A 3-Step Reaction Model of Smoldering and Flaming Combustion

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Introduction

Smoldering combustion is characterized by the slow, low temperature, flameless burning of solid fuel and is the most persistent type of combustion [4]. Flaming combustion, in contrast, involves a higher temperature burning of gaseous fuel and is rather limited in how long it can be sustained. Smoldering and flaming combustion are very interrelated, often occurring simultaneously in nature and seeming to feed into each other. Despite this inter-relatedness, the literatures of the two are somewhat sparsely connected [5]. Better understanding the mechanics of transition between smoldering and flaming combustion, and how the two work to sustain each other, is an especially relevant topic of study in fire safety, engineering, ecology, and earth science contexts alike, among others. This project expands on previously developed models, including [1], [2], and [3], complicating the combustion reaction scheme in order to be able to support both smoldering and flaming solutions in a single model.

Reactions

Because combustion involves thousands of unknown and context-specific chemical reactions, most models consider the process as happening in one or more general reaction steps. For the purposes of exploring the transition between smoldering and flaming combustion, this project uses a three step reaction scheme for opposed-flow smolder:

$$\text{oxygen} + \text{solid fuel} \rightarrow \text{char} + \text{flammable gas} \quad (1)$$
$$\text{oxygen} + \text{char} \rightarrow \text{ash} + \text{smoke} \quad (2)$$
$$\text{oxygen} + \text{flammable gas} \rightarrow \text{smoke}. \quad (3)$$

Smoldering is characterized by reaction (2), where combustion occurs within the solid medium, while flaming is characterized by reaction (3), where combustion occurs between gaseous components. Both types also include reaction (1), a process of pyrolysis and fuel oxidation, that creates the char necessary for smoldering to occur and the flammable gases necessary for flaming.

Mathematical Model

The model includes nine differential equations, nondimensionalized and converted into a moving coordinate system, that describe the energy, gas momentum, and changing masses of products and reactants. Energy (4), fuel mass (5), oxygen mass (6), and total gas mass (7) equations are included below.

$$\frac{\partial \theta_C}{\partial t} + u\frac{\partial \theta_C}{\partial x} + \frac{1}{\bar{\rho}\bar{c}}\frac{\partial\left(\frac{M}{\bar{C}}\right)\theta_C}{\partial x} = \frac{\partial^2\left(\frac{1}{\bar{C}}\right)\theta_C}{\partial x^2} + Q_1W_1 + Q_2W_2 + Q_3W_3 \quad (4)$$
$$\frac{\partial \rho_f}{\partial t} + u\frac{\partial \rho_f}{\partial x} = -W_1 \quad (5)$$
$$\frac{\partial \rho_g Y}{\partial t} + u\frac{\partial \rho_g Y}{\partial x} + \frac{\partial \rho_g v_g Y}{\partial x} = \frac{1}{Le_{ox}}\frac{\partial^2 Y}{\partial x^2} - \mu_{ox1}\bar{\rho}W_1 - \mu_{ox2}\bar{\rho}W_2 - \mu_{ox3}W_3 \quad (6)$$
$$\frac{\partial \rho_g}{\partial t} + u\frac{\partial \rho_g}{\partial x} + \frac{\partial \rho_g v_g}{\partial x} = \bar{\rho}(\mu_{c1} - 1)W_1 + \bar{\rho}(\mu_{a2} - 1)W_2 + (\mu_{sm3} - 1)W_3 \quad (7)$$

- space: x
- time: t
- speed of wave: u
- temperature: θ_C
- heat capacity: C
- gas mass flux: M
- gas density: ρ_g
- incoming gas speed: v_g
- oxygen fraction: Y
- reaction rates: W_1, W_2, W_3
- oxygen Lewis number: Le_{ox}
- solid/gas conversions: $\bar{\rho}, \bar{c}$
- stoichiometric parameters: $\mu_{c1}, \mu_{a2}, \mu_{sm3}, \mu_{ox1}, \mu_{ox2}, \mu_{ox3}$

Simulations

The full system of PDEs was simulated using a finite difference approximation scheme in MATLAB. Figures 1-3 present three solutions resulting from the use of different parameters (described further in the Results section).

Figure 1: Pyrolysis and Fuel Oxidation

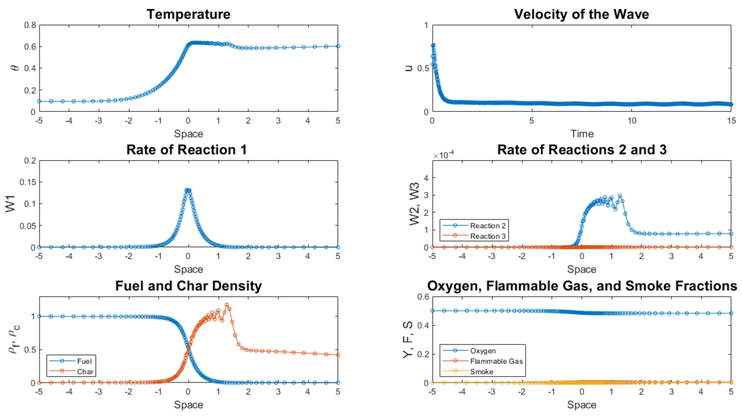


Figure 2: Smoldering

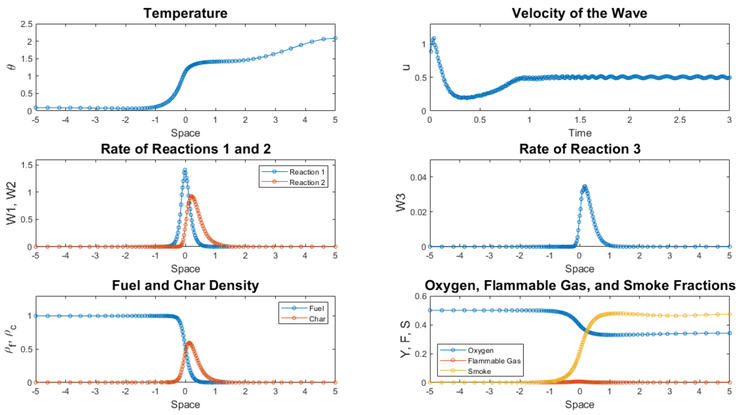
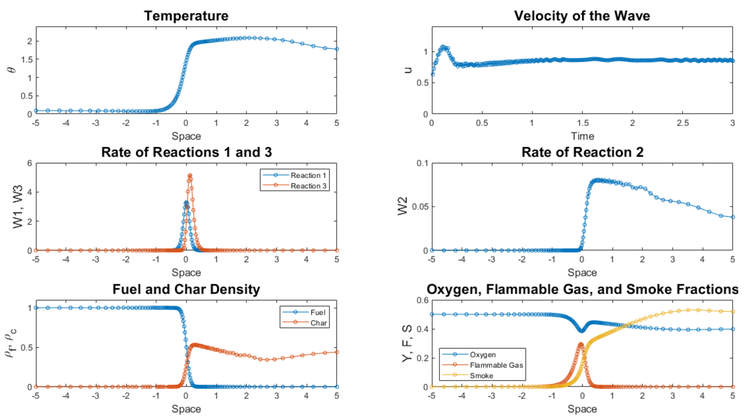


Figure 3: Flaming



Results

These simulations of pyrolysis and fuel oxidation, smoldering, and flaming solutions come from varying three parameters that control the stoichiometric ratio of flammable gas produced per unit solid burned and the ratios of reactions (2) and (3) to reaction (1). These two reaction ratios are defined as

$$Kr_{2,1} = \frac{K_2 e^{-E_2/RT_*}}{K_1 e^{-E_1/RT_*}} \text{ and } Kr_{3,1} = \frac{K_3 P_0 e^{-E_3/RT_*}}{K_1 \rho_g^0 e^{-E_1/RT_*}},$$

where T_* is the burning temperature, R is the ideal gas constant, P_0 is the initial pressure, ρ_g^0 is the initial gas density, E_1, E_2, and E_3 are the activation energies and K_1, K_2, K_3 are the pre-exponential terms of reactions (1), (2) and (3), respectively. Values used for these reaction ratios and the stoichiometric ratio are shown below for each of the three simulations.

	$Kr_{2,1}$	$Kr_{3,1}$	μ_{fg1}
Pyrolysis & Fuel Oxidation	0.01	0.5	0.02
Smoldering	1	2	0.02
Flaming	0.01	0.5	1

Because reaction rates are low, the pyrolysis and fuel oxidation solution was simulated for a longer time with a smaller time-step than the smoldering and flaming solutions. All other parameters and initial conditions were consistent across the three simulations.

In Figure 1, the rates of reactions (2) and (3) are small compared to reaction (1), indicating that mostly pyrolysis and fuel oxidation occur. Analogously, in Figure 2, the higher rates of reactions (1) and (2) indicate smoldering, and in Figure 3, the higher rates of reactions (1) and (3) indicate flaming. The flaming solution in Figure 3 maintains a higher temperature and velocity of the wave than the smoldering solution in Figure 2, as is expected physically. Pulsations in the speed of the propagating waves of each similarly match physical expectations.

Discussion

With differing parameter values, this model is able to support both smoldering and flaming combustion solutions, capturing certain relevant expected physical behaviors. Next steps (a,b) and possibilities for further work (c) include:

(a) Assessing if a region of bi-stability exists, in which a solution could develop to be either smoldering or flaming with the same set of parameters and only differing initial conditions

(b) Utilizing features of the developed system of equations to determine how unequal heat capacities of gases may affect how solutions develop

(c) Creating an adaptive time-stepping scheme and/or new adaptive spatial grid

References and Acknowledgements

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References

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