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A generalized model of flame to surface heat feedback for laminar wall flames



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ABSTRACT

In this work, experimental measurements of flame heat flux and sample mass loss rate are obtained as a diffusion flame spreads vertically upward (in the direction opposed to the vector of gravity) over the surface of seven commonly used polymeric materials, two of which are glass reinforced composites. Using these measurements, a previously developed empirical flame model specific to poly(methyl methacrylate) is generalized such that it can predict (flame to material surface) heat feedback from 3 to 20 cm tall flames supported by a wide range of materials. Model generalization is accomplished through scaling on the basis of a material's gaseous pyrolyzate heat of combustion, which can be measured using mg-sized material samples in a microscale combustion calorimeter. For all seven materials tested in this work, which represent diverse chemical compositions and burning behaviors including polymer melt flow, sample burnout, and heavy soot and solid residue formation, model-predicted flame heat flux (to a water-cooled heat flux gauge) is shown to match experimental measurements taken across the full length of the flame with an average absolute error of $3.8 \, \text{kW} \, \text{m}^{-2}$ (approximately 10–15% of peak measured flame heat flux). Coupled with a numerical pyrolysis solver, this generalized wall flame model provides the framework to quantitatively study material propensity to ignite and support early fire growth in a range of common scenarios with a level of accuracy and reduced computational cost unmatched by other currently available modeling tools.

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1. Introduction

Understanding the dynamics of fire inception and growth on organic solids is highly important for engineering fire safety in the built environment. Among organic solids, synthetic polymers and polymer based composites are used increasingly due to their low weight, highly customizable properties, low cost, and energy efficiency [1]. At the same time, it is also understood that these materials can present a greater fire safety hazard than traditional building materials [2]. Thus, understanding their resistance and reaction to fire is crucial. A variety of standard test methods have been developed by organizations such as ASTM International [3,4] and UL [5,6] to assess material flammability in terms of ignitability, heat release and surface flame spread. Although these bench scale tests are widely used, they typically provide observations of material response to a specific set of conditions. Consequently, conflicting assessments often arise from different tests [7] and they show limited ability to predict material performance in other fire scenarios

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[8]. A more rigorous approach to assessing material flammability, which would allow for the proactive design of new, safer materials, is to characterize the controlling mechanisms of a fire behavior of interest and develop models that accurately describe these constituent processes. In this manner, the behavior of a material in response to a wide range of likely fire conditions can be better understood and predicted.

Upward, concurrent-flow flame spread over the surface of a material has long been recognized in the fire safety field as a highly important process because it is a key determinant of the initial rate of fire growth [9]. It has been well established [10,11] that surface flame spread is governed by positive feedback between transient processes of solid phase degradation (pyrolysis) and gas phase combustion. As a solid is heated, it degrades and produces gaseous pyrolyzates that can react with the ambient oxidizer to form a diffusion flame. Some of the heat produced by this flame is transferred back into the solid thus allowing for continued degradation and production of flammable pyrolyzates. Upward spreading flames may grow rapidly because hot combustion products, driven upward by buoyancy, heat up a part of the solid that is not yet degrading, which causes continuous expansion of the pyrolysis region.

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Early flame spread models (e.g. Grant and Drysdale [7] or Saito et al. [12]) attempted to provide an analytical solution for flame spread rate by relying on a number of coarse assumptions including constant flame height, a single value of flame to surface heat flux (to describe the entire flame heat feedback profile), and simplified treatments of decomposition and heat transfer in the solid phase. Despite these simplifications, these early models formed a solid foundation for later works that have incorporated more detailed descriptions of the constituent processes [13]. Development of generalized numerical pyrolysis models [14–16], which include submodels for chemical reactions, phase transitions, and transient heat transfer through the condensed phase characterized by temperature- and composition-resolved thermophysical properties, has opened new opportunities for further flame spread model development.

These opportunities were explored in our recent study [17] where a generalized numerical pyrolysis model, ThermaKin2D, was coupled with an empirical model of a flame spreading upward on 17.5 cm tall samples of poly(methyl methacrylate) (PMMA). The flame model was based on highly spatially resolved measurements of flame heat flux to the sample's surface and was formulated to compute the flame's heat feedback profile solely as a function of the width-normalized mass loss rate, which was calculated by the pyrolysis model. This unified model was shown to accurately predict flame spread dynamics and mass loss evolution of 4.0 and 17.5 cm tall PMMA samples, while using a small fraction of computational resources required for a computational-fluid-dynamics-based simulation of the same system [18].

A key limitation of this flame model was that it could only be applied to PMMA. In the current study, that limitation is removed. Spatially resolved measurements of flame heat flux and mass loss rate were obtained during upward flame spread over the surface of vertically oriented solid samples, which were up to 20 cm in height. Seven polymeric solids representing a wide range of chemical compositions and burning behaviors, including melt flow, sample burnout and heavy soot and solid residue formation, were utilized in these experiments. Heats of combustion of gaseous pyrolyzates produced by these materials were also measured. Several model parameter scaling approaches based on the established theory of flame structure were examined. The approach that provides the best agreement between experimental measurements and model predictions was identified.

2. Flame model formulation and scaling

Knowledge of heat transfer across the length of a flame into a burning material's surface is required to predict the rates of upward flame spread over that material [19]. Thus, in fire science, flame height is considered to be a critical parameter describing flame structure. Flame height has been defined in the literature in multiple ways: e.g. based on visual determination of the flame tip [12] or the average location of the visible flame [20], as the position corresponding to a critical fuel concentration [21], or based on a threshold value of wall heat flux [17]. Previous analysis of PMMA wall flames [22] revealed that wall heat flux at the flame tip is about 20% of the value in the continuous region. Thus, the location of luminous flame tips is not the ideal characteristic length scale for flame heat transfer. Consequently, in our previously developed PMMA flame model [17], we defined a "heat flux flame height", y_f , as the distance from the base of the flame to the highest point where measured wall flame heat flux is within 97.5% of its steady state value, $q_{steady}^{\prime\prime}$. $q_{steady}^{\prime\prime}$ can be measured under the continuous region of the flame and it is, on average, within 2 kW m⁻² of the maximum heat flux observed at that same location. Previously, y_f was related to width-normalized mass loss rate,

 $\frac{dm'}{dt}$; however, a multitude of experimental and theoretical observations [12,20,21,23,24] indicate that, for both laminar and turbulent buoyancy driven diffusion flames, including wall fires, flame height is a function of heat release rate. Therefore, it is expected that the relationship for this heat flux flame height scales with the ratio of the heats of combustion:

$$y_f = a \left(\frac{\Delta H_c^{MATL}}{\Delta H_c^{PMMA_{EXT}}} \frac{dm'}{dt} \right)^p + b \tag{1}$$

Here, ΔH_c^{MATL} represents the heat of combustion of the gaseous pyrolyzates of the material which is being modeled; $\Delta H_c^{PMMA_{EXT}}$ represents the heat of combustion of the pyrolyzates of extruded PMMA, the material for which this flame model was originally developed; and *a*, *p*, and *b* are empirically derived constants. In this expression, mass loss rate is divided by $\Delta H_c^{PMMA_{EXT}}$ because the constant *a* already implicitly includes this value and it is multiplied by ΔH_c^{MATL} to be converted to heat release.

Net flame heat flux, q''_{flame} , is expressed in our flame model in terms of y_f and several additional parameters:

$$q_{flame}^{\prime\prime} = \begin{cases} h_{flame}(T_{fl,\max}^{MATL} - T_{surf}) & \forall y \leq y_{f} \\ h_{flame} \left(\alpha_{f} \left(T_{fl,\max}^{MATL} - T_{HFg} \right) e^{-\ln(\alpha_{f}) \times (y^{*})^{2}} + T_{HFg} - T_{surf} \right) & \forall y > y_{f} \end{cases}$$

$$(2)$$

$$y^* = \frac{y + y_0}{y_f + y_0}$$
(3)

$$T_{fl,max}^{MATL} = \begin{cases} T_{fl,adiabatic}^{MATL} & \forall \quad y \le 5 \text{cm} \\ 0.87 \times T_{fl,adiabatic}^{MATL} & \forall \quad y > 5 \text{cm} \end{cases}$$
(4)

For laminar wall flames, q''_{flame} has been shown to be primarily convective in nature [19]. Specifically, our previous measurements have shown that the radiative component of these flames accounts for less than 20% of total measured flame heat flux for $y_f \le 15$ cm [18]. Thus, in this model, q''_{flame} is defined based on a classical convection heat transfer expression. The impact of a "blowing effect" [25,26] (in which an increased flux of gaseous pyrolyzates increases flame standoff distance and reduces convective heat feedback) on measured heat transfer in this system was found to be minor [17,18,27] and thus it is not explicitly included in the model expressions.

In Eq. (2), h_{flame} is a heat transfer coefficient that captures both the dominant convective and minor radiative components of flame to surface heat transfer. h_{flame} is defined as a single constant value across the sample's surface; its calculation is detailed in a later section of this manuscript. $T_{fl, adiabatic}^{MATL}$ is the adiabatic flame temperature (in K) for the stoichiometric mixture of gaseous pyrolyzates and air, which has been shown to reasonably approximate the maximum temperature of laminar wall flames [17,28]. In the previously developed flame model, this temperature was computed for pyrolyzates of PMMA [17]. In this study, $T_{fl, adiabatic}^{MATL}$ was computed for each material of interest based on their respective ΔH_c^{MATL} values, which were measured using several techniques discussed in the following sections, together with the known atomic composition of their pyrolyzates.

 $T_{HFg} = 291$ K is the average temperature of the water used to cool the heat flux gauge utilized for flame heat flux measurements and T_{surf} is the temperature (in K) of the surface into which the flame heat flux is calculated. When T_{surf} is set equal to T_{HFg} , Eq. (2) calculates flame heat flux as measured by the water-cooled heat flux gauge, q''_{HFg} . *y* is the distance downstream from the base of

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