NUMERICAL STUDY OF INTERACTIONS OF HYDRODYNAMICS,
KINETICS AND RADIATION IN FLAMES

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DEDICATION

I would like to dedicate this thesis to my parents for their emotional and financial support.
ABSTRACT OF THE THESIS

Numerical Study of Interactions of Hydrodynamics, Kinetics and Radiation in Flames
by
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The purpose of this thesis is to simulate flame spread in zero gravity and identify different factors that can impact the flame spread rate. This was possible using the CFD code written in FORTRAN developed by Bhattacharjee. The fuel studied in this thesis is Poly (methyl methacrylate) (PMMA). A mathematical model that shows how spread rate is being calculated is explained. The importance of grids used in CFD was shown by choosing appropriate number of grids for a given domain and a rule for choosing the domain was established. Impact of boundary layer or flow development distance was deeply understood and a formula for flame tip velocity or equivalent velocity was developed. Computational spread rate was then non-dimensionalized by dividing it with spread rate obtained from de-Ris formulae and plotted against Damkohler number which was calculated based on opposed flow velocity and equivalent velocity. A large variation of opposed flow for different fuel thicknesses was plotted against spread rate to show how fuel-half thickness affects the spread rate and the impact of radiation was understood. A critical fuel-thickness up to which flame existed in a quiescent microgravity was computed using this flame code. The impact of oxygen level was also studied in detail for a given fuel thickness. Pressure was varied in the microgravity regime to see its impact on flame spread rate.
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LIST OF SYMBOLS

\( A_s \)  \quad \text{Frequency factor, } 1/\text{s}
\( B_g \)  \quad \text{Pre-exponential combustion factor, } \text{m}^3/\text{kmol.s}
\( c_g \)  \quad \text{Specific heat of gas at constant pressure, kJ/(kg.K)}
\( c_s \)  \quad \text{Specific heat of PMMA at constant pressure, kJ/(kg.K)}
\( c_{hd} \)  \quad \text{Hang distance constant}
\( Da \)  \quad \text{Damkohler number}
\( E \)  \quad \text{Activation energy, kJ/kmol}
\( F \)  \quad \text{Flame constant, } F = \frac{T_f - T_v}{T_v - T_\infty}
\( f \)  \quad \text{Velocity ratio}
\( \Delta h_v \)  \quad \text{Enthalpy of vaporization, KJ/kg}
\( \Delta h_c \)  \quad \text{Enthalpy of combustion, kJ/kg}
\( k \)  \quad \text{Rate of reaction}
\( L_r \)  \quad \text{Reference length, mm}
\( L_R \)  \quad \text{Radiation loss parameter}
\( l_g \)  \quad \text{Reference length, mm}
\( \dot{m}_F \)  \quad \text{Mass flow rate of fuel, kg/s}
\( \dot{m}_F^{''''} \)  \quad \text{Volumetric rate of fuel consumption, kg/m}^3.\text{s}
\( Pr \)  \quad \text{Prandtl number}
\( \dot{Q}_{\text{S,loss}} \)  \quad \text{Surface radiation loss, W}
\( \dot{Q}_{\text{g,loss}} \)  \quad \text{Gas radiation loss, W}
\( \dot{Q}_{\text{Released}} \)  \quad \text{Heat released, W}
\( \dot{q}_R^{''''} \)  \quad \text{Radiative source term, W/m}^3
\( R \)  \quad \text{Ryndberg’s constant, J/kg.K}
\( Re_x \)  \quad \text{Reynolds number}
\( T_s \)  \quad \text{Fuel surface temperature, K}
\( T_\infty \)  \quad \text{Ambient temperature, K}
\( T_v \)  \hspace{1cm} \text{Vaporization temperature, K}
\( T_f \)  \hspace{1cm} \text{Flame temperature, K}
\( t_{res} \)  \hspace{1cm} \text{Residence time, sec}
\( t_{comb} \)  \hspace{1cm} \text{Combustion time, sec}
\( \dot{u} \)  \hspace{1cm} \text{Velocity in x-direction, cm/s}
\( \dot{v} \)  \hspace{1cm} \text{Velocity in y-direction, cm/s}
\( V_f \)  \hspace{1cm} \text{Flame spread rate, mm/s}
\( V_g \)  \hspace{1cm} \text{Opposed flow velocity, cm/s}
\( V_r \)  \hspace{1cm} \text{Relative velocity or the velocity seen by the fuel, cm/s}
\( V_{eq} \)  \hspace{1cm} \text{Equivalent velocity or flame tip velocity, cm/s}
\( W \)  \hspace{1cm} \text{Width, mm}
\( wt \)  \hspace{1cm} \text{Grid weight factor}
\( x_d \)  \hspace{1cm} \text{Flow development distance, mm}
\( x_{O_2} \)  \hspace{1cm} \text{Mass fraction}
\( x_{st} \)  \hspace{1cm} \text{Non-dimensional domain starting position on x-axis}
\( x_l \)  \hspace{1cm} \text{Non-dimensional domain ending position on x-axis}
\( y_l \)  \hspace{1cm} \text{Non-dimensional height on y-axis}
\( y_{exp} \)  \hspace{1cm} \text{Grid weight factor in y-direction}

**Greek symbols used:**

\( \alpha \)  \hspace{1cm} \text{Thermal diffusivity, m}^2\text{/s}
\( \beta_t \)  \hspace{1cm} \text{Dimensionless parameter for de Ris solution}
\( \gamma_{hyd} \)  \hspace{1cm} \text{Hydrodynamic coefficient for various flow configurations}
\( \lambda_g \)  \hspace{1cm} \text{Thermal conductivity of gas, W/m.K}
\( \rho_g \)  \hspace{1cm} \text{Gas density, Kg/m}^3\text{ }
\( \delta \)  \hspace{1cm} \text{Boundary layer thickness, mm}
\( \epsilon \)  \hspace{1cm} \text{Radiative emittance of fuel surface}
\( \sigma \)  \hspace{1cm} \text{Stefan-Boltzman constant, 5.67x10}^{-8}\text{ W/m}^2\text{.K}^4\text{ }
\( \mathcal{V} \)  \hspace{1cm} \text{Volume, m}^3\text{ }
\( \nu \)  \hspace{1cm} \text{Kinematic viscosity, m}^2\text{/s}
\( \tau \)  \hspace{1cm} \text{Fuel half thickness, mm}
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I would like to take this opportunity to thank my parents for their continuous support during my masters at San Diego State University. I also would like to thank Dr. Subrata Bhattacharjee without whom this thesis would not have been possible. I am grateful for Dr. Fletcher Miller and Dr. Christopher Paolini for being on my thesis committee.
CHAPTER 1

INTRODUCTION

The desire to study and control fire has been in man since stone-age. Back then fire was used to cook food, provide protection from wild animals and as a light source in the dark. Today to understand and prevent wildfires, fire propagation needs to be well understood. The ambition to colonize in space at some point needs the understanding of flames in a zero gravity environment. This thesis uses computational fluid dynamics to model flames in a forced convection environment with gravitational effects neglected. In this chapter, the problem is well understood and the work done by people on flames before this thesis is briefly presented.

1.1 PROBLEM DESCRIPTION

In this problem, there is a flame propagating on a Poly(methyl methacrylate) (PMMA) sample of half-thickness $\tau$, at a spread rate of $V_f$. The flame is kept stationary by moving the fuel at a velocity of $V_f$ towards the flame. There is an opposed oxidizer flow approaching the flame at a velocity of $V_g$. The gravitational effects have been neglected and the geometry of this problem is shown in Figure 1.1. With the flame kept stationary, the flow of the oxidizer is $V_r = V_f + V_g$. The oxidizer used in our analysis is an oxygen-nitrogen mixture. The fuel is initially at a temperature of $T_\infty$. The flame heats the fuel to its vaporization temperature $T_v$. At this temperature, the fuel undergoes pyrolysis. The vaporized fuel reacts with the incoming oxidizer flow and generates heat. A part of this heat generated goes back to the unburned fuel and preheats it. So, this cycle of preheating, vaporizing and combustion must occur continuously in order to ensure that the flame propagates throughout the length of the fuel. Fuels can be classified as thermally thick or thermally thin based on the depth up to which fuel is heated. If fuel is heated throughout the entire thickness of the fuel, then the fuel is called thermally thin. Else, if fuel is heated only up to a thickness that’s less that the fuel thickness, then it is called thermally thick. For the purpose of this thesis, thermally thin fuels are used. The thickness of a fuel has been referred as half-thickness in this thesis. Half-
thickness would mean half of actual thickness. The reason being that Bhattacharjee’s flame code uses half-thickness as the input variable. All calculations are performed on one side of the fuel.

Complete reaction mole basis:

21% O₂: \( \text{C}_5\text{H}_8\text{O}_2 + 6[\text{O}_2 + 3.76\text{N}_2] \rightarrow 5\text{CO}_2 + 4\text{H}_2\text{O} + 22.57\text{N}_2 \)

50% O₂: \( \text{C}_5\text{H}_8\text{O}_2 + 6[\text{O}_2 + \text{N}_2] \rightarrow 5\text{CO}_2 + 4\text{H}_2\text{O} + 6\text{N}_2 \)

Complete reaction mass basis:

21% O₂: \( \text{C}_5\text{H}_8\text{O}_2 + 1.92\text{O}_2 + 6.32\text{N}_2 \rightarrow 2.2\text{CO}_2 + 0.72\text{H}_2\text{O} + 6.32\text{N}_2 \)

50% O₂: \( \text{C}_5\text{H}_8\text{O}_2 + 1.92\text{O}_2 + 1.68\text{N}_2 \rightarrow 2.2\text{CO}_2 + 0.72\text{H}_2\text{O} + 1.68\text{N}_2 \)
1.2 Flame Spread Regime

When flame is subjected to a wide range of opposed flow velocities, the opposed flow can be categorized into three different regimes: the microgravity regime, the thermal regime and the kinetic regime.

1.2.1 Microgravity Regime

The microgravity regime is when there is no flow or a very low velocity flow. Here effects caused by radiation cannot be neglected. The different heat transfer mechanisms present are shown in Figure 1.2. All these heat transfer mechanisms occur in parallel and the one that takes the least characteristic time is dominant. Characteristic time for a specific heat transfer mechanism is the time taken by the mechanism to preheat fuel from ambient temperature to vaporization temperature in the absence of any other heat transfer mechanism. The shortest characteristic time is $t_{\text{rad}}$. In the case of a low velocity opposed flow, gas phase residence time approaches $t_{\text{rad}}$. Gas phase residence time is the time required for the gas to be heated from ambient temperature to flame temperature. The residence time becomes so large that radiation loss could lead to extinction; i.e. the fuel could not reach vaporization temperature.

![Figure 1.2. Image showing the various heat transfer mechanisms present.](image)

1.2.2 Thermal Regime

At a relatively high flow velocity, the residence time or the time available for combustion is lesser. The flame spread in this regime, called the thermal regime, becomes heat transfer limited and a balance between conduction from the flame to the energy required
to preheat the fuel from the ambient temperature to the vaporization temperature establishes
the flame spread rate.

### 1.2.3 Kinetic Regime

At high velocity, the characteristic residence time at the flame leading edge is
comparable to the combustion time. In this regime, the Damkohler number, the ratio of the
residence time to the time needed for combustion reaction to attain equilibrium, plays an
important role. Blow-off extinction at high velocity can be correlated to the Damkohler
number.

Although theoretical work backed up by numerical simulation suggests that radiation
can be important even for very small flames in the microgravity environment, there is no
definitive work in literature, besides scaling arguments, that establishes the diminished role
of radiation in the thermal or kinetic regime [1, 2]. Another weakness in the modeling is the
use of one step overall kinetics for the combustion reaction [3]. At high oxygen levels, the
flame temperature can be significantly over-predicted unless some type of dissociation
mechanism is included in the model. Even the well known de Ris formula for the spread rate
in the thermal regime suffers from the fact that the actual flame temperature can be
substantially lower than the linearized adiabatic flame temperature, which appears in de Ris
formula, at high oxygen levels. Yet another difficulty may arise due to the presence of a
developing boundary layer in the case of a forced opposed flow. The actual flow velocity
seen by the advancing flame may depend on the length of fuel upstream, which is the
development length of the boundary layer.

### 1.3 BACKGROUND

Emmons in 1956 was the first to solve a mathematical model for a flame burning on a
solid fuel in a boundary layer flow [4]. In spite of being a burning model, it still qualified as a
flame spread model. Emmons model was capable of having variable gas density, fluid
conductivity and fluid viscosity. The highlight of this model was that it provided an
expression for burning rate of the fuel in terms of the ambient environment, opposed flow
velocity and fuel type. This formula still did not provide a flame spread rate formula.
1.3.1 Tarifa Notario and Torralbo

In 1969 Tarifa, Notario and Torralbo provided a flame spread model which was based on a simplified analysis of flame anchor with assumed functional form of heat transfer from the flame to the fuel [5]. They used this model on plastic fuels with nitrogen and oxygen as oxidizers. They also performed experiments and compared it with their theory.

1.3.2 deRis

In 1969 de RIs simplified the governing equations so that the flame spread rate calculation process could be simplified [6]. De Ris was the first to produce an analytical solution for a flame spread problem in a forced convection environment for thermally thin and thick fuels. But his model had several assumptions:

- Gravitational forces were neglected
- Instead of pyrolysis, he assumed the fuel to be vaporizing
- Infinite rate chemical kinetics was assumed
- Vaporization temperature and latent heat of vaporization were assumed constant
- Lewis number was considered to be unity
- Effects of gas and solid-phase radiation were neglected
- Oseen flow assumption (constant gas density and constant pressure in gas and solid phase)

These assumptions were necessary to complete the analysis. The analytical technique used to solve the governing equations was a Weiner-Hopf technique [7]. This mathematical technique retained the elliptical character of the governing equations in both solid fuel and gas.

So, the formulae deRis came up with for thick fuel was:

\[ V_{f,deRis-thick} = V_g \frac{\rho_g C_g A_g}{\rho_s C_s A_s} F^2 \]  \hspace{1cm} (1.1)

Where, \( F = \frac{T_f - T_v}{T_v - T_e} \)

The requirements for using this formula was that it was needed to know the Oseen velocity \( V_g \), the properties of gas and solid fuel, vaporization temperature of fuel surface and flame temperature. The flame temperature has to be determined by thermodynamic properties of fuel and environmental conditions. The problem with this solution was that it was assumed
that flame is located on the fuel surface. Fernandez-Pello and Williams in 1976 showed that real flame is lifted from the fuel surface [8].

The same procedure when applied to thin fuels, de Ris came up with a formula for thin fuels:

\[ V_{f, deRis-thin} = \sqrt{2} \frac{\lambda_g}{\rho \varepsilon_0} F \]  

(1.2)
The constant, \( \sqrt{2} \) was used because de Ris had encountered a difficulty while using the Weiner-Hopf technique.

1.3.3 Ohki and Tsuge

For thermally thick fuels, de Ris’s formula could not predict a finite spread rate in a quiescent environment. In 1974 Ohki and Tsuge provided a model where they used a premixed smoldering flame on the fuel surface followed by a lifted diffusion flame [9]. Their model implemented the Oseen flow approximation and retained elliptical energy and species conservation equation in both gas and solid phase. The combustion model used had infinite rate kinetics allowing coupling function formulation. So now their flame spread rate formula could predict the flame spread rate in quiescent environment. The problem with this model was that when oxygen level was increased, the predicted spread rate kept decreasing. Earlier experiments had shown that spread flame rate should increase with ambient oxygen.

1.3.4 Sirignano

In 1974 Sirignano presented a flame spread theory where the oxidization is a exothermic surface reaction [10]. The flame spread rate is calculated using thermo-chemical properties, fuel bed thickness and convective velocity. The theory also calculated temperature, mass fraction and heat flux as a function of position.

1.3.5 Feng and Sirignano

In 1977 Feng and Sirignano presented a flame spread model [11]. Heat transfer through both solid and gas phase was permitted in the model. It was discovered that the chemical kinetics and transport properties played a crucial role in determining spread rate. At a wide range of Peclet numbers heat transfer through gas phase was seen to be more significant than solid phase.
1.3.6 Fernandez-Pello and Williams

Fernandez-Pello and Williams in 1975 conducted experiments and realized that heat transfer through the solid fuel is the dominant mode of heat transfer [12]. This conclusion let them to generate an analytical model in 1977 [13]. Elliptical energy conservation was implemented in solid phase but parabolic model was used in gas phase. The Oseen approximation was replaced by a combination of an inner viscous solution and an outer potential solution to show the flow induced by buoyancy. Infinite rate of kinetics was no longer used. This resulted in the birth of a flame spread formula that used fuel thickness and predicted the transition from thermally thin to thermally thick fuels. De Ris formulae were only valid in the thermally thick and thermally thin limits. Also the results obtained from the new formula agreed well with experimental results.

1.3.7 Frey and T’ien

In 1979 Frey and T’ien used a numerical model to solve governing equations for flame spread on a thermally thin fuel in a forced opposing flow [3]. Their model used Oseen approximation and constant gas properties. Finite rate chemical kinetics was implemented. Because of which effect of opposing flow, oxygen level and pressure could be studied. They used Damkohler number to explain high opposed flow velocity results.

1.3.8 Wichman and Williams

Wichman and Williams in 1983 looked into thermally thick de Ris model to find out what affected the spread rate [14]. They simplified the problem by using only energy conservation in gas and solid and solved the problem analytically. This solution regenerated the flame spread formula given by de Ris and also formulae for the forward heat transfer in solid and gas. They concluded that if Peclet number was less than unity, heat transfer occurred entirely through solid where the virgin fuel was preheated and also heated the gas ahead of the flame. If Peclet number was greater than unity then heat transfer occurred through the gas which heated the oxidizer flow and aided in preheating the virgin fuel. Peclet number is a dimensionless number which is the ratio of heat transferred through convection to heat transferred by conduction. It is also defined the product of Prandtl number and Reynolds number.
1.3.9 Wichman

In 1983 Wichman had replaced the Oseen flow approximation in the de Ris solution with a linear velocity profile flow at the fuel surface [15]. Even though this made the flow more realistic, the problem with it was that as the distance from the solid surface was increased, the velocity unrealistically increased. So this flow would be valid only for a certain height. Other than this difference, the formulation was very identical to Wichman and Williams formulation presented in 1983. Using the Weiner-Hopf technique, a formula for heat flux to the fuel surface was generated. Assuming that diffusion of oxidizer into fuel surface was the only cause for heat flux, another formula for heat flux was generated. These two formulae were equated and a flame spread expression was formed.

Wichman later on generated a flame spread model with zero-streamwise diffusivity. This resulted in the surface flame to be lifted a finite distance above the fuel surface. So, in this model the functional form of downward lift-off distance was used instead of the functional form of control volume as it was shown by the work of Wichman and Wichman, Williams, and Glassman in 1982 [15, 16]. The resulting formula for spread rate had two constant unknowns, which could be found by using the experimental data from the work of Wichman, Williams and Glassman (1982).

In 1983 Wichman and Saito performed experiments to study laminar flame spread on PMMA under high oxygen levels in natural convection environment [17]. They compared their results to the existing theory. They also explored the limitation of the theory.

In 1984, Wichman showed that there existed a semi-circular premixed flame before the spreading flame [18]. His goal was to remove the assumption of infinite rate kinetics. He used a correction factor to correct the spread rate formula developed by Wichman, Williams and Glassman. There existed two unknowns in the correction factor which could be found be found by comparison with experiments.

1.3.10 Mao, Kodoma and Fernandez-Pello

The next generation of flame spread models provided numerical solutions of the coupled, elliptical conservation equations for momentum, species and energy. These models helped understanding flame spread much better. Mao, Kodoma and Fernandez-Pello in 1984 generated the first kind of this type of numerical model [19]. They used this model on a fuel
that is burning steadily on a flat vertical surface. This model had a lifted flame and it showed that flow field can be demonstrated in a numerical model.

1.3.11 Delichatsios

In 1986 using the Wiener-Hopf method and the superposition principle, Delichatsios solved the deRis problem and realized that the formulae for spread rate for thin fuels should use a different constant [20].

$$V_{f,Delichatsios-thin} = \frac{\pi \cdot \lambda g}{4 \rho_s c_s} F$$  \hspace{1cm} (1.3)

1.3.12 Di Blasi, Continillo, Crescetelli and Russo

In 1987, Di Blasi, Continillo, Crescetelli and Russo compared the flow fields of the Oseen type to the Hangen-Pousilli type for thick fuels [21]. In 1988 Di Blasi, Continillo, Crescetelli, Russo and Fernandez-Pello compared the computed results to the experimental results and concluded that the predictions of this type could regenerate the qualitative results from Fernandez-Pello, Ray and Glassman [22, 23].

1.3.13 Olson, Ferkul and T’ien

In 1988, Olson, Ferkul and T’ien were the first to use drop towers to conduct flame spread experiments [24]. They used ashless filter paper as fuel. Drop towers can provide 2.2 to 5.2 seconds of microgravity conditions. It was necessary to have steady propagating flames in this time limit. It was seen through experiment that flames appeared to be a little away from the fuel surface. They also seemed to have lower temperatures as compared to flames in normal gravity. They found out that extinction occurred in micro-gravity at an oxygen level 5% higher than the extinction in normal gravity. They generated a flammability map that was extended by Olson in 1991.

1.3.14 Bhattacharjee, Altenkirch, Vedha-Nayagam, and Srikanth

Numerical model produced by Bhattacharjee, Altenkirch, Vedha-Nayagam, and Srikanth in 1990 was capable of solving the steady, two dimensional conservation equations of momentum, species and energy [25]. The model proposed by Bhattacharjee, Altenkirch, Vedha-Nayagam, and Srikanth in 1990 explored flame spread in microgravity. This solution
neglected buoyancy effects and radiation heat transfer. The results obtained here could be correlated to Damkohler number. But the results obtained here did not match with Olson’s experimental work in 1991 [26]. This was caused mainly due to the neglect of radiation, thus showing its importance. The work proposed by Chen in 1990 also used numerical model similar to the one explained above [27]. It explored high opposed flow effect on thermally thin fuels where heat transfer is most significantly through conduction.

1.3.15 Bhattacharjee and Altenkirch

In 1991 Bhattacharjee and Altenkirch decided to include surface radiation in their model [28]. The result of adding surface radiation caused the reduction in flame spread rate and flame size. Presence of radiation was causing extinction at lower oxygen levels.

In 1991 Bhattacharjee and Altenkirch also studied the effect of surface and gas radiation through their computational model [2]. They varied opposed flow velocity over a wide range to see its effect on spread rate. They used three parameters in their model to study radiation. A planek mean absorption coefficient, the fraction of emissivity towards the surface and a shape function to depict the distribution between gas and surface radiation. Radiation was shown to be important at low opposed flow velocities.

1.3.16 Di Blasi

Di Blasi in 1994 made use of a numerical model similar to the ones explained earlier to solve for spread rate for thermally thick to thin to super thin [29]. The super thin spread rate was seen to be affected by combustion kinetics which was a new finding.

1.3.17 Hamilton

Using Bhattacharjee et al. solution for spread rate Hamilton in 1995 studied the effect of thickness on spread rate [30]. He then non-dimensionalized these results so that they can be plotted on a single graph. He also studied the zone where the fuel stops behaving thin and starts acting thick.

1.3.18 Bhattacharjee, West and Dockter

In 1996, using deRis solution as base Bhattacharjee, West and Dockter came up with a correction to the hang distance in the spread rate solution for thin fuels [31]. Hang distance
is the distance between the flame leading edge and pyrolysis front. \( c_{hd} \) is a hang distance constant.

\[
V_{f, \text{thin-EST}} = c_{hd} \frac{\lambda_g}{4 \rho_s c_v} F
\] (1.4)

### 1.3.19 Bhattacharjee, West and Altenkirch

In 1996 Bhattacharjee and West replaced the Oseen flow assumption by equivalent velocity based on boundary layer considerations and a correction factor to properly model the flame which is above the fuel bed [32]. They still maintained the assumption of infinite-rate chemistry, mass flux linearization and no radiation in thermal regime. The formula for spread rate they came up with was:

\[
V_{f, \text{thick-MEST}} = \frac{\beta_b e_2}{\beta_0' \beta_0} (\beta_3^0 e_3 (F)^{e_1} y_{\text{hyd}}) V_g
\] (1.5)

### 1.3.20 Bhattacharjee, Ayala, Wakai and Takahashi

In 2004, Bhattacharjee, Ayala, Wakai and Takahashi came up with formulae for flame spread rate in the microgravity regime for thermally thick and thin fuels [1]. The formulae included thermal limit for spread rate and a radiation number that is calculated from the parameters of the problem. They developed flammability maps which were obtained from the spread rate formulae and included fuel thickness as one of the parameters.

### 1.3.21 Sheng-Yen Hsua and James S. T’ien

In 2009 Sheng-Yen Hsua and James S. T’ien studied the pressure extinction limit on diffusion flames [33]. This was possible by inspecting the Damkohler number and heat loss parameter. It was seen that if the combustion reaction order was lesser than a critical value for a given flame, then a high pressure extinction limit existed. This was caused because of a smaller Damkohler number value. But if the combustion reaction order was greater that the critical value, then the low pressure extinction limit was seen. This was caused from the contribution of the heat loss parameter and Damkohler number.

### 1.3.22 Ya-Ting Tseng and James S. T’ien

Ya-Ting Tseng and James S. T’ien developed a two dimensional transient model to study low speed flows over thick and thin solids. For thick solids it was seen that flames are
stationary with a limiting length. For thin solids flame spread rate and flame length was seen to be the same [34].

1.3.23 Chenthil Kumar and Amit Kumar

Chenthil Kumar and Amit Kumar proposed a three-dimensional numerical flame spread model to study the effect of opposed flow over thin solid fuels inside a tunnel enclosure [35]. The goal of their study was to understand the impact of gas radiation and the tunnel wall on flame spread rate in normal and microgravity conditions. Gas radiation was seen to cause a greater impact in microgravity than normal gravity. Flame spread rate was also seen to be influenced by the wall condition and dimensionality of the simulation.

1.3.24 Tsuneyoshi Matsuoka, Shota Murakami and Harunori Nagata

Tsuneyoshi Matsuoka, Shota Murakami and Harunori Nagata studied the transition from thermal to kinetic combustion regime inside a PMMA duct [36]. It was seen that inside a duct, a blow-off limit does not occur because the combustion mode transitions to a “stabilized combustion”. In this combustion mode, the flame spread rate is very low and almost constant. A flow separation was used in front of the flame tip to show the turbulent and laminar region. The turbulent region was seen at a higher frictional velocity of the oxidizer flow on the fuel surface. The condition for laminar flow was not understood well. The combustion modes inside the duct were understood by plotting a non-dimensional spread rate against Damkohler number. They also proposed a “laminar frictional velocity” to understand if the combustion is stabilized. Blow off was seen at a very high oxidizer velocity.

1.3.25 Ying Zhang, Jie Ji, Jinhua Sun and Qingsong Wang

Ying Zhang, Jie Ji, Jinhua Sun and Qingsong Wang studied the effect of the width of a solid fuel on flame spread rate [37]. Experiments were conducted using white board samples of a fixed lengths and thicknesses but width varying from 2 cm to 12 cm. A camera was used to record the flame spread rate and to measure the flame height and thickness. For sample width’s greater than 4 cm, it was seen that the flame height increased with width. But
for sample width’s lesser than 4cm it was seen that flame height increased with decreasing width. A shape factor, which comprised of the flame height, flame thickness and sample width were used to show the influence of sample width. Shape factor using a numerical method were calculated and were seen to agree with experiment results.
CHAPTER 2

COMPUTATIONAL FLUID DYNAMICS

MODELLING

In this chapter, the mathematical model behind the flame spread analysis is presented. The operation of the two dimensional model used in the analysis is been shown. The next section in this chapter shows how the domain and grid structure is chosen. The idea was to minimize the size of the required domain and grids so that computation time is reduced.

2.1 MATHEMATICAL MODEL

The CFD code written in FORTRAN by Bhattacharjee was used to study the effects of hydrodynamics, chemical kinetics and radiation on flame spread rate. A MATLAB code uses data from the CFD code and plots the flames. A schematic of the flame spread problem (in the presence of an opposing flow) is shown in Figure 2.1. The mathematical model consists of the two-dimensional, steady, elliptic, partial differential equations describing conservation of energy, species mass, total mass, and momentum in the gas phase and ordinary differential equations for the conservation of mass and energy in the solid phase. In the numerical model, the gas and solid phases are solved sequentially using the SIMPLER algorithm, which are coupled by the interface conditions specified [38]. The solution seeks a unique value for the spread rate that anchors the flame leading edge at the desired location, \( x = x_{\text{eigen}} \), within the computational domain. This is done by requiring the solid absolute temperature to be a certain value (20% above ambient) at the \( x_{\text{eigen}} \) location. The gas-phase balance equations for total mass, fuel, oxygen and nitrogen species mass, x- and y-momentum, and energy can be expressed in the canonical form:

\[
\frac{\partial}{\partial x} (\rho u \varphi) + \frac{\partial}{\partial y} (\rho v \varphi) = \frac{\partial}{\partial x} \left( \Gamma_v \frac{\partial \varphi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \Gamma_v \frac{\partial \varphi}{\partial y} \right) + \delta^\varphi
\]

(2.1)

The meaning of each variable is defined in Table 2.1.
Figure 2.1. Numerical model for flame spread with an opposed flow.

Table 2.1. Definition of Variables Used in Equation 2.1

<table>
<thead>
<tr>
<th>Eqn.</th>
<th>φ</th>
<th>$r_p$</th>
<th>$S_p^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>x-mom</td>
<td>$u$</td>
<td>$\mu$</td>
<td>$-\frac{\partial p}{\partial x}$</td>
</tr>
<tr>
<td>y-mom</td>
<td>$\nu$</td>
<td>$\mu$</td>
<td>$-\frac{\partial p}{\partial y}$</td>
</tr>
<tr>
<td>Fuel</td>
<td>$y_F$</td>
<td>$\mu/c_g$</td>
<td>$-B_g \rho \gamma y_{0,y} \exp(-E_g/RT)$</td>
</tr>
<tr>
<td>O$_2$</td>
<td>$y_O$</td>
<td>$\mu/c_g$</td>
<td>$-B_g \rho \gamma y_{0,y} \exp(-E_g/RT)$</td>
</tr>
<tr>
<td>N$_2$</td>
<td>$y_N$</td>
<td>$\mu/c_g$</td>
<td>0</td>
</tr>
<tr>
<td>Energy</td>
<td>$T$</td>
<td>$\mu/c_g$</td>
<td>$(\dot{m}_g T_e h^o + \dot{q}_g^m)/c_h$</td>
</tr>
</tbody>
</table>
For thin fuels, with temperature $T_s$ remaining constant across the fuel thickness, a one-dimensional energy equation in terms of a variable fuel density can be written as:

$$-\tau \rho_s c_f V_f \frac{dT_s}{dx} + m_f'' \left[ \Delta h^o_c + (c_g - c_f)(T_s - T_w) \right] = \lambda_g \frac{\partial T}{\partial y}_{y=0^+} - \varepsilon_s \sigma T^4$$

(2.2)

$$m_f'' = A_s \rho_s \tau e^\frac{E_s}{R T_v} = \frac{d \left( \rho_s \tau V_f \right)}{dx}$$

(2.3)

The mass equation allows the fuel to burnout downstream when the fuel density reaches a preset burnout value. The gain from radiation is not included. The properties used for PMMA are listed in Table 2.2.

<table>
<thead>
<tr>
<th>Phase</th>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solid</td>
<td>$\rho_s$</td>
<td>1190</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td></td>
<td>$c_s$</td>
<td>1.465</td>
<td>kJ/(kg.K)</td>
</tr>
<tr>
<td></td>
<td>$\Delta h^o_c$</td>
<td>0.941</td>
<td>MJ/kg</td>
</tr>
<tr>
<td></td>
<td>$\Delta h^e_c$</td>
<td>-25.9</td>
<td>MJ/kg</td>
</tr>
<tr>
<td></td>
<td>$E_s$</td>
<td>81.867</td>
<td>MJ/kmol</td>
</tr>
<tr>
<td></td>
<td>$A_s$</td>
<td>8.78×10$^5$</td>
<td>1/s</td>
</tr>
<tr>
<td></td>
<td>$\varepsilon_s$</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Gas</td>
<td>$c_g$</td>
<td>1.183</td>
<td>kJ/(kg.K)</td>
</tr>
<tr>
<td></td>
<td>$\lambda_{g,700K}$</td>
<td>0.052</td>
<td>W/(m.K)</td>
</tr>
<tr>
<td></td>
<td>$\mu_{g,700K}$</td>
<td>40.3</td>
<td>m$^3$/(kg.s)</td>
</tr>
<tr>
<td></td>
<td>$B_g$</td>
<td>8.928×10$^7$</td>
<td>mg/(m.s)</td>
</tr>
<tr>
<td></td>
<td>$E_g$</td>
<td>83.72</td>
<td>MJ/kmol</td>
</tr>
<tr>
<td></td>
<td>$s$</td>
<td>1.92</td>
<td></td>
</tr>
</tbody>
</table>

The computation is started with an initial guess of the spread rate $V_f$ and gas phase conserved properties. After a few iterations, heat flux $q_{gs''}$ from the gas to the solid surface is calculated. The solid phase energy and mass equations are then solved to determine a spread rate that produces a specified temperature $T_{eigen} = 1.2 T_w$ at a specific location $x_{eigen}$. The temperature, mass flux distribution and the spread rate obtained from the solid phase solution
are used as boundary conditions for the gas phase equations, which are solved to produce a better heat flux distribution. Iterations between the two phases are continued until convergence is achieved in all results. The purpose of the eigen condition and the eigen temperature has no role other than pinning the flame leading edge at a location of choice.

2.2 DOMAIN AND GRID STUDY

In CFD, the accuracy of the calculated spread rate depends on the number of grids that are chosen for a particular domain. For any given domain, there has to be a sufficient number of grids to calculate the flame spread rate accurately. It is also not a very good idea to have too many grids for a domain that doesn’t actually require that many grids because doing so would take up more computation time. The objective of this study is to minimize the domain and grids as much as possible. The domain as depicted in Figure 2.2 shows an x-axis ranging from a negative value to a positive value with the flame originating at xeig and Y-axis ranging from 0 to ‘y1’. The negative and positive x-axis or the length of the domain is controlled by parameters called ‘xst’ and ‘xl’ while the ‘y1’ parameter controls the height.

The vertical and horizontal lines show the grids. The xeig- and xeig+ control the region of high grid density when non-uniform grid structure is used. A ‘wt’ factor controls the actual grid density in the non-uniform region. This factor when set to 1 causes uniform distribution. A ‘yexp’ factor controls grid density at the region closer to the fuel surface. If it is set to anything more than 1, a higher grid density closer to the surface of the fuel would be seen.

The length up to which fuel heats up from ambient temperature to vaporization temperature scales with reference length, \( L_g = \frac{a}{v_{ref}} \). Where, \( a \) is the thermal diffusivity of the
gas and $v_{ref}$ is the artificial reference velocity. This reference length gets multiplied with the x and y axis parameters thus deciding the domain size. The reference length can be adjusted by increasing or decreasing $v_{ref}$, thus changing the domain size. Higher $v_{ref}$ would mean a smaller domain and lower $v_{ref}$ would mean vice versa.

In order to choose a domain, impact of changing each length had to be well understood. For this study, a PMMA fuel of half-thickness 50 microns (mic) was used at ambient conditions of 1 atm and oxidizer of 50-50 oxygen nitrogen by volume. A very dense non-uniform grid structure of 360x70 grids was used on a large domain as the starting point of this study. Figure 2.3 shows this domain for a flame that is facing an opposed flow velocity of 100 cm/s. Now, keeping the same number of grids the domain is reduced. The white contour lines indicate fuel mass fraction 0.1, 0.2, 0.3 and 0.4.

The height was first studied. Figure 2.4 shows the height being reduced from 60 mm to 20 mm. With the reduction of height, a very insignificant change of spread rate from 8.9 mm/s to 9 mm/s was seen.

**Figure 2.3.** MATLAB image showing a large domain with very high grid with flame facing an opposed flow velocity of 100 cm/s.

**Figure 2.4.** MATLAB image showing a domain with reduced height.
Also when the back length or xst was reduced from 150 mm to 100 mm, spread rate still remained nearly the same. When the flow development length or xl was increased or decreased, a significant change in spread rate was seen. For this purpose, a boundary layer study is done in the next chapter. The flow development distance or the positive x-axis limit was chosen in such a way that the product of the opposed flow velocity and the positive x-axis length stayed constant at every opposed flow velocity, thus maintaining a constant Reynolds number. Reynolds number was chosen to be 392. This is explained in detail in the next chapter.

So this domain, where the height is about two times the height of the flame and whose negative x-axis limit is about two and a half times the length of the hottest part of the flame was chosen for a grid study. So for all opposed flow velocities this rule had to be obeyed thus calling this rule from now on as the domain rule. Figure 2.5 shows an image of a flame obeying this rule.

![Figure 2.5. MATLAB image showing the domain rule.](image)

Now to perform the grid study, the opposed flow velocity varied from 0 cm/s to 400 cm/s. As mentioned earlier, the grids are spread out non-uniformly throughout the domain. This means that it possible to have more densely packed grids at the flame origin. The ‘wt’ factor and the ‘yexp’ factor are set to 0.7 and 1.5. Now using the non-uniform high grids solution, the grids were reduced to find a low grid that would give us the same result as high grid. It was found that a grid of 120x70 was sufficient enough to find an accurate spread rate. These results are also compared with a uniform grid structure with 360x70 grids. The three different grid structures are shown in Figure 2.6.
Figure 2.6. Plot comparing different grids used for an opposed flow velocity study.

Figure 2.7 shows an image of a flame plotted with non-uniform grid. It could be seen that xeig- and xeig+ are set in a way that high grid density occurs in the region between -20 mm and 10 mm on the x-axis.

Figure 2.7. Zoomed in MATLAB image of a flame facing an opposed flow velocity of 100 cm/s plotted using non-uniform grids (120x70).

On plotting images for flames facing different opposed flow velocities, it was found that flames initially get bigger with opposed flow velocity and then smaller after opposed flow velocities of 100 cm/s. Radiation becomes less significant as opposed flow velocity is increased thus causing spread rate to first increase. After reaching a certain opposed flow velocity, the fuel and oxidizer get lesser and lesser time to react causing the spread rate to decrease. Blow off occurs when the fuel and oxidizer get absolutely no time to react. So as
reference velocity $V_r$ is increased, the reference length gets smaller thus making the computation domain smaller. In Bhattacharjee’s flame code, the opposed flow velocity can be increased along with the reference velocity by a factor. The flame sizes have been seen to get smaller at around 100 cm/s opposed flow. The reason being that at higher oxidizer flow the fuel and oxidizer do not get enough time to react. On doubling the opposed flow velocity, the reference velocity is also doubled and the domain is made to half of its original size. When this flame is plotted, the domain rule is automatically followed provided the starting domain was obeying domain rule.
CHAPTER 3
BOUNDARY LAYER AND DAMKOHLER
NUMBER STUDY

3.1 IMPACT OF BOUNDARY LAYER ON SPREAD RATE

It was discovered that at high opposed flow velocities, a change in the flow development length could cause a significant difference in spread rate. This was noticed for opposed flow velocities that were beyond 100 cm/s. The lesser the flow development distance, smaller was the flame size and flame spread rate. It could be quickly understood that at an opposed flow velocity of say 200 cm/s, the flame would feel the flow to be much stronger at a smaller flow development distance, thus causing a smaller flame than at a larger flow development distance.

Figure 3.1 and Figure 3.2 show images of flames that are facing an opposed flow velocity of 100 cm/s at flow development length’s or $x_d$ of 30 mm and 60 mm on which a boundary layer is shown by drawing a white line. A boundary layer is the height above the solid surface above which the effects of viscosity are important. The thickness of boundary layer is the distance from the fuel surface at which 90% of free steam velocity is seen. It could be seen that at a smaller flow development distance, the velocity at the flame tip was higher which resulted in a smaller boundary layer as compared to a case with longer flow development length.

![Figure 3.1. MATLAB image showing flame facing opposed flow velocity at an xd of 30 mm on which a boundary layer is shown.](image)
Figure 3.2. MATLAB image showing flame facing opposed flow velocity at an xd of 60 mm on which a boundary layer is shown.

Figure 3.3 shows how velocity changes with height at different locations on the horizontal axis. The black line indicates the starting position of the flow. At starting position, it could be seen that at every height the velocity is the same. The blue lines indicate positions that are a little further from the starting point and closer to the flame. It could be seen that the velocity profile is greatly affected at different heights. The red lines indicate positions inside the flame and the green line shows velocity versus height in the greenish-blue zone of the flame. Since the gas density decreases at the hot region, the oxidizer flow gets accelerated. At x = -15 mm, a greater velocity is seen when development length is 30 mm.

To understand this better, it was decided to keep the flow development length constant for an entire range of opposed flow. A fixed flow development distance of 60 mm was decided to be used at all opposed flow velocities. The same study was then repeated keeping the flow development distance fixed at 30 mm. Spread rate was then plotted against opposed flow for these cases. Results for these computations are shown in Figure 3.4.

As expected, it could be seen that spread rates calculated at opposed flow velocities more than 100 cm/s did not fall on the same line for the two cases. At lower opposed flow velocity spread rate however did fall on the same line. A separate plot for spread rate versus opposed flow at lower velocities at different flow development lengths is shown in Figure 3.4 (b).

In order to correlate the spread rates obtained from the different flow development length’s studies, a formula to calculate the equivalent velocity i.e. flow velocity at the flame tip had to be developed. The objective was to plot spread rate against equivalent velocity for different flow development cases.
Figure 3.3. MATLAB plot showing how velocity changes with height at different locations on the horizontal axis when (a) \( x_d = 30 \text{ mm} \) and (b) \( x_d = 60 \text{ mm} \).

The purpose of calculating the equivalent velocity was to see if the two flow development length cases could fall on the same line when spread rate is plotted against equivalent velocity. Figure 3.5 shows an image of a boundary layer on a flame. This figure shows the opposed flow velocity or free stream velocity and equivalent velocity at flame tip.
Figure 3.4. Plot showing impact on spread rate when different flow development lengths are used over a wide range of opposed flow velocity.

Figure 3.5. Image showing a boundary layer over a flame.

Velocity reduction fraction can be written as:

\[
\frac{V_{eq}}{V_g} = \frac{L_g}{\delta}
\]  

(3.1)

Momentum equation gives:
Boundary layer thickness can be written as:

$$\delta = \frac{x_d}{v d a} = \sqrt{\frac{v x_d}{v g}}$$  \hspace{1cm} (3.3)$$

Kinematic viscosity can be written in terms of Prandtl number and thermal diffusivity:

$$\nu = Pr \cdot \alpha$$

$$\delta = \sqrt{\frac{Pr \cdot \alpha \cdot x_d}{v g}}$$  \hspace{1cm} (3.4)$$

$L_g$ is length over which fuel pyrolyzes and is given as, $L_g = \frac{\alpha}{V_r}$

$$\alpha = L_g \cdot V_r$$

$$\delta = \sqrt{\frac{Pr \cdot L_g \cdot V_r \cdot x_d}{v g}} = \sqrt{x_d \cdot L_g \cdot Pr \cdot \left(\frac{V_r}{v g}\right)}$$  \hspace{1cm} (3.5)$$

Velocity ratio can be written as:

$$f = \frac{V_{eq}}{V_g} = \frac{L_g}{\delta} = \frac{L_g}{\sqrt{x_d \cdot L_g \cdot Pr \cdot \left(\frac{V_r}{v g}\right)}} = \frac{\alpha}{\sqrt{V_r \cdot x_d \cdot Pr \cdot \left(\frac{V_r}{v g}\right)}}$$

$$f = \frac{V_{eq}}{V_g} = \frac{\nu}{\sqrt{V_r \cdot x_d \cdot Pr^2 \cdot \left(\frac{V_r}{v g}\right)}} = \frac{\nu V_g}{\sqrt{V_r \cdot x_d \cdot Pr^2 V_r}}$$

$$f = \frac{V_{eq}}{V_g} = \frac{\nu V_g}{\sqrt{V_r^2 \cdot x_d \cdot Pr^2}}$$  \hspace{1cm} (3.6)$$

If $V_r = V_g$. 
To test out this formula, opposed flow studies where different flow development lengths of 30 mm and 60 mm were used. It could be seen that velocity ratio, \( f \) was highly dependent on Reynolds number as Prandtl number was almost equal to unity. A third case where flow development length or \( x_d \) was adjusted such that Reynolds number was kept constant was also used. Keeping the Reynolds’s number constant would ensure that the velocity ratio is constant. Figure 3.6 shows spread rate plotted against opposed flow velocity where different flow development lengths are used.

\[
\begin{align*}
    f &= \frac{V_{eq}}{V_g} = \frac{1}{(Re_x)^{\frac{1}{4}}} \frac{1}{Pr} \\
    V_{eq} &= \frac{V_g}{(Re_x)^{\frac{1}{4}}} \frac{1}{Pr} 
\end{align*}
\]

**Figure 3.6.** Plot showing impact on spread rate when different flow development lengths are used over a wide range of opposed flow velocity.

Using the two formulae for equivalent velocity, spread rate versus equivalent velocity plots for the three flow development length cases were plotted hoping that one of them would make all three cases to coincide. Figure 3.7 (a) shows spread rate versus equivalent velocity...
Figure 3.7. Spread rate versus equivalent velocity when (a) relative velocity is equal opposed flow velocity (b) and when relative velocity is equal to equivalent velocity.

when relative velocity is equal to opposed flow velocity. It could be seen that the three curves are closer than before, but not close enough to say we are using the correct formula. Figure 3.7 (b) shows a plot where spread rate is plotted against equivalent velocity when relative velocity is considered to be equal to the equivalent velocity.

On plotting, it was seen that both the formulae don’t agree that well. It was then realized that the correct formula could be attained if the exponent of the Reynolds number
was iterated. On iterating, it was seen that when the exponent of Reynolds number was 1/3, the three curves fall together very well. So, the correct formula was found to be:

\[ V_{eq} = \frac{V_g}{(Re_x)^{\frac{1}{3}} Pr} \]  

(3.9)

The Figure 3.8 shows spread rate plotted against equivalent velocity calculated with this new formula.

![Figure 3.8. Plot showing spread rate versus equivalent velocity for different flow development length using Equation 3.9.](image)

Using the formula that worked, Figure 3.9 shows how \( f \) changes with Reynolds number. Since it was desired to keep the boundary layer effect constant, Reynolds number had to be kept constant as opposed flow velocity is varied. For all parametric studies from here on, a constant Reynolds number of 392 was chosen at all opposed flow velocities which corresponds to a velocity ratio of 0.15. This Reynolds number was chosen because it was convenient. If a different Reynolds number is desired, a different velocity ratio has to be picked from Figure 3.9.

### 3.2 The Damkohler Number

The Damkohler number as discussed briefly in Chapter 1 is defined as the ratio of the residence time of reactants in gas phase to the time required for the combustion reaction to achieve chemical equilibrium. This number shows the importance of the interaction between chemistry and turbulence. When Damkohler number is much lesser than one, the turbulence
Figure 3.9. Plot showing how velocity ratio changes with Reynolds number. Marker indicates velocity ratio chosen in Equation 3.5.

(opposed flow in our case) is faster than the chemistry. It shows that there is not enough time for the reaction to take place. So as opposed flow increases the Damkohler number reduces.

\[ Da = \frac{t_{res,g}}{t_{comb}} \]  \hspace{1cm} (3.10)

Where the gas phase residence time and combustion time are given as,

\[ t_{res,g} = \frac{L_g}{V_r} \sim \frac{\alpha_d}{V_r^2} \]

\[ t_{comb} = \frac{\bar{m}_{O_2}}{x_{O_2} \rho_{O_2} B_{g e} \left( \frac{f}{V_f} \right)} \]  \hspace{1cm} (3.11)

Figure 3.10 shows residence and combustion time on a flame. From the formulae it was seen that residence time and combustion time are closer as Damkohler number reduces. The lower limit of Damkohler number shows extinction.

Figure 3.10. An image of a flame showing residence and combustion time.
In this work, dimensionless spread rate is plotted against Damkohler number for three different flow development lengths at 50% oxygen level. The dimensionless spread rate is the ratio of the spread rate calculated by Bhattacharjee’s flame code to the thermal spread rate. The thermal spread rate is given by [1]:

$$V_{f,\text{thermal}} = \frac{\lambda_g}{\rho_s c_s \tau} \left( \frac{T_f - T_v}{T_v - T_{\infty}} \right)$$ (3.12)

Figure 3.11 and Figure 3.12 show these plots when Damkohler number is based on opposed flow velocity and equivalent velocity respectively at different flame temperatures. The Damkohler number axis is chosen to be logarithmic. When Damkohler number is based on opposed flow velocity, as expected the curves don’t agree at high velocities. But, when Damkohler number is based on equivalent velocity, all three curves agree well at every flame temperature. Maximum computation temperature calculated by the CFD code, complete combustion flame temperature and equilibrium combustion temperature were used [39].

Later on, it was decided to plot dimensionless spread rate against Damkohler number for different thicknesses, flow development lengths and oxygen levels at the complete combustion temperature calculated by the flame code. Curves for a 50 mic half-thickness PMMA at oxygen level 50% and 70% at constant Reynolds number were compared with the two different flow development length cases of 30 mm and 60 mm shown earlier. Also another curve with a higher thickness was compared to these 4 curves. In Figure 3.13, Damkohler number is calculated based on the opposed flow velocity and in Figure 3.14 Damkohler number is calculated based on equivalent velocity. It could be seen that when Damkohler number is based on equivalent velocity, all five curves agree well as compared to when Damkohler is based on opposed flow velocity.
Figure 3.11. Plot showing dimensionless spread rate versus Damkohler number based on opposed flow velocity calculated using (a) Maximum computation temperature = 4336 K (b) Complete combustion flame temperature = 4118 K and (c) Equilibrium flame temperature = 2850 K.
Figure 3.12. Plot showing dimensionless spread rate versus Damkohler number based on equivalent velocity calculated using (a) Maximum Computation temperature= 4336 K, (b) Complete combustion= 4118 K and (c) Equilibrium temperature= 2850 K.
Figure 3.13. Dimensionless spread rate versus Damkohler number based on opposed flow velocity calculated using complete combustion temperature.

Figure 3.14. Dimensionless spread rate versus Damkohler number based on equivalent velocity calculated using complete combustion temperature.
CHAPTER 4

PARAMETRIC STUDIES

In this chapter, different parameters in the input file of the CFD program have been modified to see its impact on spread rate. In all opposed flow studies shown in this chapter, Reynolds number is held constant. The first section shows a flame spread model that does not include effects caused by radiation losses. Using this model, an opposed flow study on spread rate was performed. In the same section, the model is coupled with radiation to show the importance of radiation. A blow off extinction was studied for different thicknesses of PMMA fuel. The spread rate and flame temperature were compared for different thicknesses. A critical fuel thickness limit was found in a quiescent environment where there is no opposed flow velocity. This was followed by an opposed flow study with oxygen level changed to see impact on flame spread rate. Finally, different PMMA thicknesses were studied in the microgravity regime at different pressure levels.

4.1 THE IMPACT OF RADIATION ON FLAMES

The impact of radiation has been studied on flame spread rate at different opposed flow velocities. For the purpose of this study, a PPMA fuel of 50 mic fuel half thickness was chosen. The computation was initially performed excluding the effects of radiation. The results for this computation are shown in Figure 4.1. It was seen that the spread rate in the microgravity regime was very high and flame sizes were huge. The flame sizes could not be captured in a computation domain. In the thermal and kinetic regime the flames could be captured in a computational domain. The microgravity results did not make much sense and it was soon realized that it was necessary to couple the flame spread model with radiation. Radiation losses were then included in the computation to see how flame spread rate was affected. Bhattacharjee’s code calculates both gas and solid radiation losses along with the total heat released. Equation Figure 4.1 also compares the no radiation model to with radiation model. A significant difference in flame spread rate was observed in the microgravity regime.

Through Figure 4.2 it could be seen that with the inclusion for radiation losses flame temperatures were lowered. The microgravity regime showed a significant change in both
Figure 4.1. Plot comparing impact of opposed flow velocity on spread rate performed for cases without and with radiation.

Figure 4.2. Plot comparing impact of opposed flow velocity on flame temperature performed for cases without and with radiation.

spread rate and flame temperature thus proving the importance of radiation effects in this regime. Extinction in the microgravity regime is called radiative extinction.

Figure 4.3 compares images of flames without and with radiation loss effects facing an opposed flow of 100 cm/s (thermal regime). It could be seen that flames are a lot larger, hotter and have a higher spread rate when radiation losses are neglected. Flame temperature seen with radiation neglected was 4820 K as against 3673 K when radiation is present. Also, flame spread
Figure 4.3. (a) MATLAB images of a flame facing an opposed flow of 100 cm/s with radiation effects neglected and (b) with radiation losses present. These figures do not follow the domain rule because they were shown to illustrate the impact of radiation on flame size in the thermal regime for a PMMA fuel of half-thickness of 50 mic.

rate seen when radiation effects were neglected was 10.9 mm/s as against 9.24 mm/s with the inclusion of radiation losses.

Figure 4.4 compares images of flames with without and with radiation loss effects facing opposed flow velocity of 400 cm/s (Kinetic regime). Without radiation, flame temperature was observed to be 4636 K as against 4233K when radiation is present. It could be seen that flame size is nearly the same and the difference in flame temperature is lesser as compared to the 100 cm/s opposed flow case thus showing that radiation losses are minimal and don’t affect the flame. Difference in spread rate calculated for both models was seen to be only 0.7 mm/s.
To explore the relative importance of radiation losses in comparison with the heat released, the surface radiation loss, gas radiation loss and the heat released were computed as follows:

\[
\dot{Q}_{s,\text{loss}} = W \sigma \int_{-\infty}^{\infty} T_s^4 \, dx
\]  

(4.1)

\[
\dot{Q}_{g,\text{loss}} = \iiint \dot{q}_g \, d\mathcal{V}
\]  

(4.2)

\[
\dot{Q}_{\text{release}} = \iiint \dot{m}_v \Delta h^0 \, d\mathcal{V}
\]  

(4.3)

These values are evaluated from the computed solutions and plotted in Figure 4.5, which showed that the bulk of the radiation losses take place through emissions from the gas. At low opposing flow velocity, however, the surface radiation loss can be seen to be significant relative
Figure 4.5. Plot compares the heat released to radiation losses over an entire range of opposed flow on a PMMA fuel of 50 mic half-thickness.

To quantify the importance of radiation losses, a non-dimensional radiative loss parameter is defined by dividing the total radiative losses by the flame power:

\[ L_R = \frac{\hat{Q}_{g,\text{loss}} + \hat{Q}_{s,\text{loss}}}{\hat{Q}_{\text{release}}} \]  

(4.4)

The loss parameter is computed as a function of three different fuel thicknesses for the entire range of opposing flow values and presented in Figure 4.6. The plot clearly establishes the increased importance of radiation loss in the microgravity regime. In a quiescent environment almost all of the heat generated is radiated away. One surprising finding of this study is that even in the kinetic regime, radiation loss is not insignificant. About 15-20% of the heat is released during extinction.

It was then decided to study the impact of surface and gas radiation on spread rate individually in the thermal and kinetic regime. So Figure 4.7 shows spread rate versus opposed flow velocity ranging from 100 cm/s to 400 cm/s where contribution of surface and gas radiation loss is clearly shown. It shows that the inclusion of gas radiation loss in our model is good enough to model flame spread as surface radiation loss has minimal effect.
4.2 THE STUDY OF OPPOSED FLOW VELOCITY ON SPREAD RATE

The opposed flow effect on spread rate was studied for fuel half-thicknesses of 100mic, 50mic, and 25mic. Opposed flow was varied over a wide range. The computation showed the operation of the three opposed flow regime i.e. Microgravity regime, thermal...
regime and kinetic regime. A MATLAB code was employed to plot the flames and it was ensured that the domain rule was obeyed as described in the grid study chapter. The grid structure used for this study was uniform distribution with 360 grids in x-direction and 70 grids in y-direction. It was realized from theory that the boundary layer thickness keeps reducing as opposed flow increases. So as per the discussion in Chapter 3, flow development length was adjusted such that the Reynolds number is kept constant.

On variation of opposed flow velocity for the 50 mic half-fuel thickness, the spread rate and flame size was first seen to increase reaching a maximum value at an opposed flow velocity of 100 cm/s, and then decrease and reach extinction or blow off at 400 cm/s. Figure 4.8 shows MATLAB images of flames on a 50 mic half-thickness PMMA fuel facing opposed flow. The maximum flame spread rate seen was 9.18 mm/s.

So, using the 50mic fuel half-thickness case as baseline, the next step was to see how opposed flow would affect the spread rate when fuel half-thickness is doubled and halved. On doubling the fuel half-thickness, the peak spread rate seen was 5.1 mm/s at an opposed flow velocity of 100 cm/s. While, on reducing the half-thickness to 25mic the peak spread rate seen was 14.8 mm/s at an opposed flow velocity of 50 cm/s. This shows that the peak gets shifted to the left i.e. peak spread rate has occurred at a lower velocity as thickness is reduced. It could also be clearly seen that blow off extinction occurs at the same opposed flow velocity for all three thicknesses thus proving that blow-off does not depend on thickness. The results for these computations are shown in Figure 4.9. Lesser fuel thickness showed higher spread rate because theory suggests that fuel thickness is inversely proportional to flame spread rate. This is shown below:

The thermal spread rate is given by [1],

$$V_{f, thermal} = \frac{\lambda g}{\rho_s C_s} \left( \frac{T_f - T_v}{T_v - T_e} \right)$$  \hspace{1cm} (4.5)

The plot for flame temperature is plotted against opposed flow velocity in Figure 4.10. The computation shows us that all three thicknesses have nearly the same flame temperature at a given opposed flow velocity thus proving that fuel thickness has very less impact on flame temperature.

To test out the equivalent velocity formula shown in Chapter 3, it was decided to implement it at different thicknesses with different flow development lengths. Constant flow
Figure 4.8. MATLAB images of flames on a PMMA fuel of half-thickness 50 mic facing an opposed flow velocity of (a) 50 cm/s (b) 200 cm/s and (c) 400 cm/s.
development distance of 40 mm was used for 100 mic, 50 mic and 25 mic and compared with a changing flow development length where Reynolds number is kept constant at 392 as shown earlier in Figure 4.9. Figure 4.11 compares these cases.

Spread rate was then plotted against equivalent velocity as shown in Figure 4.12. It could be seen that both curves for each thickness are hugging each other, thus verifying the correctness of the new formula.
4.3 THE STUDY OF THICKNESS ON SPREAD RATE IN A QUIESCENT ENVIRONMENT

The goal of this study was to find the maximum thickness of PMMA fuel that has a flame propagating on its surface in a quiescent environment. So, a fuel at ambient condition of 1 atm with 50% oxygen and 50% nitrogen by volume is used for this analysis. The grid structure used here was uniform with 360x70 grids. The thickness of fuel was varied in this environment and the results for the computation are shown in Figure 4.13. The plot clearly shows that as thickness is increased, the spread rate and maximum temperature both decrease in a quiescent environment. The reason for spread rate to decrease as shown earlier was that...
Figure 4.13. Plot showing how spread rate and maximum temperature are changing with fuel half-thickness in a quiescent environment.

flame spread rate is inversely proportional to fuel thickness. The maximum half-thickness at which spread rate could be computed was found to be 55 mic thus showing that flame extinction can occur by increasing fuel thickness. So, 55 mic fuel half-thickness is the critical thickness in quiescent environment. Figure 4.14 shows MATLAB Images of these flames.

4.4 THE STUDY OF OXYGEN LEVEL ON SPREAD RATE

The goal of this study was to change the oxygen level and vary opposed flow velocity to see how spread rate is affected. Oxygen level was changed from 21% to 70% by volume in three levels for a 50 mic fuel half-thickness and the spread rate was plotted against opposed velocity. The grid structure used here was uniform with 360x70 grids. The results for this computation are shown in Figure 4.15. It could be seen that as oxygen level is increased, spread rate reaches much higher values and extinction occurs at a higher opposed flow velocity. The reason for a higher spread rate is that as oxygen level is increased, the flame temperature increases. Equation 8 tells us that spread rate is directly proportional to flame temperature. The Reynolds number was kept constant at 392.

The maximum spread rate seen for the 21%, 50% and 70% oxygen level cases were 2.92 mm/s, 9.235 mm/s and 13 mm/s respectively. Extinction for 70% oxygen level occurs at a very high opposed flow velocity of 600 cm/s and 21% oxygen level at 60 cm/s. Extinction for 50% oxygen level was shown earlier to be happening at 400 cm/s. MATLAB images of flames facing an opposed flow of 300 cm/s at 50% and 70% oxygen level on a PMMA fuel of 50 mic half-thickness are shown in Figure 4.16. Clearly the 70% oxygen level flame
Figure 4.14. MATLAB images showing flames propagating on PMMA fuel of different half thicknesses (a) 5 mic, (b) 20 mic, (c) 40 mic and (d) 55 mic.
Figure 4.15. Plot showing impact of oxygen concentration on spread rate over a wide range of opposed flow.

(a)

(b)

Figure 4.16. MATLAB images comparing sizes of flames facing an opposed flow of 300 cm/s with oxygen level of (a) 50% (T_f = 4123 K) and (b) 70% (T_f = 4931 K) for a PMMA fuel of half-thickness of 50 mic.
appears to be larger. As discussed earlier, the radiative loss parameter is plotted against opposed flow velocity to show the importance of radiation in Figure 4.17.

![Figure 4.17. Plot showing radiation loss parameter plotted against opposed flow velocity at different oxygen levels.](image)

### 4.5 The Study of Spread Rate in Micro-Gravity

The spread rate of a flame at low opposed velocity was studied in detail. At an ambient pressure of 1 atm and 50-50 oxygen-nitrogen composition, the opposed flow velocity was varied from 0 cm/s to 10 cm/s for different fuel half-thicknesses to see how the spread rate was affected. Fuel half-thicknesses of 200mic, 100mic, 50mic and 25mic were used in this study. It was seen that more the thickness, lesser was the spread rate for a given oxidizer composition and pressure which agrees with theory as mentioned earlier. Figure 4.18 shows how spread rate changes for different thicknesses at a pressure of 1 atm. It was found that at an opposed flow of 1 cm/s and 2 cm/s the flame code did not find a converged solution for 100 mic and 200 mic fuel half thicknesses. This meant that flame did not exist for fuel-half thicknesses of 100 mic and 200 mic at these velocities. Figure 4.19 shows MATLAB images of flames facing an opposed flow velocity of 10 cm/s for different fuel thicknesses. Flame appears to be longer for higher thickness.

Pressure was then varied from 0.5 atm to 2 atm to see how spread rate is affected for various thicknesses. For a fuel half-thickness of 50 mic, spread rate is plotted at different pressures keeping the oxygen level at 50% in Figure 4.20. It was found that for any fixed...
half-thickness, higher the pressure, higher is the spread rate and larger are the flames. The reason being that as pressure is increased; the gas density is affected because of which the thermal diffusivity increases. As thermal diffusivity increases, reference length or the length over which fuel pyrolyzes to increases, thus causing the spread rate to increase. Figure 4.21 shows MATLAB images of flames facing an opposed flow of 2 cm/s at different pressures for a PMMA fuel of 50 mic half-thickness.
Figure 4.19. MATLAB images comparing flames facing an opposed flow of 10 cm/s propagating on half-thicknesses (a) 200 mic (b) 100 mic (c) 50 mic and (d) 25 mic of PMMA fuel.
Figure 4.20. Plot shows how pressure variation affects spread rate in the microgravity regime for a PMMA fuel of half-thickness of 50 mic.
Figure 4.21. MATLAB images showing flames facing an opposed flow velocity of 2 cm/s at pressure of (a) 0.5 atm (b) 1 atm and (c) 2 atm for a PMMA fuel of half-thickness of 50 mic.
CHAPTER 5

CONCLUSIONS

It was seen that at a given opposed flow velocity, the variation of the flow development distance caused a significant change in flame spread rate. Due to this, the impact of boundary layer had to be well understood. An expression for flame tip velocity or equivalent velocity was developed and spread rate was plotted against it for different flow development lengths. Curves for different flow development lengths appeared to be hugging each other thus verifying the correctness of this new expression. This expression was further tested for different fuel thicknesses where different flow development lengths were used for each thickness. As expected the formula agreed well here too. It was seen that the velocity ratio was highly dependent on the Reynolds number. In order to keep the velocity ratio constant, it was decided to keep the Reynolds number constant at every opposed flow velocity.

A non dimensional spread rate was plotted against Damkohler number and it was seen that when Damkohler number was based on equivalent velocity a change in thickness, oxygen level or flow development length barely caused an impact on the shape of the curve.

It was shown that radiation losses played a very important role in the microgravity regime. If these losses were neglected, flames were seen to have very high spread rates and ridiculous flame sizes. An opposed flow study for different fuel thicknesses proved that blow-off or extinction is independent of fuel thickness. Lesser the fuel thickness, higher was the flame spread rate as theory suggests that flame spread rate is inversely proportional to fuel thickness. As oxygen level was increased, it was seen that flame spread rate and flame sizes increased. This was because the increased oxygen level resulted in higher flame temperature, which was directly proportional to flame spread rate. A brief study in the microgravity regime, showed that higher pressure resulted in higher spread rates and larger flame sizes.
REFERENCES


