt flowing along the catch plate was obtained by measuring the rheometry of a melt sample extracted from below the melt feeder. This is the purple curve in the viscosity plot in Figure 4. Ideally, a melt sample taken from the far end of the catch plate would show the same rheometry. The fact that it does not, as shown by the green curve in Figure 4, indicates that further polymer degradation is taking place during spreading.

Figure 4. Melt spread experiment. The viscosity plot superimposes curves for melt samples taken below the melt feeder and at the end of the catch plate onto Figure 3

Computation

The Particle Finite Element Method (PFEM) was developed by the International Center for Numerical Methods in Engineering (CIMNE) in Barcelona, Spain. The purpose was to solve problems involving large continuous deformations of the free surface or complicated contacts between different fluids or between fluids and solids. This method has been used to solve a variety of free surface, fluid-structure interaction, and multiphase problems, including dam bursting, wave breaking, ship hydrodynamics, and mold filling.
In the PFEM, all domains, fluid or solid, are modeled using an updated Lagrangian formulation, in which all variables in both fluid and solid domains are known at time $t$ and sought for time $t+\Delta t$. The finite element method is used to solve the continuum equations specific to each domain. This requires a mesh that discretizes the fluid and solid domains and defines the free surfaces and interfaces between them. The fluid and solid regions are not required to be stationary, so the nodes defining the elements are allowed to move. Each node becomes a material particle, with its own density, acceleration, and velocity, subject to gravity and other forces in the problem. In a single time step, the nodes move to a new position dictated by their individual forces. The new boundaries for the fluid and solid domains are then identified. This is not a trivial task because some boundaries may be severely distorted (such as the free surface of fluids) and some particles or groups of particles may have separated from the bulk of the material. The alpha-shape method, described below, is used to define the boundaries of all domains. The domains are then discretized with a finite element mesh using a method based on the extended Delaunay tessellation, in which a random collection of particles is divided into a mesh of elements of arbitrary polyhedral shapes, including triangles and quadrilaterals. The Lagrangian equations of motion for the fluid and solid domains can then be solved for state variables, including velocities, pressure, and viscous stresses in the fluid, displacements, stresses, and strains in the solid, and temperature throughout, and the next time step proceeds.

The alpha-shape method for boundary detection is illustrated in Figure 5. To determine which particles are on the surface of a domain, circles (or spheres in three dimensions) are drawn touching two or more points. Any nodes that are on an empty circle with radius greater than $a h$, where $h$ is the local minimum distance between two particles and $a$ is a parameter close to but greater than one, are considered to be boundary nodes. Figure 5 illustrates the detection of the boundary of a large domain with a hole in it and two separated droplets, one defined by three nodes and the other by a single particle.

Figure 5. Alpha shape determination of domain boundaries

Of particular interest for the dripping problem is the process by which the particles falling off the thermoplastic object land on the catch plate. Figure 6 illustrates the approach of a fluid mass toward a wall. In this illustration, $C$ denotes the cloud of particles, $G$ the boundary of the fluid mass derived from the particle locations, and $V$ the analysis domain for the fluid, with superscripts $n$ and $n+1$ denoting times $t_n$ and $t_{n+1}$. The alpha-shape method detects when a particle approaches to a point $h^c$ within a critical distance $h_{crit}$ of the wall. When this occurs, the incompressibility constraint prevents the particle from going through the wall and converts momentum toward the wall into momentum parallel to the wall. The particle experiences two additional forces: a normal force proportional to the difference ($h^c - h_{crit}$) in the direction away from the wall and a tangential force proportional to viscosity times the normal force pointed in the same direction as the original tangential velocity. This procedure puts a limitation on the time step for the dripping thermoplastic problem, since drops must be detected before they travel through the catch plate.
MODEL

In the two-dimensional PFEM model of the melt spread experiment, the initial computational space is an upright rectangle representing the thermoplastic object mounted above a rectangular catch plate, as illustrated in Figure 7. For ease of defining the distinction between melt belonging to the object and that in the melt pool, the catch plate always extends along the x-axis. A catch plate that is tilted with respect to the horizontal is therefore modeled by tilting the object with respect to the y-axis, with the gravity vector tilted as well to keep it parallel to the object. The object is initially 2.5 cm thick by 10 cm high. This is half the thickness of the samples subjected to experimental testing but with the same mass loss rate during the quasi-steady state flow period.

The left surface of the object and the top surface of the catch plate are designated as free surfaces, which are subject to heat losses from radiation and convection. A steady heat flux is applied only to the free surface of the object, whose drips are distinguished from the melt on the catch plate by location above a specified value of y. All other faces in the problem, identified by dark lines in Figure 7, obey no-slip conditions. These faces are adiabatic, except for the bottom surface of the catch plate, which is maintained at a fixed heater temperature. The thermoplastic object is initially at room temperature, and the linear temperature distribution within the catch plate balances the heat losses from the upper surface. The temperature of the top surface, given the heater temperature and the thermal conductivity of the catch plate, was found to agree with the experimental value.

Material properties for the polymer are identical to the values used to obtain mass loss rates in Figure 2. Viscosity follows the black curve in Figure 4 until the melt drips onto the catch plate, after which the viscosity of the degraded melt tracks the purple line. Density, thermal conductivity and specific heat are considered constant. The ceramic catch plate is assigned the thermal properties reported by the manufacturer.

The spatial resolution of the finite element mesh is initially uniform throughout the thermoplastic object. Figure 7 shows a relatively coarse grid with initial spacing between particles of 2.0 mm, and results are reported for a fine grid with initial spacing of 1.0 mm. For the catch plate, the mesh size at the top surface must be small enough to catch the particles dripping from the object, but the mesh can be coarser further in-depth since only thermal diffusion needs to be resolved.
RESULTS

Figure 8 shows a snapshot of flow onto a horizontal catch plate at time $t = 600$ s. Directly below the base of the object where the polymer melt is dripping, the temperature of the melt pool is around 340 °C. This equals the set temperature of the melt feeder used in the experiments. The temperature of the melt pool cools as it flows away from the line of dripping and loses heat to the catch plate and to the surroundings. At far enough distances the surface temperature of the melt pool drops below the temperature of the catch plate. If the plate was not heated, the polymer would continue to cool, until its viscosity may be high enough to interfere with the flow. Note that beneath the dripping the catch plate itself is heating – different thermal properties or different boundary conditions for the plate will change the thermal transport and may also affect the flow.

Figure 8. Thermoplastic object dripping into horizontal catch pan at $t = 600$ s
Figure 9 shows the evolution of the melt pool with time as the object continues to drip. The spread rate is determined by a balance between the potential energy caused by the accumulation of melt under the drip line, the kinetic energy of the flow and the viscous drag on the melt as it moves over the catch plate.\textsuperscript{11}

Figure 9. Spread of melt pool over horizontal catch plate

In Figures 10 and 11, the catch plate has been tilted at an angle of 1.8°. The slope of the plate adds to the potential energy of the melt, and the spread rate increases in the downslope direction while it decreases in the upstream direction where the accumulation of fluid must counter the potential energy due to the slope.

Figure 10. Thermoplastic object dripping into tilted catch plate at t = 600 s
The spread rate can be measured as the slope of the locations of the particles at the right and left ends of the flow plotted against time. The blue markers in Figure 12 track the progress of the melt fronts in each direction with time for the horizontal and tilted cases. After about 100 s to 150 s in each case the spread rate becomes constant. A linear fit to the data under the blue lines gives spread rates of 0.194 and 0.195 mm/s in the horizontal case and 0.111 and 0.233 mm/s in the tilted case.

These values must undergo two adjustments before they can be compared to the experimental values. First, from Figure 2 it is known that the mass loss rate from the thermoplastic object calculated by the PFEM model is about 25 % too high relative to experiment. Further, a significant fraction of the mass loss rate is due to gasification, which is not included in the model. The melt flow rate onto the catch plate is measured in the experiment as 0.098 g/s for the horizontal case and 0.090 g/s for the tilted case. The quasi-steady state mass loss rates calculated by the model over the time periods used for the linear fits are 0.147 g/s and 0.132 g/s for the horizontal and tilted cases respectively. Thus the flow onto the catch plate calculated by the model needs to be corrected by a factor of 0.098/0.147 or 0.090/0.132, which each equal about 0.67.
The second adjustment is the dimensional mismatch in the experiment, from the 10 cm wide object to the 7 cm wide catch plate. Since the model assumes an equal (infinite) width for both object and catch plate, the flow onto the catch plate must be multiplied by $10/7 = 1.43$ to proportionately increase the flow.

The flow onto the catch plate calculated by the model must be corrected by multiplying these two factors together in order to provide a good comparison with experiment. The two factors combine to give 0.96, or nearly 1. Remarkably, then, the dimensional mismatch in the experiment almost exactly balances the lack of gasification and other discrepancies in the calculation of flow onto the catch plate, and the model results can be compared directly with the experimental results. This is done in Table 1.

<table>
<thead>
<tr>
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<th>Melt Front Velocity (mm/s)</th>
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<tr>
<td></td>
<td>Horizontal</td>
<td>1.8° Tilt, upward</td>
<td>1.8° Tilt, downward</td>
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<tr>
<td>Experiment</td>
<td>0.22 – 0.24</td>
<td>?</td>
<td>0.35</td>
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<td>PFEM model</td>
<td>0.19, 0.20</td>
<td>0.11</td>
<td>0.23</td>
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<tr>
<td>PFEM model using 0.5 µ</td>
<td>0.20, 0.22</td>
<td>0.12</td>
<td>0.33</td>
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</table>

The melt front velocities calculated by the PFEM model and measured in the experiment for the horizontal catch plate are in reasonably good agreement. However, for the tilted catch plate the model calculates a spread rate only two-thirds that measured in the experiment. The viscosity plot in Figure 4 provides a possible answer to this discrepancy. Recall that the rheometry of the melt sample taken from the end of the catch plate differed from that taken under the melt feeder, indicating that the melt continued to degrade as it spread. From Figure 4, the viscosity is approximately halved from the beginning to the end of the catch plate. If the viscosity over the catch plate is halved in the model, the results, plotted in red in Figure 12 and listed in Table 1, increase only slightly for the horizontal case and the upward spread over the tilted catch plate, but the downward spread is now very close to the experimental result. So the differences between the experimental and modeling results may be explained by the difficulties of finding a catch plate temperature that both keeps the melt pool fluid and prevents continuing decomposition.

**CONCLUSION**

Despite difficulties in setting up an experiment that represents two-dimensional melt flow over a catch plate and heats the spreader and catch plate sufficiently to prevent cooling and re-solidification of the melt, the spread rate calculated for horizontal and slightly tilted catch plates is within 10% of experimental results when continuing degradation of the polymer is taken into account. Although the model used here does not yet include gasification, in-depth heat absorption, and other phenomena, the temperatures of the melt pool are low enough that many of these factors do not have a large effect.

**ACKNOWLEDGMENTS**

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REFERENCES

16 Eugenio Onate presentation, by permission.