



A flame spread simulation based on a comprehensive solid pyrolysis model coupled with a detailed empirical flame structure representation



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ABSTRACT

A new model, which represents a unified description of material thermal degradation and burning under thermally thin (non-dimensional), surface radiant heating (one-dimensional) and upward flame spreading (two-dimensional) conditions, has been developed by coupling the numerical pyrolysis solver ThermaKin2D, whose function is to compute the transient rate of gaseous fuel production of a material in response to external heat transfer, with an empirical flame model that predicts a wall flame's heat feedback profile as a function of material mass loss rate. A previously developed pyrolysis model of poly(methyl methacrylate), which was parameterized using a combination of milligram-scale simultaneous thermal analysis experiments and gram-scale gasification tests, was validated in this study using gasification experiments distinct from those utilized in the parameterization process. A previously developed wall flame model was reformulated to include results of new heat flux measurements from 3 to 20 cm above the base of the flame. Inclusion of these results improved the model's predictive capabilities at ignition and across a larger range of flame sizes. The new unified model was employed to predict vertical burning and upward flame spread on 4 and 17.5 cm tall samples of poly(methyl methacrylate). The model predictions – including time to ignition and initial, peak, and rate of rise of sample mass loss rate – were found to closely match experimental results. The impacts of melt flow effects and uncertainties in the flame model formulation on the unified model predictions were examined and found to be moderate.

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1. Introduction

Upward flame spread has long been recognized in the fire safety field as a highly important process, one that frequently defines the early stages of fire growth. Not only is flame spread over a material's surface typically present following ignition [1], but it is most rapid, and thus most hazardous, in the upward direction [2]. As synthetic polymers are used in a multitude of applications across a wide and growing range of built environments, understanding how these materials behave in upward flame spread scenarios becomes increasingly important. Unfortunately, common test standards used to provide some measure of material flammability typically provide only qualitative observations of material response to specific test conditions and consequently show limited ability to predict material performance in other fire scenarios [3]. Additionally, conflicting assessments often arise from different tests [4].

Despite these complications, the fundamentals of flame spread governing dynamics have been understood for decades [5]. Flame

spread is known to be controlled by a positive feedback between coupled processes of solid degradation and gas phase combustion. As gaseous degradation products react with the ambient oxidizer in a diffusion flame, a fraction of the heat produced in this reaction is transferred back to the solid, causing further degradation and production of flammable gases. In vertical wall fires, this process has the potential for rapid growth because gaseous fuel moves upward, driven by buoyancy, and burns downstream from where it was created, thus heating a region of the solid that is not yet degrading.

Challenges that continue to limit attempts at producing an accurate flame spread model include the inherent difficulties associated with obtaining experimental measurements of the key properties of the system [6] and maintaining a balance between including every feature of phenomenological significance and only those of primary importance [7] to maintain computational feasibility. The ultimate goal, when studying flame spread, is to be able to predict flame spread rate, and thus determine how quickly a fire grows. Early attempts to do so, such as those by Saito et al. [8] or Sibulkin and Kim [9] which have repeatedly been used as frameworks in numerous later works, offer simplified descriptions of the system in order to obtain an analytical solution. These descriptions rely upon a number of assumptions such as constant flame height, single values

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of flame to surface heat flux to describe the heat feedback profile, and simplified solid heat transfer and degradation mechanisms.

As time progressed and both computational power and understanding of the controlling mechanisms of flame spread increased, models of constituent processes have correspondingly improved in detail and accuracy. Solid phase pyrolysis models have evolved from one-dimensional, steady-state formulations to multi-dimensional, time-resolved solvers with multi-reaction degradation chemistry and temperature and composition resolved thermophysical properties [10,11]. Flame heat flux models have also advanced from prescribing a single, constant value between the flame's base and some effective measure of flame height, to predicting flame height as a function of material burning rate and capturing variation in the heat flux with height [12–14]. Recently, promising results were obtained by applying Direct Numerical Simulations to modeling of laminar wall flames [15] and Large Eddy Simulations to modeling turbulent wall fires [16]; however, the computational costs associated with the necessity to resolve near-wall convection and conduction for laminar wall flames and soot production and radiation for turbulent fires remain high.

Here we report the results of the first attempt to combine a highly spatially resolved empirical model of flame heat feedback with a state-of-the-art pyrolysis model to simulate the early stages of the upward flame spread process. The heat feedback model was formulated based on detailed measurements of heat flux from a flame spreading on 15 cm tall, 5 cm wide samples of poly(methyl methacrylate) (PMMA) [17]. This sample size was selected as it represents the critical length scale at which, in likely ignition scenarios, flame spread is the most important hazard determining fire growth. Additionally, experimental studies on the burning behavior of PMMA have indicated that 5 cm is the minimum width that, when samples are ignited uniformly across their base, produces the same width-normalized burning rate as observed for wider samples [18]. The flame model consists of an analytical expression that calculates flame heat feedback, expressed as a function of the distance from the base of the flame, based on width-normalized material mass loss rate. At this point, this model is material specific; however, mounting evidence indicates that it can be generalized to an arbitrary solid through straightforward scaling [19, 20].

In the current study, the flame heat feedback model has been reformulated to include results of measurements of flame heat flux from 3 to 20 cm above the base of the flame and combined with a recently developed numerical pyrolysis solver, ThermaKin2D [10], whose function is to compute the transient rate of gaseous fuel production of a material in response to boundary conditions defined, primarily, by the flame heat feedback. The pyrolysis model was parameterized using a combination of milligram-scale thermal analysis experiments [21] and gram-scale gasification tests performed earlier [22]. The parameterization of this model is summarized in this work and further validated under the range of different boundary conditions supported by the experiments conducted here. The newly developed pyrolysis/flame spread model represents a unified description of material degradation and burning under thermally thin (non-dimensional), surface radiant heating (one-dimensional) and upward flame spreading (two-dimensional) conditions. This model bridges a range of length scales and offers a unique path for development of rigorous quantitative relationships between various flammability test standards.

2. Methods

2.1. Material selection

The PMMA used in the current study was purchased in the form of 5.9 mm thick, clear, extruded sheets produced by Evonik Industries and distributed by US Plastics. PMMA was selected because it is a widely used, easily ignitable, non-charring material that does not

form excessive amounts of soot while burning. Although cast PMMA is often utilized in research because it does not soften and flow during heating in the vertical configuration, which makes it easier to study, this form of the material is seldom used in common engineering applications. Thus, in this work, extruded PMMA was studied to better understand the behavior of a material that is representative of commodity plastics. During flame spread experiments, this material exhibited a moderate melt flow, which was analyzed and accounted for as described in later sections of this manuscript. In all bench scale tests conducted in this work, samples were mounted onto sheets of Kaowool PM insulation, which has well-defined thermophysical properties [23]. Both PMMA samples and insulation were dried in a desiccator in the presence of Drierite for a minimum of 24 h prior to use in any experiments.

2.2. Thermal analysis and gasification experiments

In a previous work, 4–7 mg samples of PMMA (cut from the extruded sheets) were subjected to linear heating at a rate of 10 K min⁻¹ in a nitrogen atmosphere using a Netzsch F3 Jupiter simultaneous thermal analyzer capable of thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). Mass of and heat flow into these samples were recorded as a function of time and temperature and a careful analysis was conducted to derive both kinetics and thermodynamics of the material's thermal decomposition. A complete description of these experiments and analysis is provided in a recent publication [21].

In a follow-up work [22], bench scale gasification experiments were conducted to parameterize heat transfer through PMMA. Radiation absorption coefficient, α , was determined by exposing the top surface of a 2.0 mm thick PMMA sample to 35 kW m⁻² of collimated incident radiant heat. Radiation transmitted through the sample was measured by a water-cooled Schmidt-Boelter heat flux gauge and a Beer-Lambert-law based expression (taking into account reflected radiation at the polymer-air interfaces) was used to compute α . Material thermal conductivity, k , was also determined in this work by exposing 6.0 mm thick PMMA samples to 20 kW m⁻² of incident radiant heat and measuring temperature rise at their back surfaces using an infrared camera. Inverse modeling was employed to derive temperature dependent k from these measurements. Collectively, these results fully parameterize a pyrolysis model that was used to predict mass loss rate histories of 6.0 mm thick PMMA samples exposed to 20–60 kW m⁻² of external radiant heat flux. Predicted mass loss rates were found to be, on average, within 10% of the experimental values.

In the aforementioned work, the radiation driven gasification experiments were conducted with samples mounted on a 0.8 mm thick aluminum mesh, which exposed their back surface to the ambient atmosphere. In flame spread experiments performed in this study, samples were mounted on Kaowool PM insulation. To ensure that boundary conditions employed in earlier tests did not affect the pyrolysis model parameterization and to validate its ability to simulate the tests conducted in this study under these new back surface boundary conditions, a series of gasification experiments were conducted at several radiant heat fluxes and simulated in ThermaKin2D. Here, 80 × 80 × 5.9 mm³ samples of PMMA were gasified using controlled radiant heating in a Govmark CC-1 cone calorimeter [24] equipped with the Controlled Atmosphere Pyrolysis Apparatus (CAPA) as seen in Fig. 1. The cone calorimeter radiant heater was used to deliver a nearly uniform and steady heat flux to the top surface of a horizontally mounted sample, while the calorimeter's precision balance system monitored sample mass. The CAPA was used to provide a controlled gaseous environment in the immediate vicinity of the sample. A detailed description of the CAPA design and operation is provided in a recent publication [25].

In all current experiments, the CAPA was operated at 225 L min⁻¹ of nitrogen (measured at 1 atm and 298 K). The cone calorimeter

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