A Three Step Reaction Model of Smoldering and Flaming Combustion

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Investigating Two Types of Combustion

Smoldering Combustion

- burning of solid fuel
- slow
- low temperature

Flaming Combustion

- burning of gaseous fuel
- fast
- high temperature

These two types of combustion are intimately related, occurring together in nature and seemingly feeding into each other. The aim of this project was to give further insight into this relationship and the transition from smoldering to flaming.

Reaction Steps

Pyrolysis and Fuel Oxidation:

$$\text{oxygen} + \text{solid fuel} \rightarrow \text{char} + \text{flammable gas}$$

Char Oxidation:

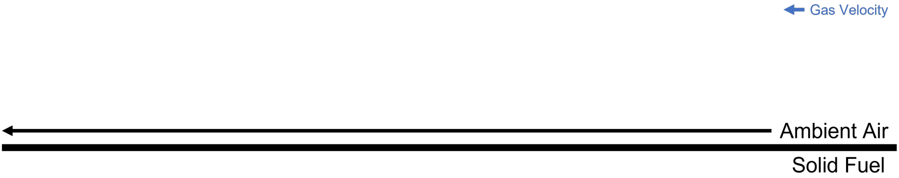
$$\text{oxygen} + \text{char} \rightarrow \text{ash} + \text{smoke}$$

Gas Oxidation:

$$\text{oxygen} + \text{flammable gas} \rightarrow \text{smoke}$$

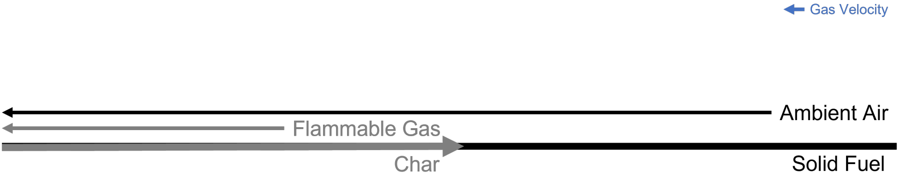
Model

Initial State of the System



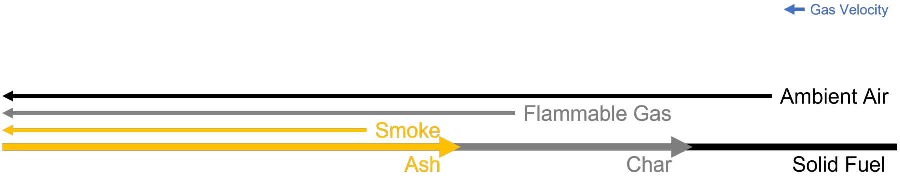
Model

Reaction 1: Pyrolysis and Fuel Oxidation



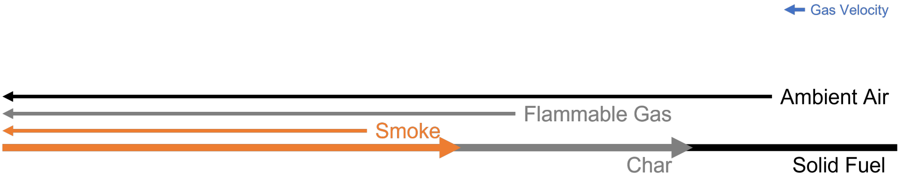
Model

Reaction 1: Pyrolysis and Fuel Oxidation
Reaction 2: Char Oxidation



Model

Reaction 1: Pyrolysis and Fuel Oxidation
Reaction 3: Flammable Gas Oxidation



Mathematical Model: Reaction Rates

Reaction rates (W_i) are assumed to be have an Arrhenius dependence on temperature.

$$W_1 = K_1 P Y \rho_f e^{-\frac{E_1}{RT}}$$

$$W_2 = K_2 P Y \rho_c e^{-\frac{E_2}{RT}}$$

$$W_3 = K_3 P^2 Y F e^{-\frac{E_3}{RT}}$$

P	pressure	ρ_f	solid fuel density
Y	oxygen fraction	ρ_c	char density
F	flammable gas fraction	T	temperature
K_i	pre-exponential terms	E_i	activation energies
R	ideal gas constant		

Mathematical Model: Heat Capacity Terms

Heat capacity terms are constructed such that we can consider unequal heat capacities for each of the products, reactions, and inert gas species in the system:

$$C = c_f\rho_f + c_c\rho_c + c_a\rho_a + c_{ox}Y\rho_g + c_{fg}F\rho_g + c_{sm}S\rho_g + c_i(1 - Y - F - S)\rho_g$$

$$M = \rho_g v_g[c_{ox}Y + c_{fg}F + c_{sm}S + c_i(1 - Y - F - S)]$$

C	weighted heat capacity	M	weighted heat capacity flux
Y	oxygen fraction	F	flammable gas fraction
S	smoke fraction	v_g	gas velocity

ρ densities (for fuel, char, ash, total gas)

c heat capacities (for fuel, char, ash, oxygen, flammable gas, smoke, inert gas)

Mathematical Model: Conservation of Energy

Energy is assumed to be conserved in an adiabatic system with no heat losses:

$$\frac{\partial CT}{\partial t} + \frac{\partial MT}{\partial x} = \lambda \frac{\partial^2 T}{\partial x^2} + Q_1 W_1 + Q_2 W_2 + Q_3 W_3$$

t	time	x	space
C	weighted heat capacity	M	weighted heat capacity flux
T	temperature	W_i	reaction rates
Q_i	heat of reactions	λ	thermal conductivity

Mathematical Model: Solid Masses

Fuel Mass:

$$\frac{\partial \rho_f}{\partial t} = -W_1$$

Char Mass:

$$\frac{\partial \rho_c}{\partial t} = \mu_{c1} W_1 - W_2$$

Ash Mass:

$$\frac{\partial \rho_a}{\partial t} = \mu_{a2} W_2$$

t	time	T	temperature
ρ_f	solid fuel density	ρ_c	char density
ρ_a	ash density	W_i	reaction rates
μ_{c1}	char produced per unit fuel	μ_{a2}	ash produced per unit char

Mathematical Model: Gas Masses

Total Gas Mass:

$$\frac{\partial \rho_g}{\partial t} + \frac{\partial \rho_g v_g}{\partial x} = (\mu_{c1} - 1)W_1 + (\mu_{a2} - 1)W_2 + (\mu_{sm3} - 1)W_3$$

Oxidizer Mass:

$$\frac{\partial \rho_g Y}{\partial t} + \frac{\partial \rho_g v_g Y}{\partial x} = D_{ox}\rho_g \frac{\partial^2 Y}{\partial x^2} - \mu_{ox1}W_1 - \mu_{ox2}W_2 - \mu_{ox3}W_3$$

t	time	x	space
ρ_g	gas density	v_g	gas velocity
Y	oxygen fraction	W_i	reaction rates
μ_{c1}	char produced per unit fuel	μ_{a2}	ash produced per unit char
μ_{sm3}	smoke produced per unit gas	μ_{oxi}	oxygen consumed per reaction
D_{ox}	oxygen diffusion coefficient		

Mathematical Model: Gas Masses

Flammable Gas Mass:

$$\frac{\partial \rho_g F}{\partial t} + \frac{\partial \rho_g v_g F}{\partial x} = D_{fg} \rho_g \frac{\partial^2 F}{\partial x^2} + \mu_{fg1} W_1 - W_3 \qquad (1)$$

Smoke Mass:

$$\frac{\partial \rho_g S}{\partial t} + \frac{\partial \rho_g v_g S}{\partial x} = D_{sm} \rho_g \frac{\partial^2 F}{\partial x^2} + \mu_{sm2} W_2 + \mu_{sm3} W_3 \qquad (2)$$

t	time	x	space
ρ_g	gas density	v_g	gas velocity
F	flammable gas fraction	S	smoke fraction
W_i	reaction rates	μ_{fg1}	flam-gas produced per unit fuel
μ_{sm2}	smoke produced per unit char	μ_{sm3}	smoke produced per unit gas
D_{fg}	flam-gas diffusion coefficient	D_{sm}	smoke gas diffusion coefficient

Mathematical Model: Gas Momentum and Equation of State

This model assumes Darcy's law for fluid flow through a porous medium and the ideal gas law to give the following two equations.

Gas Momentum:

$$\frac{\partial P}{\partial x} = -k_f v_g$$

Equation of State:

$$P = \rho_g RT$$

x	space	P	pressure
v_g	gas velocity	ρ_g	gas density
T	temperature	k_f	friction coefficient
R	ideal gas constant		

Further Developing Equations

Nondimensionalization

To reduce parameters and simplify the system, these equations were combined and nondimensionalized to create a system of nine PDEs

Moving Coordinate System

Then, this system was converted to moving coordinates of the form $\hat{x} = x + ut$, $\hat{t} = t$

- a uniformly propagating wave would then appear as a solution independent of time in this system
- u is the speed of the propagating wave; it is constant in space, but may vary in time with pulsations of the wave
- $\hat{x} = 0$ defined where $\rho_f = \frac{1}{2}$ (where half of fuel is consumed)

to keep the reaction front defined at $x = 0$

Results and Limitations

Results

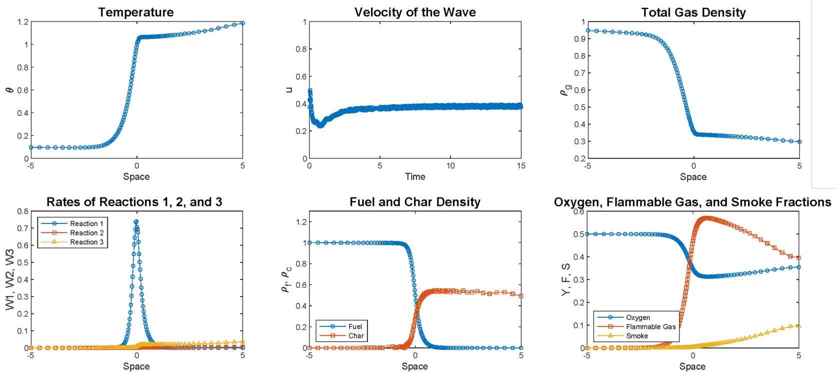
It was found

- this system could support pyrolysis/fuel-oxidation, smoldering, and flaming solution types
- considering unequal gas heat capacities did have qualitative effects on the solutions

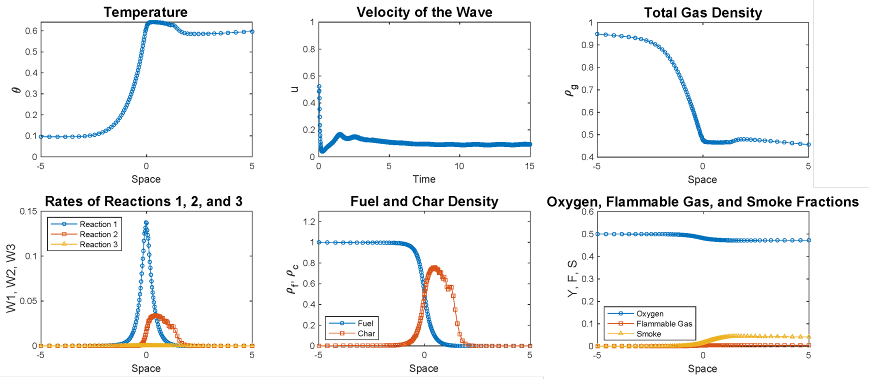
Limitations

- Changing dt significantly affects how the solutions evolve
- Very close to the ending of this project, a sign change mistake was found in the coded finite difference schemes of the oxygen, flammable gas, and smoke fractions. Initial simulations with this error fixed did not seem to help the system's sensitivity to the time-step size, or to dramatically change the types of solutions that can evolve.

Pyrolysis and Fuel Oxidation

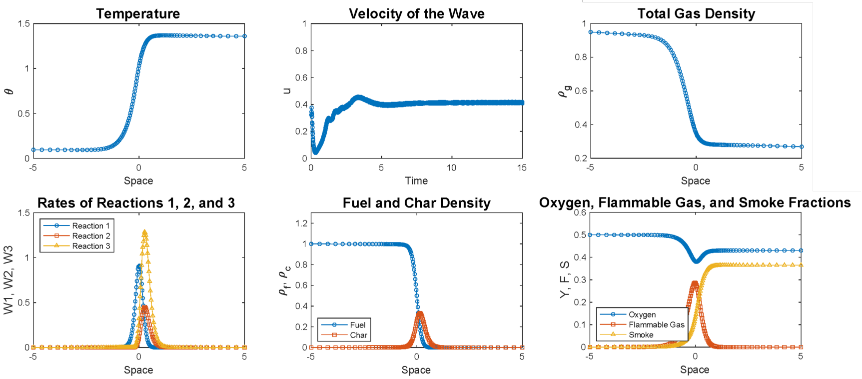


Smoldering



Temperature
θ
Space
Velocity of the Wave
u
Time
Total Gas Density
ρ_g
Space
Rates of Reactions 1, 2, and 3
Reaction 1
Reaction 2
Reaction 3
W1, W2, W3
Space
Fuel and Char Density
Fuel
Char
ρ_f, ρ_c
Space
Oxygen, Flammable Gas, and Smoke Fractions
Oxygen
Flammable Gas
Smoke
Y, F, S
Space

Flaming



Temperature
θ
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Velocity of the Wave
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Time
Total Gas Density
ρ_g
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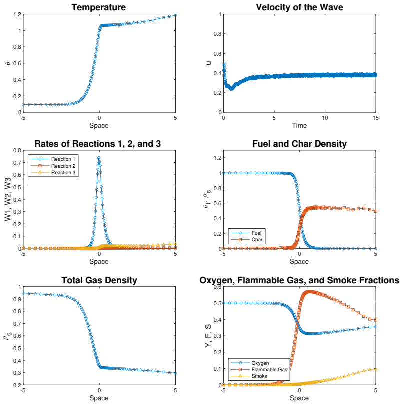
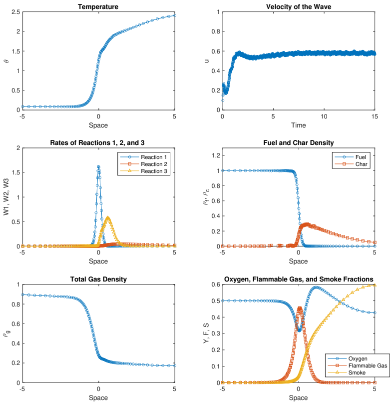
Rates of Reactions 1, 2, and 3
W1, W2, W3
Reaction 1
Reaction 2
Reaction 3
Space
Fuel and Char Density
ρ_f, ρ_c
Fuel
Char
Space
Oxygen, Flammable Gas, and Smoke Fractions
Y, F, S
Oxygen
Flammable Gas
Smoke
Space

Different Gas Capacities: Pyrolysis and Fuel Oxidation

Equal Gas Heat Capacities

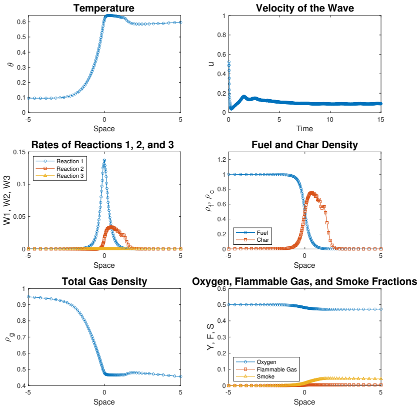


Unequal Gas Heat Capacities

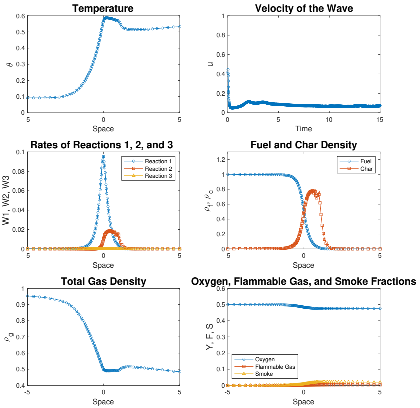


Different Gas Capacities: Smoldering

Equal Gas Heat Capacities

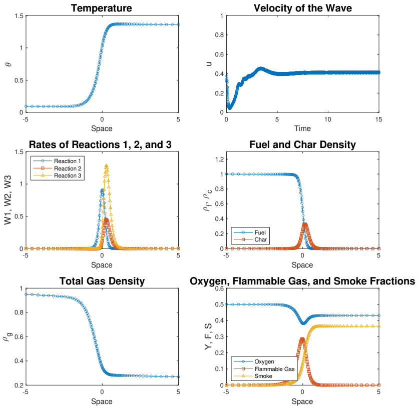


Unequal Gas Heat Capacities

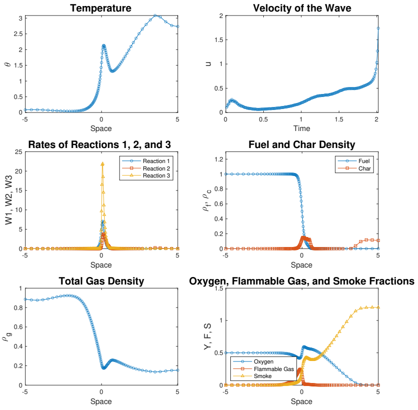


Different Gas Capacities: Flaming

Equal Gas Heat Capacities



Unequal Gas Heat Capacities



Further Work

- Exploring the parameter space with corrected code
- Further looking into changing the effect of dt
- Adding an adaptive time-stepping scheme, that could perhaps help to support more dramatic flaming solutions
- Looking for a region of bi-stability in the parameter space, where either type of solution could form based only on differences in the initial conditions