AN EMBEDDED UPWARD FLAME SPREAD MODEL USING 2D DIRECT NUMERICAL SIMULATIONS

by

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Department of Mechanical and Aerospace Engineering
To my parents, Ruiyun Fu and Chunming Xie
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Nomenclature

*Italic*:

\[ C \quad \text{thermal capacity } (J \cdot kg^{-1} \cdot K^{-1}) \]

\[ D \quad \text{molecular diffusivity } (m^2 \cdot s^{-1}) \]

\[ g \quad \text{gravity } (m \cdot s^{-2}) \]

\[ k \quad \text{thermal conductivity } (W \cdot m^{-1} \cdot K^{-1}) \]

\[ \dot{m}'' \quad \text{mass flux} (kg \cdot m^{-2} \cdot s^{-1}) \]

\[ \dot{m}''' \quad \text{mass generation rate} (kg \cdot m^{-3} \cdot s^{-1}) \]

\[ Pr \quad \text{Prandtl number} \]
\( q'' \) : heat flux (\( W \cdot m^{-2} \cdot s^{-1} \))

\( \dot{q}''' \) : heat generation rate (\( W \cdot m^{-3} \cdot s^{-1} \))

\( Re \) : Reynolds number

\( Sc \) : Schmidt number

\( S_p \) : pyrolysis length (\( m \))

\( S_f \) : flame length (\( m \))

\( T \) : temperature (\( K \))

\( Y_i \) : species mass fraction

\( Z \) : mixture fraction
Greek:

\[\alpha : \text{thermal diffusivity}(m^2 \cdot s^{-1})\]

\[\omega : \text{vorticity} (m^{-1})\]

\[\psi : \text{steam function} (m^2 \cdot s^{-1})\]

\[\phi : \text{level set function}\]

\[\rho : \text{density}(kg \cdot m^{-3})\]

\[\xi : \text{arbitrary scalar}\]

\[\mu : \text{dynamic viscosity}(kg \cdot m^{-1} \cdot s^{-1})\]

\[\nu : \text{kinematic viscosity}(m^2 \cdot s^{-1})\]
Vectors:

\( \vec{V} \) : velocity

\( \vec{t} \) : unit vector in the tangential direction

\( \vec{n} \) : unit vector in the normal direction

\( \vec{e}_x \) : unit vector in the \( X \) – axis direction

\( \vec{e}_y \) : unit vector in the \( Y \) – axis direction
Abstract

A fully coupled 2D fluid-solid direct numerical simulation (DNS) approach is developed to simulate fluid-solid heat and mass transfer processes using Cartesian grids. The solid geometry is identified using level set based embedded interface method. The flow field is described by the 2D Navier Stokes equations using a vorticity-streamfunction approach.

First a fluid-solid coupling formulation for the thermal and momentum fields is developed that is robust, computationally efficient and second-order accurate. Solutions for several example problems are presented for flow over stationary and moving cylinders to benchmark the current approach. Heat transfer for an isolated cylinder and two cylinders in series are then examined to explore the Nusselt number dependence on cylinder spacing and unsteady conjugate heat transfer processes.

Secondly, the methodology is extended to simulate flame spread over poly(methyl methacrylate) (PMMA) at different angles of inclination. Comparison of simulations and experimental measurements are conducted for flame spread rates. Results show
that the heat flux to the preheating region varies considerably in time - contradicting often employed assumptions used in established flame spread theories. Accounting for the time dependent behavior is essential in accurate predictions of flame spread, however, a universal characterization in terms of easily defined parameters is not found. Alternatively, a reaction progress variable based embedded flame model is developed using mixture fraction, total enthalpy and surface temperature. State maps of the gas-phase properties and surface heat flux are constructed and stored in pre-computed lookup tables. The resulting model provides a computationally efficient and a local formulation to determine the flame heat flux to the surface resulting in excellent agreement to DNS and experiments for predictions of flame spread rate and position of the pyrolysis front.
Chapter 1

Introduction

The overall goal of this research is to predict flame spread over solid materials. This is an important topic for addressing fire safety concerns. One of the current challenges in fire research is the prediction of flame spread over solids. Upon heating, the solid materials release combustible gases that burn with the surrounding air resulting the phenomena of flame spread. A fully coupled fluid-structure simulation methodology is developed to model conjugate heat and mass transfer processes with different solid geometries.

The first part of this research is to develop a computational algorithm which can predict conjugate heat transfer involving a fluid and a solid for 2D geometries and moving interfaces. Moving fluid-solid interfaces arise in a large variety of settings, most notably in combustion applications that often consist of burning, ablating, and
melting surfaces. The movement of the fluid-solid interface from heat and mass transfer affects the flow by changing the thermo-physical properties and geometry at the boundary. The change in the flow, in turn, modifies the gradients of temperature and species concentration near the interface which modify the rate at which the interface will move. This interaction is non-linear and depends on the kinematic and thermodynamic interface conditions that couple the fluid and solid systems. The solution to such problems remains largely intractable to analytical approaches.

Alternatively, a numerical approach may be pursued for which there are several solution methods available. Perhaps the earliest are arbitrary Lagrangian-Eulerian formations (ALE) for which the interface is tracked (see references in Belytschko et al. [4]). These methods are known to work well for small boundary displacements. For larger displacements, however, ALE methods may suffer from grid entanglement and require regridding that introduces additional computational cost.

As an alternative to ALE, interface capturing methods have become popular for treating interfaces using fixed Cartesian grids. In this approach, the fluid-solid interface is constructed using some sort of geometrical description of the interface that is within each cell or element. Several methods have been developed to represent the interface which include volume-of-fluid (VOF), marker-and-cell (MAC), and level set method. These methods can be grouped into two general classes: i) immersed boundary method (IBM), where the effects of the interface are introduced by applying
additional source terms [5, 6, 7, 8, 1, 9, 10, 11], and ii) embedded interface methods (EIM) where the effects of the interface are introduced by modifying the spatial discretization [12, 13, 14, 15, 16]. Each of these methods has relative advantages and disadvantages depending on the problem of interest. In this study, a level set based embedded interface method is pursued where the zero\(^{th}\) level set defines the location of the fluid-solid interface. Modifications to standard finite difference operators are developed to account for the presence of the interface and applied to the problem of moving and conjugate heat transfer of cylinders.

The development of this methodology begins with the mathematical formulation using a vorticity-streamfunction approach to describe the flow. Flow discretization for the spatial operators are then discussed along with interface matching conditions. While the current approach is limited to 2D flows, many of the approximations discussed can also be used for 3D applications in the context of other pressure based primitive variable formulations since the finite difference operators are formed from 1D constructs. Results are presented first for flow over stationary and translating cylinder to benchmark this approach and demonstrate second-order accuracy. Heat transfer applications are then discussed for an isolated cylinder and cylinders in series.

The next step of this research is to extend the algorithm developed above to study flame spread. Flame spread is often classified as either counter-current (opposed) or concurrent. For counter-current flame spread the direction of flame spread is
opposite to that of oxygen diffusion resulting in a steady flame spread rate that has been well described by previous extensive theoretical [17, 18, 19, 20], numerical [21] and experimental [21, 22] studies. Concurrent flame spread for vertically oriented surfaces (upward) in buoyancy driven flames are however much less understood. The fundamental challenge with upward flame spread is an adequate description of the time dependent coupled fluid-solid processes as the flame grows.

Early theoretical estimates of upward flame spread for laminar flames rely on approximate similarity solutions for the flow using a translating coordinate system located at the pyrolysis front (the flame spread rate is assumed constant) and steady-state heat conduction solutions for the solid phase are obtained by assuming either a thermally thick or thin material [23]. Orloff et al. [24] employed a “leap-frog” description of a turbulent flame where a power law relation between the flame height \( S_f \) and pyrolysis length \( S_p \), i.e., \( S_f(t) = \beta S_p^n(t) \), to couple the the fluid and solid phases - a useful approximation that is still commonly used. The time-to-ignition for each stage of the leap-frogging time is determined using a thermally-thick solution for the temperature in the solid phase by assuming a constant heat flux during each stage. More recently, Delichatsios et al. developed similarity solutions for turbulent upward flame spread assuming the time-to-ignition is a linear function of time [25]. Flame spread solutions are determined for three cases: constant heat flux, an assumed power law dependence of heat flux, and constant ignition time. In all cases, an
assumed power-law relation between $S_f$ and $S_p$ is employed, similar to that of Orloff et al. Excellent agreement is reported between the theory and detailed numerical predictions of $S_p$ for constant heat flux, however, less satisfactory agreement is shown between the theory and experimental measurements.

Recent numerical studies of Kumar et al. [26] and Consalvi et al. [27] have confirmed the importance of temporally varying heat flux in detailed numerical calculations. In the latter study, the time dependent evolution of both the solid and gas phases are solved simultaneously for flame spread over PMMA in the context of a Reynolds-Averaged Navier-Stokes equations (RANS) formulation. Predictions of heat flux show a rapid rise and then gradual decay with time for a given spatial location. These results are in agreement with recent findings of Rangwala et al. [28] who have shown the impact of a time dependent heat flux by using a revised definition of the $B$ number in Emmons solution [29]. Improved predications of pyrolysis growth are reported with the time dependent $B$ number when compared to experiments.

Experimentally, Quintiere [30] and Dysdale [3] have examined upward and downward flame spread over PMMA at several angles of inclination. Quintiere identifies two categories of upward flame spread corresponding to gravity assisted (i.e., flame below material) and gravity opposed configurations (i.e., flame above material). In both of these studies, as much as a factor of two decrease in flame spread rates is
observed for both configurations when the material is oriented from a vertical position to $\pm 60^\circ$. A flame spread theory is developed by Quintiere for thermally thin materials using a modified Grashof number to account for the inclination angle along with experimentally developed heat transfer correlations from Ahmad and Faeth [31] and Roper [32]. The resulting heat flux to the preheating region of the material is given in terms of the pyrolysis length, cosine of inclination angle, etc., but the spatial distribution of the heat flux within the preheating zone is assumed constant. The resulting predictions are shown to be in qualitative agreement with experiments.

With the advent of high performance computing, direct numerical simulation (DNS) of reacting flow is shedding new light on existing flame theories and providing guidance for the construction of subgrid scale (SGS) models for use with either large eddy simulation (LES) or Reynolds-averaged Navier-Stokes (RANS) [33]. The use of DNS for the fire related problems is in its infancy and provides a rich area to explore the limits of existing theories of flame spread and develop new SGS models for use with LES and RANS. The scope of the current study is to use 2D DNS to examine the process of flame spread for gravity opposed material orientations. The objectives for using this level of detail is two-fold. The first is to explore commonly used assumptions in flame spread modeling theory that can be explored in detail using DNS (e.g., constant heat flux in preheating zone, 1D heat transfer in solid, power-law dependence between $S_f$ and $S_p$, etc.). One of the findings that will be presented
from this activity is the importance of the time and spatial dependent descriptions of wall heat flux to obtain quantitative predictions of flame spread rate using existing flame spread theories. The limitation of these theories is they are often non-local – depending on distance such as ”flame height” and ”pyrolysis length” that are often not well defined. The non-local nature of these formulations limits them for use as SGS models for LES and RANS formulations. The second objective of this study is therefore to develop a local modeling formulation that can be used with LES and RANS and what is termed in this study an ”embedded flame spread” model. The model is based on a reduction in the degrees of freedom from that used in DNS using flamelet libraries that depend on a few conditioning variables. The heat flux to the wall and near-wall species and temperature in the flame are shown to be unique functions of these variables. Predictions using the embedded flame spread model are shown to beat in excellent agreement with the DNS demonstrating the viability of this approach.

The organizations of this dissertation are as follows: The first chapter will be introduction. In this chapter the motivation of this study and a review of what has been done is summarized. In chapter 2 the mathematical formulations used in this study are listed. It is followed by chapter 3, numerical discretization. The numerical method and discretized equations is discussed. In the next two chapters, the problems of interest of this dissertation, conjugate heat transfer and flame spread
are introduced and the findings are discussed. The last chapter is the conclusions of this dissertation.
Chapter 2

Mathematical Formulations

2.1 Governing Equations for 2D Incompressible Flow and Solid Phase

This research starts with the study of conjugate heat transfer between fluid and solid for 2D geometries and moving boundaries. Here the fluid flow is described by the 2D, unsteady Navier-Stokes equations for an incompressible fluid expressed in terms of a streamfunction ($\psi$) and vorticity ($\omega = \nabla \times \vec{V}$). These equations are supplemented with a temperature equation when convective heat transfer is considered. The result is the following system of non-dimensional equations,
where $Re(= U_{\infty} D/\nu)$ and $Pr(= \nu/\alpha)$ are the fluid Reynolds and Prandtl numbers, respectively. All fluid properties are assumed to be constant. The variables in the equations above are non-dimensionalized by the following transformations,

$$\omega^* = \frac{\omega L}{U_{\infty}}$$  \hspace{1cm} (2.5a)

$$\psi^* = \frac{\psi}{U_{\infty} L}$$  \hspace{1cm} (2.5b)

$$t^* = \frac{t U_{\infty}}{L}$$  \hspace{1cm} (2.5c)

$$x^* = \frac{x}{L}$$  \hspace{1cm} (2.5d)

$$y^* = \frac{y}{L}$$  \hspace{1cm} (2.5e)

$$T^* = \frac{T - T_{\infty}}{T_i - T_{\infty}}$$  \hspace{1cm} (2.5f)
where \( T_\infty \) is the inflow temperature and \( T_i \) is the initial solid temperature.

For the solid phase, the convective velocity is set equal to zero, resulting in the unsteady heat condition for the temperature equation,

\[
\frac{\partial T^*}{\partial t^*} = \frac{\alpha_s}{\alpha_f Pr Re} \nabla^2 T^* \tag{2.6}
\]

where \( \alpha_s/\alpha_f \) is solid to fluid thermal diffusivity ratio.

Boundary conditions are required at the boundaries of the computational domain and at the fluid-solid interface. At the inlet, the velocity \((U_\infty)\) and temperature \((T_\infty)\) are prescribed. At the outlets, convective based boundary conditions are used resulting in the following set of conditions for \( \psi^*, \omega^* \) and \( T^* \).

\[
\frac{\partial \omega^*}{\partial t^*} + V^*_n \frac{\partial \omega^*}{\partial \bar{n}} = 0 \tag{2.7a}
\]
\[
\frac{\partial T^*}{\partial t^*} + V^*_n \frac{\partial T^*}{\partial \bar{n}} = 0 \tag{2.7b}
\]
\[
\frac{\partial \psi^*}{\partial \bar{n}} = 0 \tag{2.7c}
\]

where \( \bar{n} \) is a unit normal vector directed outward from the boundary of the computational domain. At the fluid-solid interface, the fluid velocity \( V^*_{f} \) is used to specify \( \psi^* \) using the relations,
where $\mathbf{\tau}^I$ and $\mathbf{n}^I$ denote unit vectors in the tangential (oriented counter-clockwise) and normal (directed outward from the solid) directions, respectively. Imposing a no-slip condition on the interface gives $\mathbf{V}^* = \mathbf{V}^I$, where $\mathbf{V}^I$ is the velocity of the interface and is prescribed for all problems considered. The numerical implementation of these conditions is non-trivial since there are two conditions for a single unknown ($\psi^*$) and the problem appears to be over-prescribed. One of the conditions, however, is used to determine the vorticity on the boundary, via, $\nabla^2 \psi^I = -\omega^I$. The implementation of this condition will be discussed later in section 3.2 with regard to the evaluation of the properties at the interface.

The temperature at the interface, $T^I$, is determined from a balance of heat conduction,

$$k_s \frac{\partial T^s}{\partial n^I} \bigg|_s = k_f \frac{\partial T^f}{\partial n^I} \bigg|_f$$

where $k$ is the thermal conductivity.

In summary, Eqs. (2.1)-(2.4) along with the boundary conditions (2.7)-(2.9) define
the problem of interest. What still remains to be defined is a geometrical representation of the interface for which in this study a level set function is used.

### 2.2 Governing Equations for Flame Spread Problem

The second part of this research is flame spread. To take advantage of solver developed from the previous study, vorticity ($\omega$) -streamfunction ($\psi$) formulation is again used to solve the Navier-Stokes equations but with a dimensional form along with supplementary equations for scalar transport to describe the combustion processes and necessary modification to account for variable density. This is done by following that of Ashurst and Barr [34],

\[
\frac{\partial \omega}{\partial t} + (\vec{u} \cdot \nabla) \omega + \omega (\nabla \cdot \vec{u}) = \nu \nabla^2 \omega - \frac{\rho_0}{\rho^2} g \frac{\partial \rho}{\partial x}
\]  

(2.10)

where $\rho_0$ is density of air at the normal condition. Dilatation of the velocity field from thermal expansion is accounted for by using a Helmholtz decomposition of the velocity field [35], i.e., $\vec{u} = \vec{v} + \nabla \phi$ with $\nabla \times \vec{v} = \omega$ and $\nabla \cdot \vec{v} = 0$. The streamfunction and expansion component of the velocity are determined from solution to the Poisson equations [36].
\[ \nabla^2 \psi = -\omega \]  
\[ \nabla^2 \phi = \frac{1}{\rho C_{p,g} T} (\dot{q}'' + k \nabla^2 T) \]  

where \( \dot{q}'' (= \dot{m}'',\Delta h_c) \) is the heat release per unit volume from combustion. Energy and species transport equations are solved in conjunction with the momentum field,

\[ \mathcal{L}(T) = \frac{\nu}{Pr} \nabla^2 T + \frac{\dot{q}''}{\rho g C_p} \]  
\[ \mathcal{L}(Y_k) = \frac{\nu}{Sc} \nabla^2 Y_k + \frac{\dot{m}''}{\rho} \]  

where \( \mathcal{L}(\cdot) = \partial(\cdot)/\partial t + \bar{u} \cdot \nabla(\cdot) \) is the material derivative operator. Schmidt number, \( Sc \), and Prandtl number, \( Pr \), are both assumed to be unity in the current study. The density in Eqs.(2.12)-(2.14) is determined from an ideal gas equation of state assuming the pressure is everywhere constant. The value of the specific heat in Eq.(2.12) is chosen to be \( 1.31 \text{ kJ/kg - K} \) to match the measured adiabatic flame temperature of \( 2442 \text{ K} \).

The chemical reaction rate term for each species is determined from an assumed single-step chemical kinetics mechanism,

\[ F + r_{Ox} Ox + r_I I \rightarrow (1 + r_{Ox}) P + r_I I \]  

(2.15)
with a prescribed global Arrhenius reaction rate given as

\[ \dot{m}_F'' = -B_c \rho Y_F Y_{Ox} \exp(-T_{a,c}/T) \]  

(2.16)

where parameter constants \( B_c = 5.928 \times 10^9 \text{m}^3/(\text{kg} \cdot \text{s}) \) and \( T_{a,c} = 10,700 \text{K} \) are adopted from West et al. for the burning of MMA vapor in air [37]. Soot formation and radiation heat transfer are not explicitly accounted for in the model but rather its effects are introduced as two adjustments. The first is based on the experiments of MMA pool fire of Hamins et al. where the radiative heat loss is estimated to be 30% of the total heat release [38]. The heat release rate is therefore scaled accordingly as: 

\[ \dot{q}'''' = \chi \dot{m}_F'' \Delta h_e, \]

where \( \chi = 0.7 \) and \( \Delta h_e = 2.601 \times 10^4 \text{kJ/\text{kg}} \). The second is a modification of the heat flux to the solid surface that is discussed below.

Standard convection boundary conditions are employed at the open boundaries of the domain for all transported quantities (i.e., \( \mathbf{L}(\cdot) = 0 \)) and the normal derivatives of \( \psi \) and \( \phi \) are assumed equal to zero. At the solid-gas interface, energy and mass balances are enforced for the preheat and pyrolysis zones. In the preheat zone the heat and mass fluxes at the solid-gas interface are balanced, i.e., 

\[ k_s \partial T/\partial n = k_g \partial T/\partial n + \dot{q}_{\text{rad}}''', \]

and 

\[ \partial Y_k/\partial n = 0, \]

where \( n \) is the normal direction directed outward from the solid surface. The heat flux from the flame to the surface from radiation, \( \dot{q}_{\text{rad}}''' \), is assumed to be equal to that from conduction, \( \dot{q}_{\text{rad}}''' = k_g \partial T/\partial n \) based on the measurements of Tewarson et al. [39] where he found that the ratio of heat flux from conduction and
radiation to be close to unity for standard air conditions. During the pre-heating stage a non-slip condition is imposed for the velocity. In the pyrolysis zone, the temperature is assumed to be constant and set equal to the decomposition temperature of $653K$. The mass flux is determined from the overall energy balance,

$$
\dot{m}'' = \frac{\dot{q}_{\text{net}}''}{L_v}
$$

(2.17)

where $L_v$ ($= 1.62 \times 10^4 kJ/kg - K$) is the latent heat of vaporization of PMMA and $\dot{q}_{\text{net}}'' = k_g \partial T/\partial n + \dot{q}_{\text{rad}}'' - k_s \partial T/\partial n$ is the net heat flux used for gasification of PMMA. Species jump relations at the gas-solid interface in the pyrolysis zone result in the balance relation for all species,

$$
-\rho \partial Y_F/\partial n = \dot{m}'' (1 - Y_F)
$$

(2.18)

$$
-\rho \partial Y_k/\partial n = \dot{m}'' (0 - Y_k)
$$

(2.19)

In the solid phase, the Fourier law of conduction is used,

$$
\partial T/\partial t = (k_s/\rho_s C_s) \nabla^2 T
$$

(2.20)

where the thermal conductivity ($k_s$), density ($\rho_s$), and specific heat ($C_s$) are equal to $0.19 W/m - K$, $1190 kJ/m^3$ and $1420 J/kg - K$, respectively. At the solid-gas
interface, the net heat flux from the gas phase is imposed. The remaining boundaries are assumed adiabatic. The solid surface is fixed in space for each case (regression and fuel swelling are not modeled).

2.3 Level Set Description of Interface

The level set method was devised by Osher and Sethian and is a simple and versatile method for computing and analyzing the motion of an interface in two or three dimensions [40]. Sethian, Osher, and others have popularized this method for use in a wide range of applications in combustion, incompressible flow [41, 42], compressible flow [43], solidification, and Stefan problems [44]. In this approach, a scalar function, $\phi(\vec{x}, t)$, is defined whose magnitude is the shortest distance from the point $\vec{x}$ to the interface. By definition then, the value $\phi$ equals zero for a point which lies on the fluid-solid interface. For locations off of the interface, the sign of $\phi$ depends on the orientation of the interface normal, $\vec{n}^I$, and is determined from the condition,

$$\frac{\nabla \phi}{|\nabla \phi|} = \vec{n}^I$$

(2.21)

For this study, $\vec{n}^I$ is directed into the solid, therefore $\phi$ has the following sign convention.
\[
\phi(\vec{x},t) > 0 \text{ for } \vec{x} \text{ in the solid-phase}
\]
\[
\phi(\vec{x},t) < 0 \text{ for } \vec{x} \text{ in the fluid-phase}
\]
\[
\phi(\vec{x},t) = 0 \text{ for } \vec{x} \text{ on the interface}
\]

In this study, the interface is rigid and the interface of cylinder can be exactly imposed. Therefore no level set movement equations are solved. Our motivations for pursuing the level set approach for interface capturing is to be able to readily incorporate melting or surface decomposition phenomena (e.g., ablation or charring) in our future research, however, this is not addressed in the present study.
Chapter 3

Numerical Discretization

3.1 Flow Discretization

Finite difference discretization with two-stage Runge-Kutta time integration is used to solve Eqs. (2.1)-(2.4) on a Cartesian grid. The convective terms are discretized using a third order accurate QUICK [45] scheme and second order centered differences are used for viscous/conduction terms. The Poisson equation for the streamfunction given in Eq. (2.2) is discretized using standard centered differences and solved using a multigrid solver with four levels of grid refinement employing a “V” cycle [46].

For nodes neighboring the zeroth level set, the finite difference equations are modified to account for the presence of the interface. Figure 3.1(a) shows one of eight possible fluid-solid configurations. Node \((i, j)\) is the point of interest on the numerical
interface for which Eqs. (2.1)-(2.4) are modified. The points 1 and 2 identify the intersection of the mesh lines from node \((i, j)\) with the interface. The distances \(\delta x\) and \(\delta y\) are the distances from points 1 and 2 to node \((i, j)\), respectively. Approximating the interface between points 1 and 2 as a line, expressions for the complementary interior angles \(\theta_1\) and \(\theta_2\) can be obtained in terms of \(\delta x\), \(\Delta x\), \(\phi_{i,j}\), \& \(\phi_{i+1,j}\) and \(\delta y\), \(\Delta y\), \(\phi_{i,j}\), \& \(\phi_{i,j-1}\), respectively. Setting these expressions equal to each other results in,

\[
\begin{align*}
\sin(\theta_1) &= \frac{\phi_{i,j}}{\delta x} = -\frac{\phi_{i+1,j}}{\Delta x - \delta x} \\
\sin(\theta_2) &= \frac{\phi_{i,j}}{\delta y} = -\frac{\phi_{i,j-1}}{\Delta y - \delta y}
\end{align*}
\] (3.1)

Rearranging these results, expressions for \(\delta x\) and \(\delta y\) in terms of the level function can be determined that are similar to those of Marella et al. \[16\],

\[
\begin{align*}
\delta x &= -\left(\frac{\phi_{i,j}}{\phi_{i+1,j} - \phi_{i,j}}\right) \Delta x \\
\delta y &= -\left(\frac{\phi_{i,j}}{\phi_{i,j-1} - \phi_{i,j}}\right) \Delta y
\end{align*}
\] (3.2)

Once \(\delta x\) and \(\delta y\) are known, then second-order accurate finite differences are developed for \(\nabla \xi\) and \(\nabla^2 \xi\) for locations near the fluid-solid interface, where \(\xi\) is an arbitrary scalar. For the case shown in Fig. 3.1(b) these approximations are,
\[ \nabla \xi = \frac{\partial \xi}{\partial x} \hat{e}_x + \frac{\partial \xi}{\partial y} \hat{e}_y \]
\[ = \frac{\xi_i - (1 - \alpha^2)\xi_{i,j} - \alpha^2 \xi_{i-1,j}}{\alpha(1 + \alpha)\Delta x} \hat{e}_x + \frac{\xi_2 - (1 - \beta^2)\xi_{i,j} - \beta^2 \xi_{i,j+1}}{\beta(1 + \beta)\Delta y} \hat{e}_y \]
\[ \nabla^2 \xi = \frac{\partial^2 \xi}{\partial x^2} + \frac{\partial^2 \xi}{\partial y^2} \]
\[ = \frac{1}{(\Delta x)^2} \left( \frac{\alpha - 1}{\alpha + 2} \xi_{i-2,j} + \frac{4 - 2\alpha}{\alpha + 1} \xi_{i-1,j} + \frac{\alpha - 3}{\alpha} \xi_{i,j} + \frac{6}{\alpha(\alpha + 1)(\alpha + 2)} \xi_1 \right) \]
\[ + \frac{1}{(\Delta y)^2} \left( \frac{\beta - 1}{\beta + 2} \xi_{i,j+2} + \frac{4 - 2\beta}{\beta + 1} \xi_{i,j+1} + \frac{\beta - 3}{\beta} \xi_{i,j} + \frac{6}{\beta(\beta + 1)(\beta + 2)} \xi_2 \right) \]
\[ (3.3) \]

where \( \alpha = \delta x / \Delta x \) and \( \beta = \delta y / \Delta y \). A similar set of discrete operators are determined for the remaining seven possible interface configurations for \( \nabla \xi \) and \( \nabla^2 \xi \). These cases are subdivided into four edge configurations and four corner configurations. Tables 3.2 and 3.3 show one edge and one corner configuration for \( \nabla \xi \) and \( \nabla^2 \xi \), respectively. For ease of implementing these operators into a computer code, a switch function, \( S \), is introduced. This switch function is equal to 1 in the flow field and equal to zero in the solid side and is defined as,

\[ S = \begin{cases} 1 & \text{if } \phi_{i,j} < 0 \\ 0 & \text{if } \phi_{i,j} \geq 0 \end{cases} \]  
\[ (3.4) \]
For example, the finite difference approximation of $\nabla^2 \xi$ can be completely expressed for all eight possible cases as,

\[
\nabla^2 \xi = \frac{S_{i-1,j}}{(\Delta x)^2(S_{i+1,j} + S_{i-1,j})} \left( \frac{\alpha - 1}{\alpha + 2} \xi_{i-2,j} + \frac{4 - 2\alpha}{\alpha + 1} \xi_{i-1,j} + \frac{\alpha - 3}{\alpha} \xi_{i,j} + \frac{6}{\alpha(\alpha + 1)(\alpha + 2)} \xi_1 \right)
\]

\[
+ \frac{S_{i+1,j}}{(\Delta x)^2(S_{i+1,j} + S_{i-1,j})} \left( \frac{\alpha - 1}{\alpha + 2} \xi_{i+2,j} + \frac{4 - 2\alpha}{\alpha + 1} \xi_{i+1,j} + \frac{\alpha - 3}{\alpha} \xi_{i,j} + \frac{6}{\alpha(\alpha + 1)(\alpha + 2)} \xi_1 \right)
\]

\[
+ \frac{S_{i,j-1}}{(\Delta y)^2(S_{i,j+1} + S_{i,j-1})} \left( \frac{\beta - 1}{\beta + 2} \xi_{i,j-2} + \frac{4 - 2\beta}{\beta + 1} \xi_{i,j-1} + \frac{\beta - 3}{\beta} \xi_{i,j} + \frac{6}{\beta(\beta + 2)} \xi_2 \right)
\]

\[
+ \frac{S_{i,j+1}}{(\Delta y)^2(S_{i,j+1} + S_{i,j-1})} \left( \frac{\beta - 1}{\beta + 2} \xi_{i,j+2} + \frac{4 - 2\beta}{\beta + 1} \xi_{i,j+1} + \frac{\beta - 3}{\beta} \xi_{i,j} + \frac{6}{\beta(\beta + 2)} \xi_2 \right)
\]

(3.5)

Direct implementation of these operators into the explicit two-stage Runge-Kutta results in reasonable results for coarse grids. However, with increased grid refinement numerical instability is observed. The source of this instability is from the small cut-cell distances, $\delta x$ and $\delta y$, which require small time steps for numerical stability using an explicit method. It was found that the time step, $\Delta t$, had to be chosen small enough to ensure CFL conditional stability at the interfaces, i.e., $\Delta t \leq \text{MIN}(\delta x, \delta y)/|\vec{V}|_{\text{max}}$, where $|\vec{V}|_{\text{max}}$ is the maximum velocity associated with the nodes closest to the fluid-solid interface. This limitation becomes especially problematic since the time step, $\Delta t$ become prohibitively small as $\delta x, \delta y \to 0$. Previous studies using level set interface methods suggest modifying the spatial operators to
get around this issue by replacing \( \delta x \) and \( \delta y \) with \( \delta x + (\Delta x)^2 \) and \( \delta y + (\Delta y)^2 \), respectively, or adding some arbitrary small value to \( \delta x \) and \( \delta y \) [16]. These approaches were found to be unsatisfactory and therefore an alternative point implicit approach is pursued. In this approach, the spatial operators near the interface are evaluated at the current, \((n + 1)\), time level resulting in a coupled system of equations. To avoid the computational costs and complexity of inverting this system, a point-implicit approach is pursued where all of the nodes except those lying near the interface are first updated using an explicit method to the current \((n + 1)^e\) time level, where the superscript “e” indicates a value using an explicit method. These values are then used to update the nodes that bound the fluid-solid interface where the spatial operators that contain information at node \((i,j)\) are evaluated at \((n + 1)^i\), where the superscript “i” indicates a value using the point-implicit method. The resulting finite difference expression at node \((i,j)\) is inverted analytically to solve for the quantity. As an example, for the configuration considered in Fig. 3.1(b), the value of vorticity is updated as follows,
The use of this point-implicit method results in a robust integration approach with conditional stability using time steps based on the uncut cell distances, $\Delta x$ and $\Delta y$.

The source terms in Eqs. (2.13) and (2.14) are integrated using the LSODE solver [47] then integrated in time using a fractional stepping procedure. In the study of flame spread over PMMA, the solid phase PMMA region of the the domain is solved using standard finite differences and the grid is aligned with the material interface therefore no special treatment of cut-cells is required.
3.2 Property Evaluation at Interface

3.2.1 For 2D Conjugate Heat Transfer Between Incompressible Flow and Solids

The values of \(\psi\), \(\omega\), and \(T\) are required where the Cartesian grid intersects with the fluid-solid interface. These intersections are labeled as points 1 and 2 for the case considered in Fig. 3.1(a). For stationary bodies, the value of \(\psi\) on the interface is a constant. For moving boundaries \(\psi\) changes along the interface and appears to be over-specified using Eqs. (2.8a) and (2.8b) - two relations for one unknown. However one of these relations, \(\partial \psi / \partial n^I = -\vec{V}_f \cdot \vec{n}^I\), may be used to determine the wall vorticity therefore the system of equations is well-posed. This is accomplished by using Eq. (2.2) to update \(\omega\) at the fluid-solid interface. As an example, consider the fluid-solid intersection point 1 in Fig. 3.1. The Poisson equation at this location is,

\[
\omega_1 = - \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) \bigg|_1 \tag{3.7}
\]

which requires evaluation of the second derivatives of \(\psi\). Using Taylor series expansions for \(\psi\) at points \(N1, N2, W1\) and \(W2\) shown in Fig. 3.1(b) in the “north” and “west” directions gives,
\[ \psi_{N_1} = \psi_1 + \Delta y \frac{\partial \psi}{\partial y} \bigg|_1 + \frac{\Delta y^2 \partial^2 \psi}{2! \partial y^2} \bigg|_1 + \frac{\Delta y^3 \partial^3 \psi}{3! \partial y^3} \bigg|_1 + O(\Delta y^4) \quad (3.8) \]

\[ \psi_{N_2} = \psi_1 + 2\Delta y \frac{\partial \psi}{\partial y} \bigg|_1 + 4 \frac{\Delta y^2 \partial^2 \psi}{2! \partial y^2} \bigg|_1 + 8 \frac{\Delta y^3 \partial^3 \psi}{3! \partial y^3} \bigg|_1 + O(\Delta y^4) \quad (3.9) \]

\[ \psi_{W_1} = \psi_1 - \Delta x \frac{\partial \psi}{\partial x} \bigg|_1 + \frac{\Delta x^2 \partial^2 \psi}{2! \partial x^2} \bigg|_1 - \frac{\Delta x^3 \partial^3 \psi}{3! \partial x^3} \bigg|_1 + O(\Delta x^4) \quad (3.10) \]

\[ \psi_{W_2} = \psi_1 - 2\Delta x \frac{\partial \psi}{\partial x} \bigg|_1 + 4 \frac{\Delta x^2 \partial^2 \psi}{2! \partial x^2} \bigg|_1 - 8 \frac{\Delta x^3 \partial^3 \psi}{3! \partial x^3} \bigg|_1 + O(\Delta x^4) \quad (3.11) \]

Rearranging the above expressions and substituting in \( \psi_x = -v \) and \( \psi_y = u \) then results in approximations for the second derivatives,

\[ \left. \frac{\partial^2 \psi}{\partial x^2} \right|_1 = \frac{8\psi_{W_1} - 7\psi_1 - \psi_{W_2}}{2\Delta x^2} - 3 \frac{v_1}{\Delta x} + O(\Delta x^2) \quad (3.12) \]

\[ \left. \frac{\partial^2 \psi}{\partial y^2} \right|_1 = \frac{8\psi_{N_1} - 7\psi_1 - \psi_{N_2}}{2\Delta y^2} - 3 \frac{u_1}{\Delta y} + O(\Delta y^2) \quad (3.13) \]

The values of \( \psi \) at points \( N_1, N_2, W_1 \) and \( W_2 \) in Eqs. (3.12) and (3.13) are determined from fourth-order accurate Lagrange interpolating polynomials using the closest neighboring nodes. Fourth-order accuracy is required because second-order accuracy is desired for estimating \( \frac{\partial^2 \psi}{\partial x^2} \) and \( \frac{\partial^2 \psi}{\partial y^2} \) (Note, the \((\Delta x)^2\) and \((\Delta y)^2\) that appear in the denominators of the first term on the r.h.s. of Eqs. (3.12) and (3.13),
respectively). Substituting Eqs. (3.12) and (3.13) into Eq. (3.7) then results in the following second-order accurate expression for $\omega$ at point 1.

$$
\omega_1 = - \left( \frac{8\psi_{W1} - 7\psi_1 - \psi_{W2}}{2\Delta x^2} + \frac{8\psi_{N1} - 7\psi_1 - \psi_{N2}}{2\Delta y^2} \right) + 3 \left( \frac{u_1}{\Delta x} + \frac{u_1}{\Delta y} \right) \quad (3.14)
$$

Equation (3.14) is one out of eight possible configurations. The approximations used for $\nabla^2 \psi$ for one of the edge and corner configurations is summarized in Table 3.5.

For conjugate heat transfer problems, a numerical approximation for the heat flux balance across the fluid-solid interface given in Eq. (2.9) is required. The surface normal derivatives are first expressed in terms of the level set function,

$$
\frac{\partial T}{\partial n} = \nabla T \cdot \hat{n} = \nabla T \cdot \nabla \phi = \frac{\partial T}{\partial x} \frac{\partial \phi}{\partial x} + \frac{\partial T}{\partial y} \frac{\partial \phi}{\partial y} \quad (3.15)
$$

where $\partial \phi / \partial x$ and $\partial \phi / \partial y$ are determined using second order centered finite differences and $\partial T / \partial x$ and $\partial T / \partial y$ are determined using second order one-sided finite differences. The finite difference stencils for one of the edge and corner configurations are summarized in Table 3.4. As an example, the approximations for Eq. (3.15) at point 1 in Fig. 3.1(b) (corner configuration in Table 3.4) are,
\[
\frac{\partial T}{\partial n^I}_{1,1} = \frac{3T_1 - 4T_W W_1 + T_W W_2 \frac{\partial \phi}{\partial x}}{2\Delta x} + \frac{-3T_1 + 4T_N N_1 - T_N N_2}{2\Delta y} \sqrt{1 - \left( \frac{\partial \phi}{\partial x} \right)^2} \tag{3.16}
\]

and

\[
\frac{\partial T}{\partial n^I}_{s,1} = -3T_1 + 4T_E E_1 - T_E E_2 \frac{\partial \phi}{\partial x} + \frac{3T_1 - 4T_S S_1 + T_S S_2}{2\Delta y} \sqrt{1 - \left( \frac{\partial \phi}{\partial x} \right)^2} \tag{3.17}
\]

where

\[
\frac{\partial \phi}{\partial x} = \frac{\phi_{i+1,j} \alpha^2 - \phi_{i,j} (1 - \alpha^2)}{\alpha (1 - \alpha) \Delta x}. \tag{3.18}
\]

Substituting Eqs. (3.16) and (3.17) into Eq. (2.9) allows the temperature at point 1 to be determined,
where \( B = \Delta x / \Delta y \). The discrete operators for \( \dot{q}_s''(= -k_s \nabla T \cdot \hat{n}_s^I) \) and \( \dot{q}_f''(= -k_f \nabla T \cdot \hat{n}_s^I) \) for an edge and corner configurations are summarized in Table 3.4. These expressions are equated to determine the interface temperature for all mesh-interface intersection point configurations.

### 3.2.2 For Flame Spread Problem

Unlike the problem of conjugate heat transfer between liquid and solids, the temperature at the interface is solved by heat conduction in PMMA instead of the direct heat balance equation such as 3.19. Because in that problem equations 2.4 and 2.6 are both solved at each flow time step. In flame spread problem, the solid phase is solved with a time step of 0.1 second [48] which is also the coupling time step between gas phase solver and solid phase solver. A time averaged heat flux from the gas phase over this coupling time step is applied as the heat flux boundary condition for the solid. Then the temperature on the solid-gas boundary is obtained by solving 2.20. The mass flux is solved from 2.17. Then species on the solid-gas interface is solved by 2.18 and 2.19 where the normal derivatives are approximated in a similar manor as 3.16.
3.3 Grid Convergence Test

A series of benchmark problems suggested by LeVeque and Li [5] are first considered to examine the accuracy of the interface capturing method. A circular interface is considered on a uniform grid. The diameter of the circle is unity and is centered on a square domain of length 2. The distribution of \( \psi \) is as following,

\[
\psi = \begin{cases} 
1 & \text{inside the circle} \\
1 + \ln(2r) & \text{outside the circle}.
\end{cases}
\]  

(3.20)

The objective is to calculate \( \nabla^2 \psi = \frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r} \frac{\partial \psi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \theta^2} = \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \) at the zeroth level set and compare to the exact solution. The exact solution for \( \nabla^2 \psi \) is equal to zero at the zeroth level set. This operator is developed similar to the other operators discussed and summarized in Table 3.6. Several levels of grid-refinement are employed using a uniformly spaced \( n \times n \) grid where \( n = 20, 40, 160, 320, 640, 1280 \) and \( 2560 \). Table 3.1 summarizes the results in terms of \( L_1, L_2 \) and \( L_\infty \) error norms for different grid refinement ratios. A clear second-order asymptotic convergence rate emerges where the ratio of successive errors is observed to approach four.
Table 3.1: Results for convergence tests of Leveque’s problem.

<table>
<thead>
<tr>
<th>Grids</th>
<th>$L_1$</th>
<th>Ratio</th>
<th>$L_2$</th>
<th>Ratio</th>
<th>$L_\infty$</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>$6.02 \times 10^{-1}$</td>
<td>-</td>
<td>$6.37 \times 10^{-1}$</td>
<td>-</td>
<td>$7.86 \times 10^{-1}$</td>
<td>-</td>
</tr>
<tr>
<td>40</td>
<td>$1.94 \times 10^{-1}$</td>
<td>3.103</td>
<td>$2.15 \times 10^{-1}$</td>
<td>2.967</td>
<td>$3.17 \times 10^{-1}$</td>
<td>2.477</td>
</tr>
<tr>
<td>80</td>
<td>$5.78 \times 10^{-2}$</td>
<td>3.356</td>
<td>$6.45 \times 10^{-2}$</td>
<td>3.327</td>
<td>$9.43 \times 10^{-2}$</td>
<td>3.368</td>
</tr>
<tr>
<td>160</td>
<td>$1.58 \times 10^{-2}$</td>
<td>3.662</td>
<td>$1.77 \times 10^{-2}$</td>
<td>3.653</td>
<td>$2.57 \times 10^{-2}$</td>
<td>3.670</td>
</tr>
<tr>
<td>320</td>
<td>$4.14 \times 10^{-3}$</td>
<td>3.813</td>
<td>$4.61 \times 10^{-3}$</td>
<td>3.826</td>
<td>$6.67 \times 10^{-3}$</td>
<td>3.852</td>
</tr>
<tr>
<td>640</td>
<td>$1.06 \times 10^{-3}$</td>
<td>3.907</td>
<td>$1.18 \times 10^{-3}$</td>
<td>3.912</td>
<td>$1.69 \times 10^{-3}$</td>
<td>3.936</td>
</tr>
<tr>
<td>1280</td>
<td>$2.68 \times 10^{-4}$</td>
<td>3.954</td>
<td>$2.98 \times 10^{-4}$</td>
<td>3.956</td>
<td>$4.27 \times 10^{-4}$</td>
<td>3.970</td>
</tr>
<tr>
<td>2560</td>
<td>$6.73 \times 10^{-5}$</td>
<td>3.977</td>
<td>$7.49 \times 10^{-5}$</td>
<td>3.978</td>
<td>$1.07 \times 10^{-4}$</td>
<td>3.986</td>
</tr>
</tbody>
</table>

Table 3.2: Finite-difference operators for $\nabla \xi$ at the node $(i, j)$ near the fluid-solid interface for edge and corner configurations.

\[
\begin{array}{c|c|c}
\text{Configuration} & \nabla \xi & \\
\hline
\theta = \beta & \hat{e}_x & \hat{e}_y \\
\hline
\frac{1}{\alpha(\alpha+1)}(\xi_i + \frac{1}{\alpha} \xi_{i+1} - \frac{\alpha}{\alpha+1} \xi_{i-1}) & & \frac{\xi_{i+1} - \xi_{i+1-1}}{2\Delta y}
\end{array}
\]
Table 3.3: Finite-difference operators for $\nabla^2 \xi$ at the node $(i, j)$ near the fluid-solid interface for edge and corner configurations.

<table>
<thead>
<tr>
<th>Configuration</th>
<th>$\nabla^2 \xi$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\vec{c}_x$</td>
</tr>
<tr>
<td></td>
<td>$\frac{\alpha-1}{\alpha+2} \xi_{i-2,j} + \frac{4-2\alpha}{\alpha+1} \xi_{i-1,j} + \frac{\alpha-3}{\alpha} \xi_{i,j} + \frac{6}{\alpha(\alpha+1)(\alpha+2)} \xi_{i+1,j}$</td>
</tr>
<tr>
<td></td>
<td>$(\Delta x)^2$</td>
</tr>
</tbody>
</table>

*Diagram showing edge and corner configurations.*
Table 3.4: Finite-difference approximations for $\bar{q} \cdot \bar{n} = \bar{q} \cdot \nabla \phi = q''$ for the solid and fluid side of the interface at point 1 for edge and corner configurations.

<table>
<thead>
<tr>
<th>Configuration</th>
<th>$q_s'' = -k_s \left( \frac{\partial T_s}{\partial x} \frac{\partial \phi}{\partial x} + \frac{\partial T_s}{\partial y} \frac{\partial \phi}{\partial y} \right)$</th>
<th>$q_f'' = -k_f \left( \frac{\partial T_f}{\partial x} \frac{\partial \phi}{\partial x} + \frac{\partial T_f}{\partial y} \frac{\partial \phi}{\partial y} \right)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Edge</td>
<td>$-k_s \frac{-3T_1 + 4T_{E1} - T_{E2}}{2\Delta x}$</td>
<td>$-k_f \frac{3T_1 - 4T_{W1} + T_{W2}}{2\Delta x}$</td>
</tr>
<tr>
<td>Corner</td>
<td>$-k_s \frac{-3T_1 + 4T_{E1} - T_{E2}}{2\Delta x} \cdot \frac{\alpha^2 \phi_{i+1,j} - (1-\alpha)^2 \phi_{i,j}}{\alpha(1-\alpha)\Delta x}$</td>
<td>$-k_f \frac{3T_1 - 4T_{W1} + T_{W2}}{2\Delta x} \cdot \frac{\alpha^2 \phi_{i+1,j} - (1-\alpha)^2 \phi_{i,j}}{\alpha(1-\alpha)\Delta x}$</td>
</tr>
<tr>
<td></td>
<td>$-k_s \frac{-3T_1 + 4T_{S1} + T_{S2}}{2\Delta y} \left[ -\sqrt{1 - \left( \frac{\partial \phi}{\partial x} \right)^2} \right]$</td>
<td>$-k_f \frac{-3T_1 + 4T_{N1} - T_{N2}}{2\Delta y} \left[ -\sqrt{1 - \left( \frac{\partial \phi}{\partial x} \right)^2} \right]$</td>
</tr>
</tbody>
</table>
Table 3.5: Finite-difference approximations for $\nabla^2 \psi = \partial^2 \psi / \partial x^2 + \partial^2 \psi / \partial y^2$ on the fluid-solid interface at point 1 for edge and corner configurations.

| Configuration | $\nabla^2 \psi|_1$ |
|---------------|-------------------|
| ![Diagram](image1.png) | $-\frac{8\psi_{N1} - 7\psi_1 - \psi_{N2}}{2(\Delta y)^2} + \frac{3\psi_1}{\Delta y} - \frac{8\psi_{W1} - 7\psi_1 - \psi_{W2}}{2(\Delta x)^2} + \frac{3\psi_1}{\Delta x}$ |
| ![Diagram](image2.png) | $-\frac{8\psi_{N1} - 7\psi_1 - \psi_{N2}}{2(\Delta y)^2} + \frac{3\psi_1}{\Delta y} - \frac{8\psi_{W1} - 7\psi_1 - \psi_{W2}}{2(\Delta x)^2} + \frac{3\psi_1}{\Delta x}$ |
Table 3.6: Finite-difference approximations for \( \nabla^2 \xi = \frac{\partial^2 \xi}{\partial x^2} + \frac{\partial^2 \xi}{\partial y^2} \) on the fluid-solid interface at point 1 for edge and corner configurations.

| Configuration | \( \nabla^2 \xi |_1 \) |
|--------------|------------------|
| ![Configuration diagram](image1) | \( \frac{2\xi_1-5\xi_{N1}+4\xi_{N2}-\xi_{N3}}{2(\Delta y)^2} + \frac{2\xi_1-5\xi_{W1}+4\xi_{W2}-\xi_{W3}}{2(\Delta x)^2} \) + \( \frac{2\xi_1-5\xi_{S1}+4\xi_{S2}-\xi_{S3}}{2(\Delta y)^2} \) |
| ![Configuration diagram](image2) | \( \frac{2\xi_1-5\xi_{N1}+4\xi_{N2}-\xi_{N3}}{2(\Delta y)^2} + \frac{2\xi_1-5\xi_{W1}+4\xi_{W2}-\xi_{W3}}{2(\Delta x)^2} \) |
Figure 3.1: Details of the fluid-solid interface showing (a) the definitions of $\delta x$ and $\delta y$ along and associated interior angles and (b) intersection points for constructing high order approximations to gradients at fluid-solid interface.
Chapter 4

Conjugate Heat Transfer

4.1 Flow Over a Stationary Cylinder

A commonly used test problem for examining embedded grid techniques is flow over a circular cylinder where numerical solutions [8, 1] and experimental data [49] are readily available for comparison. Two Reynolds numbers of 20 and 40 are chosen to compare against the previous studies of Calhoun [8] and Russel and Wang [1]. Simulations are performed using $n \times n$ grid where $n = 80, 160, 320$ and 640 corresponding to 16, 32, 64 and 128 grid points across the diameter of the cylinder, respectively.

Figures 4.1 and 4.2 show the contours of streamfunction and vorticity at steady-state for $Re = 20$ and 40, respectively, using the finest mesh. A pair of counter-rotating vortices form on the downstream location of the cylinder and increase in
length with increasing $Re$. At these low $Re$ numbers no vortex shedding is expected. Figure 4.3(a) presents the cross-stream velocity at the center of the recirculation zone for the $Re = 20$ case. As shown, the solutions for the $n = 320$ and $640$ cases are identical indicating a grid converged solution (all other variables are less sensitive to grid refinement). Figure 4.3(b) shows the normalized streamfunction error as a function of mesh refinement. Consistent with the previous LeVeque test case, second-order grid convergence is observed. Similar results are also obtained for the $Re = 40$ case (not shown). Calculations of the recirculation length ($L$), separation angle ($\theta$) and drag coefficient compare favorably with the previous numerical investigations of Calhoun [8] and Russell and Wang [1], as well as to the experiments of Coutanceau and Bouard [49], and summarized in Table 4.1.

4.2 Flow Over a Translating Cylinder

The major difficulty concerning moving boundaries using a vorticity-streamfunction approach is the evaluation of the streamfunction at the boundary, since the boundary can no longer be considered as a streamline. In this case, the value of the streamfunction at the fluid-solid interface is no longer constant. One approach to determine $\psi$ is to integrate along the interface, as discussed by Russell and Wang [1]. In this study, a simpler approach is devised for a translating cylinder problem. Figure 4.4 shows a sketch of the moving cylinder employing a control volume that translates at
the same speed as the cylinder. The control volume surface area is defined in terms of the segments \(A - B, B - C, C - D, D - E E - F\) and \(F - A\). Mass conservation for the control volume is enforced as,

\[
\frac{\partial}{\partial t} \int_{CV} \rho dV + \int_{CS} \rho (\vec{V} - \vec{V}_{CS}) \cdot \vec{n} dA = 0.
\] (4.1)

where \(\vec{V}_{CS} = -U_{cyl} \vec{e}_x\) is the velocity of the control volume surface. Since the density of the flow is assumed to be constant and the volume of the CV is fixed, then the first term in Eq. (4.1) is equal to zero. After dividing through by the density the second term may be expanded as,

\[
\int_{CS} (\vec{V} - \vec{V}_{CS}) \cdot \vec{n} dA = - \int_{BA} (u + U_{cyl}) dy - \int_{BC} v dx + \int_{CD} (u + U_{cyl}) dy
\]

\[
+ \int_{DE} (\vec{V} + U_{cyl} \vec{e}_x) \cdot \vec{n} dA + \int_{EF} (u + U_{cyl}) dy + \int_{AF} v dx.
\] (4.2)

In the limit as the CS height approaches a large value, the upper and lower surfaces of the control volume become the same streamline. In this limit, the velocity component normal to the surface is very small, therefore the second and last term on the r.h.s. of Eq. (4.2) is equal to zero. The fourth term on the r.h.s. involving the integration along DE is also zero because of the no-slip condition. The remaining terms may be integrated and expressed in terms of differences in the streamfunction at the ends of
Chapter 4: Conjugate heat transfer

the surface areas.

\[-(\psi_A - \psi_B) + \psi_D - \psi_C + \psi_F - \psi_E = \int_{BA} U_{cyl} dy - \int_{CD} U_{cyl} dy - \int_{EF} U_{cyl} dy \quad (4.3)\]

Since the upper and lower boundaries of the control volume are streamlines, \(\psi_A = \psi_F\) and \(\psi_B = \psi_C\) which results in the cancellation of the \(\psi_F, \psi_C\) and \((\psi_A - \psi_B)\) terms in Eq. (4.3). Arbitrarily choosing \(\psi_D = 0\), setting \(y_D = 0\) and recognizing that the r.h.s. of Eq. (4.3) is simply the vertical distance from point E to the centerline of the cylinder, then the final expression for the streamfunction at point E is obtained,

\[\psi_E = -U_{cyl}y. \quad (4.4)\]

Since the CV chosen is quite general, the same analysis may be repeated for which point E may be any arbitrary point along the cylinder surface, therefore the condition imposed for \(\psi\) on any point along the surface of the translating surface is \(\psi^I = -U_{cyl}y\).

Figures 4.5 through 4.7 show results for a translating cylinder for \(Re = 40\) at \(t = 16\) using a \(32 D \times 16 D\) domain. These conditions are chosen to match those of Russell and Wang [1] in order to facilitate the comparison of results. The total number of grid points is \(640 \times 320\) (20 grid points per diameter). Figures 4.5 and 4.6 show the streamfunction and vorticity, respectively. Two recirculation regions are observed, one above and one below the cylinder. For comparison purposes, the
results of Russell and Wang are also shown in these figures and agree well with the present study. At this time in the simulation the streamfunction is steady therefore if the streamfunction in Fig. 4.5(a) is re-plotted with respect to the moving coordinate system then it may be compared directly to the results for flow over a stationary cylinder. Figure 4.7(a) shows the stream function after the mapping. Excellent agreement is observed between this result, Fig. 4.2, and the result of Russell and Wang given in Fig. 4.7(b).

4.3 Conjugate Heat Transfer of Cylinders

The final set of results is the flow over cylinders in series that include conjugate heat transfer processes. The interest here is to examine the time response of the cylinders and the influence of a cylinders wake on the heat transfer of a cylinder downstream. A $20D \times 8D$ computational domain is considered using $320 \times 128$ grid points (16 grid points per diameter). The initial non-dimensional temperature of each cylinder is chosen as unity and the rest of the flow-field is equal to zero. The inlet, upper, and lower boundaries are assumed to be isothermal and a convective boundary condition is used at the outlet.

As a baseline, Fig. 4.8 shows the Nusselt number ($Nu$) as a function of $Re$ for an isolated cylinder (solid line) with experimental correlations of Hilpert ($Nu = C Re^n_D$), where $C = 0.821$ \& $n = 0.385$ for $4 < Re < 40$ and $C = 0.615$ \& $n = 0.466$ for
40 < Re < 4000) [2]. As shown, the overall agreement is excellent with maximum differences of 5.8% for the highest Reynolds number case considered.

To understand the effects of upstream cylinder wake on heat transfer, an additional cylinder is added directly downstream at a distance $L$. Three cases are considered with spacings of $L/D = 1, 5,$ and $10$ at $Re = 60$. Figure 4.9 shows $Nu$ number comparisons for these cases early in time when the flow is steady. As expected, the $Nu$ is lower for the rear cylinder due to the preheating of the flow from the first cylinder. For $L/D = 5$ and $10$, the $Nu$ for the front cylinder is identical to the isolated cylinder case in Fig. 4.8. For the case of $L/D = 1$, the heat transfer on the front cylinder is also reduced by 3.2% because of the influence of the second cylinder which serves to increase the temperature on the leeward side of the first cylinder.

Later in time the flow transitions to an unsteady flow resulting in vortex shedding. The time history of the $Nu$ is shown in Fig. 4.10. For $L/D = 1$ the flow remains steady. For $L/D = 5$ and $10$, however, the flow becomes unsteady at $t = 80$ and $110$, respectively. After transition, the $Nu$ for the rear cylinder oscillates due to the vortices shed from the first cylinder. This is clearly shown in Fig. 4.11, comparing the temperature fields (a) before and (b) after transition for $L/D = 5$. Figure 4.10 also shows that after transition, the average $Nu$ for the rear cylinder increases by 51% & 36% to values of 3.51 & 3.85 for $L/D = 5$ & $10$, respectively. The $Nu$ number is larger for $L/D = 10$ since the shed vortices have a longer residence time with which
to entrain ambient fluid resulting in a reduction of the effective ambient temperature for the rear cylinder. The variation in the $Nu$ for the $L/D = 5$ case, however, is larger because the temperature variations are greater due to its closer proximity to the first cylinder.

Figures 4.12 and 4.13 present results for the conjugate heat transfer cases. For these cases, $\alpha_s/\alpha_f = 0.07$, $Pr = 0.7$, and $Re = 60$. Figure 4.12 shows the time history for $Nu$ for $L/D = 5$ with comparison to the isothermal case. The $Nu$ number decreases for both the front and rear cylinder as they cool. Early in time the $Nu$ number for the rear cylinder is lower than the front cylinder, consistent with the isothermal cases. After $t \simeq 100$, the flow around the rear cylinder undergoes transition resulting in a slightly higher $Nu$ number than the front cylinder. This interesting role reversal is from the higher temperature of the rear cylinder after transition due to unsteady transient heating processes as shown in Fig. 4.13.
Table 4.1: Comparisons of wake bubble length, angle of separation and drag coefficient.

<table>
<thead>
<tr>
<th></th>
<th>Re=20</th>
<th>Re=40</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>L</td>
<td>θ</td>
</tr>
<tr>
<td>Tritton [50]</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Coutanceau and Bouard [49]</td>
<td>0.73</td>
<td>42.3°</td>
</tr>
<tr>
<td>Fornberg [51]</td>
<td>0.91</td>
<td>-</td>
</tr>
<tr>
<td>Calhoun [8]</td>
<td>0.91</td>
<td>45.5°</td>
</tr>
<tr>
<td>Russel and Wang [1]</td>
<td>0.94</td>
<td>43.3°</td>
</tr>
<tr>
<td>Present</td>
<td>1.00</td>
<td>43.9°</td>
</tr>
</tbody>
</table>
Figure 4.1: Contour plots for flow over a cylinder at $Re = 20$ showing (a) streamlines with contour levels of -2.5:0.1:2.5 and -0.02:0.002:0.02 and (b) vorticity with contour levels of -12:0.5:12. Solid vertical lines represent the spatial location for the velocity comparisons in Fig. 4.3(a).
Figure 4.2: Contour plots for flow over a cylinder at $Re = 40$ showing (a) streamlines with contour levels of $-2.5:0.1:2.5$ and $-0.05:0.005:0.05$, and (b) vorticity with contour levels of $-16:0.5:16$. 
Figure 4.3: Convergence test for flow over cylinder at $Re = 20$ showing (a) cross-stream velocity at the downstream location indicated in Fig. 4.1 (vertical straight lines) and (b) streamfunction error as a function of grid refinement.
Figure 4.4: Control volume of translating cylinder for developing condition for the streamfunction at the fluid-solid interface.
Figure 4.5: Streamlines for $Re = 40$ translating cylinder from (a) present study and (b) Russell and Wang [1].
Figure 4.6: Vorticity for $Re = 40$ translating cylinder from (a) present study and (b) Russell and Wang [1].
Figure 4.7: Adjusted streamlines of translating cylinder from (a) present study and (b) Russell and Wang [1].
Figure 4.8: Comparison of Nusselt number prediction to experimental correlations of Hilpert for an isolated cylinder [2].
Figure 4.9: Comparison of Nusselt number predictions for two-cylinder for $L/D = 1, 5$ and 10. Dashed line is primary cylinder and solid line is secondary cylinder positioned downstream.
Figure 4.10: Nusselt number vs. time for $L/D = 1, 5$ and 10 at $Re = 60$. The vertical lines indicate the times where the flow snapshots in Fig. 4.11 are taken for the $L/D = 5$ case.
Figure 4.11: Instantaneous snapshots of temperature contours for $Re = 60$ (a) before and (b) after flow transition corresponding to the times indicated by the vertical lines in Fig. 4.10.
Figure 4.12: Nusselt number vs. time for $L/D = 5$ and $Re = 60$ comparing the isothermal and conjugate heat transfer cases. The vertical lines indicate the times where the flow snapshots in Fig. 4.13 are taken for the $L/D = 5$ case.
Figure 4.13: Instantaneous snapshots of temperature contours for \( Re = 60 \) for the conjugate heat transfer case (a) before and (b) after flow transition corresponding to the times indicated by the vertical lines in Fig. 4.12.
Chapter 5

2D Flame Spread

5.1 Numerical Model Validation

Figure 5.1 shows the problem considered in this study of upward flame spread over PMMA slab with thickness, \( l \), at an orientation angle, \( \theta \). A simplified coupled system of gas and solid phase equations are considered for solution in a 2D domain. The specific heats of both phases are assumed to be constant. Composition and temperature dependent transport properties are simplified using prescribed \( Sc \) and \( Pr \) dependencies and Sutherland’s Law for the viscosity [52]. For gas-phase energy transport, a unity Lewis number is employed and pressure and viscous work terms are neglected.
Figures 5.2 and 5.3 show representative comparisons of the DNS with the experiments of Drysdale and Macmillan using \( l = 6 \text{ mm} \) thick samples at inclination angles ranging from \( \theta = 0^\circ \) (horizontal) to \( 90^\circ \) (vertical) [3]. DNS is conducted using a \( 0.5 \text{ mm} \) mesh resolution for grid independent results. The computational domain is different case by case to fit different inclination angles. It is \( 0.14m \times 0.06m \) for 30 degree case then change to \( 0.04m \times 0.1m \) for 90 degree case. Time step is determined from CFL condition while \( U_{\text{max}} \Delta t/\Delta x = 0.3 \).

Figure 5.2 shows comparisons of flame structure at inclination angles of \( 10^\circ \) and \( 45^\circ \) from the (a) experimental and (b) DNS predictions of gas and solid phase temperatures. DNS results reproduce the qualitative changes in flame structure observed in the experiments with a detached flame for lower angles and an attached flame for higher angles. The transition from detached to attached flame at \( 20^\circ \) is also reproduced in Fig. 5.3 showing a comparison of the average flame spread rate from the experiments (symbols) and the DNS (lines) with increasing inclination angle. The corresponding flame spread rate increases by a factor of four due to the increased size of the preheating region seen in the solid phase temperature contours in Fig. 5.2(b). In general, the flame is more stable for higher angles of inclination. For example the flame is quasi-steady at 90 degree while will be fluctuating at 30 degree due to the balance of momentum force and buoyancy force.
5.2 Comparisons with Flame Spread Theory

To better quantify the effect of the flame structure on the preheating zone, the flame height, $S_f$, is computed based on the surface heat flux criterion suggested by Consalvi et al. [53]. In this study, a value of $q'' = 20 \, \text{kW/m}^2$ is used as the threshold for defining the flame height measured along the surface. The preheat zone, $S_{\text{pre}} = S_f - S_p$, can then be defined along with a local ignition time $\tau_{ig}(S) = t(S_f) - t(S_p)$ where $S_p$ is defined as the distance from the bottom of the PMMA slab to the pyrolysis front which is defined as the front point where surface temperature reaches $T_p$. Figures 5.4 and 5.5 summarize the time history of $S_{\text{pre}}$ and $\tau_{ig}$, respectively. The preheat zone is shown to increase with increasing orientation angle because the flame stand-off distance is reduced resulting in an increase in $\tau_{ign}$. Those points do not follow the overall trend in Fig. 5.4 are where the flame is going away from the surface or getting back to the surface. For low inclination angles, $\tau_{ign}$ is somewhat erratic because of the unsteady nature of the detached flame. However, for $\theta > 50^\circ$, an approximately linear increase in $\tau_{ign}$ is observed - consistent with the assumption of Delichatsios et al. in the development of their self-similar solutions [25]. The reason for this can be understood as in Fig. 5.6 showing the average heat flux in the preheat zone as a function of time. The heat flux is observed to decrease by nearly 30% which has a pronounced effect on the flame spread rate shown in Fig. 5.7. Previous experimental [54, 55] and numerical [27] studies have also confirmed the importance
of the exponentially decaying heat flux away from the flame into the preheat zone and is the main source of difficulty for analytically describing upward flame spread.

Existing theories of flame spread either implicitly or explicitly specify the spatial and temporal behavior of the heat flux from the flame to the surface. In the early theoretical work of Fernandez-Pello [23], the heat flux while changing spatially in the preheat zone, is implicitly assumed to be time independent since the rate of flame spread is assumed constant. In the similarity theory of Delichatsios et al. [25] the heat flux is either assumed to be a constant or has a prescribed power-law spatial distribution. As pointed out in their study, simpler descriptions of flame spread of the form: \( V_p = dS_p/dt = S_{pre}/\tau_{ign} \), also suffer from the same limitations since they are only valid when \( S_{pre} \) is a constant. A plot of \( S_f \) vs. \( S_p \) from the DNS is given in Fig. 5.8. A constant slope of unity would indicate that \( S_{pre} \) is a constant. It is clear however that such a trend is not observed. It appears that one of the main challenges in improving quantitative predictions is to develop a better descriptions of the time dependent nature of the heat flux in the preheating region. This was confirmed recently by Rangwala et al. [28] where an experimentally determined time dependent B-number is included into the Emmons solution for steady-state flame spread. Predictions using the modified B-number are reported to yield significantly better predictions of flame spread.

The heat flux and surface temperature time history from the DNS for the \( \theta = 90^\circ \)
case is shown in Fig. 5.9 at $S = 5, 7$ and $9 \text{cm}$. The heat flux grows exponentially until a peak value, $q''_{\text{max}}$, is attained followed by a linear decay at every location along the surface which is consistent with the recent study of Consalvi [27]. The reason for the peak value in heat flux can be better understood in the contour plots of Fig. 5.10 showing instantaneous temperature contours of the solid and gas-phases for the three times of 40, 55 and 64 s. Also on this plot is a contour line for normalized heat release rate of $q''/\rho_gC_{P,g} = 50 \text{K/s}$ indicating the location of the flame. Comparing Figs. 5.9(a) with 5.10 shows the peak heat flux corresponds to location of the flame impingement, as indicated by the line contour (yellow arrow indicated approximate location for clarity) of the normalized heat release rate. A similar trend is also observed for the other orientation angles, showing that the flame impingement is a well defined flame feature that can serve as an indicator of flame height.

For engineering estimates of flame growth, two main inputs are required. The first is an estimate of the heat flux in the preheating region. Figure 5.9(b) shows the heat flux re-plotted as $\log(q'')/S^n = \log(t)$ up to the time of flame impingement, $t_{\text{imp}}(S)$. For a value of $n = -0.356$ the data collapses for the $\theta = 90^\circ$ case. A similar collapse in the data is observed for $\theta = 80^\circ, 70^\circ, 60^\circ, 50^\circ, 40^\circ$ and $30^\circ$ cases with $n = -0.353, -0.346, -0.341, -0.337, -0.325$ and $-0.318$ respectively. An estimation of the time history of the surface heat flux can then be constructed using a piecewise composite
function for $t \leq t_{imp}$ and $t > t_{imp}$,

$$q'' = [1 - H(t - t_{imp})](t^{S_0}) + H[t - t_{imp}]C(S)(t - t_{imp})$$ (5.1)

where $H$ is the Heaviside function and $C(S) = A S + B$ is a linear function of $S$ where the constants $A$ and $B$ are orientation dependent.

The second input required for engineering estimates of flame spread is a model for the heat conduction in the solid phase which ranges from detailed numerical discretization [56, 57] to semi-analytical solutions for 1D thermally thick or thin materials [30, 58]. A priori estimates of thermal thickness is given in the Appendix as expressed in terms of a transitional thickness, $l_{trans} = k_s(T_{ig} - T_o)/q'' = 2.3 \text{ mm}$. For $l << l_{trans}$ the material may be considered thermally thin and for $l >> l_{trans}$ the material may be considered thermally thick. In this study $l = 6 \text{ mm} > l_{trans}$ therefore the material may be assumed thermally thick. Using 1D infinitely thick solution of heat conduction and setting the surface temperature equal to the decomposition temperature, $T_p$, results in the following integral relation for $t_p(S)$ in terms of $t_{heating}(S)$ and $q''$,

$$T_p - T_o = \frac{1}{\sqrt{\pi} k_s C_s} \int_{t_{heating}(x)}^{t_p(S)} \frac{q''(S, \tau)}{\sqrt{t_p(S) - \tau}} d\tau$$ (5.2)

where $\tau = t - t_{heating}$ with $t_{heating}$ defined as the time when the material at location $S$ is first heated. Substituting Eq.(5.1) into (5.2) and integrating numerically yields
in engineering estimates of $S_p$ that can be compared to the DNS results. Figure 5.11 presents these comparisons for all inclination angles. The overall agreement between the simplified model predictions and DNS is excellent with slightly larger differences observed for the $\theta = 30^\circ$ case. The reason for this is that the average flame heat flux to the surface is lower for this case (see Fig. 5.6) resulting in a larger value of $l_{\text{trans}}$. Therefore the assumption of a 1D thermally thick solid is no longer strictly valid and multi-dimensional heat conduction becomes more important. Also in Fig. 5.11 are engineering predictions assuming $\dot{q}^* = \dot{q}^\circ = \text{constant}$ which is consistent with assumptions often made in simplified theories. As shown, the predictions of flame spread rate are in error by factors of two to three. It is clear from these results that accounting for the time dependent nature of the heat flux is critical in obtaining quantitatively accurate predictions of flame spread. Unfortunately, it is difficult to arrive at a universal description of the heat flux which can be readily expressed in terms of simple quantities, i.e., $S_p$, $S_f$, etc. While empirically derived correlations are available such as in Eq.(5.1), they often rely on either experimentally (or numerically) derived constants or depend on ill defined quantities, such as the flame height. A localized solution methodology is therefore desirable that allows for accurate predictions of heat flux which doesn’t necessarily require sub-millimeter DNS resolution of the flame structure and integration of detailed chemical kinetics.
5.3 Embedded Flame Spread Model

To obtain accurate estimates of heat flux and reduce the degrees of freedom in the problem, a reaction progress variable is explored. Figures 5.12 and 5.13 are scatter plots of gas-phase species mass fraction, $Y_k$, and $T$ vs. mixture fraction ($Z$), respectively. The mixture fraction in this context is defined as the local mass fraction which originated from the pyrolysis zone. The data is shown to collapse reasonably well for $Y_k$ because the influence of finite rate chemistry is minimal, and also the transport equations and boundary conditions are nearly the same (i.e., differences are a constant multiple). The temperature scatter in Fig. 5.13, however, varies considerably over the entire mixture fraction space. The reason for these variations is from the differences in boundary conditions between $T$ and $Z$ transport, therefore a second conditioning variable of total enthalpy of the mixture, $h$, is introduced to account for the boundary differences. Figure 5.14 shows the gas-phase temperature vs. $h$ for five bins of $Z$. A collapse of the data is observed indicating that the temperature is a unique function of $Z$ and $h$.

For flame spread predictions, $q''$ is required at the surface. Figure 5.15 shows a scatter plot of $q''$ vs. $\partial h/\partial n$ at the surface for five ranges in $\partial Z/\partial n$. A collapse of the data is observed for most of the data except for low values of $\partial Z/\partial n$ that corresponds to the preheating region. In this region $\partial Z/\partial n \equiv 0$ therefore the heat flux is no longer uniquely defined. However, these data may be further uniquely partitioned in terms
of surface wall temperature as shown in Fig. 5.16. A collapse of the data is observed - indicating that the heat flux in this region is a unique function of \( \partial h / \partial n \) and surface wall temperature.

Using the DNS results, tables are constructed for gas-phase properties (e.g., \( Y_k \), \( T \), etc.) and surface heat flux as a function of \( Z \), \( h \) and gradients of each. Flame tables along with transport of \( Z \) and \( h \) then completely define the flame structure and wall heat flux thereby replacing Eqs. (2.13) and (2.14). Figure 5.17 presents comparisons of the embedded flame modeling to the DNS for predictions of \( S_p \) using the flame table created from the \( \theta = 90^\circ \) case. Overall, the agreement is excellent for both cases indicating that the tables constructed are applicable over a range of orientation angles. The advantage of the embedded flame model is a factor of two computational cost reduction comparing to the DNS. Even larger savings are expected for 3D. Also for reference are the constant heat flux cases shown in Fig. 5.17 showing the significant over prediction of the flame spread rate by factors of 2-3 that are often used in more simplified flame spread theories.
Figure 5.1: Sketch of gravity opposed flame spread at a given inclination angle, $\theta$. 
Figure 5.2: Comparisons of flame structure for orientation angles of 10° and 45° from (a) experiments of Drysdale and Macmillan [3] and (b) DNS showing temperature contours of gas and solid phases.
Figure 5.3: Comparisons of average flame spread rates from experiments (symbols) [3] and DNS (line) with increasing orientation angle.

Figure 5.4: Preheating length, $S_{pre} = S_f - S_p$, time history with increasing orientation angle.
Figure 5.5: Time to ignition ($t_{ign}$) time history with increasing orientation angle.
Figure 5.6: Average heat flux time history in preheating region with increasing orientation angle.
Figure 5.7: Flame spread rate time history with increasing orientation angle.

Figure 5.8: $S_f$ vs. $S_p$ with increasing orientation angle.
Figure 5.9: Heat flux time history at several locations along PMMA surface for $\theta = 90^\circ$ plotted in (a) physical coordinates and (b) $\log(q')/S^n$ vs. $\log(t)$ where $n=-0.356$. 
Figure 5.10: Instantaneous temperature contours and heat release rate contour for $\theta = 90^\circ$ at times of (a) 40 s, (b) 55 s and (c) 64 s.
Figure 5.11: Comparisons of current model predictions and numerical simulations for different angle of orientations: (a) $90^\circ$, (b) $80^\circ$, (c) $70^\circ$, (d) $60^\circ$, (e) $50^\circ$ and (f) $40^\circ$. 
Figure 5.12: Scatter plots of gas-phase $Y_k$ vs. $Z$. 
Figure 5.13: Scatter plots of gas-phase $T$ vs. $Z$. 
Figure 5.14: Scatter plot of temperature vs. total enthalpy for five ranges in mixture fraction.

Figure 5.15: Scatter plot of $q''$ vs. surface temperature and $\partial h/\partial n$ for five ranges of $\partial Z/\partial n$. 
Figure 5.16: Scatter plot of $\dot{q}''$ vs. surface temperature for five ranges of $\partial h/\partial n$ for $-1 < \partial Z/\partial n < 0$.

Figure 5.17: Comparison of $S_p$ time history using DNS vs. embedded flame model vs. constant heat flux for orientation angles of 90° and 50°.
Chapter 6

Conclusions

In this study, an interface embedding technique is first developed to simulate moving fluid-solid interfaces for low speed 2D flows. The interface is described using a level set function and finite difference operators are developed for constructing interface conditions across the fluid-solid interface. Systematic grid convergence studies reveal that the method is second order accurate. A point-implicit time integration methodology is developed that removes the numerical stiffness associated with cut-cells - avoiding previous *ad hoc* treatments that have been developed to treat this problem. Results using this novel approach reproduce existing solutions for flow over stationary and non-stationary cylinders. Application to heat transfer of cylinders shows predictions are in excellent agreement with experimental correlations for an isolated isothermal cylinder. Extensions to two cylinders reveal a complex heat
transfer behavior for cylinders located in the wake of another cylinder from vortex
sheddng and time dependent conjugate heat transfer processes.

Then the computational tool is extended to simulate flame spread over PMMA at
a given angle of inclination. Overall the DNS predictions are in good agreement with
the experimental data - reproducing detachment flame angle and flame spread rates.
The DNS reveals the importance of the time dependent nature of the heat flux along
the wall consistent with recent findings of [26, 27]. A power-law description of the
heat flux resulted in significantly improved engineering estimates of flame spread when
compared to DNS, however, this approach is non-local. To overcome these limitations,
an embedded flame model is developed using a reaction progress variable approach.
State maps for species mass fraction, temperature and heat flux to the surface are
constructed in terms of mixture fraction, total enthalpy and surface temperature.
Results using the embedded model agree well with DNS predictions over a range of
orientation angles indicating the approach is robust and potentially applicable for
more complex geometries. Another potential advantage of this modeling approach
is with the extension to turbulent flows. Because both $Z$ and $h$ are passive scalars,
established boundary layer scaling theories could potentially be used to estimate these
quantities and their wall normal gradients for buoyancy driven wall bounded flows
[59, 60]. Such an approach could be used in the construction of near-wall models for
LES and RANS in application to simulations of turbulent upward flame spread.
Appendix: *A priori* Estimates of thermal thickness

For solid phase heat transfer, two limits of either thermally thick or thin materials are often used in theoretical estimates and modeling of upward flame spread. For a given material thickness, however, there doesn’t appear to be readily available metrics to define if the material may be *a priori* considered thin or thick. An estimate of the thermal thickness of the material may be determined by taking the ratio of ignition times assuming a thermally thin, \[ \tau_{\text{ign-thin}} = \frac{\rho_s C_s (T_{ig} - T_o) l}{q''} \] \hspace{1cm} (1)

and thick material, \[ \tau_{\text{ign-thick}} = \frac{\pi k_s \rho_s C_s (T_{ig} - T_o)^2}{4q''^2} \] \hspace{1cm} (2)

where \( l \) is the thickness of material. Setting the ratio of \( \tau_{\text{ign-thin}} / \tau_{\text{ign-thick}} = 4q'' l / [\pi k_s (T_{ig} - T_o)] \) to unity provides an estimate of a transition thickness, \( l_{\text{trans}} \),

\[ l_{\text{trans}} = \frac{\pi k_s (T_{ig} - T_o)}{4q''} \] \hspace{1cm} (3)

for which if \( l << l_{\text{trans}} \) then the material may be considered thermally thin and for
$l \gg l_{\text{trans}}$ then the material may be considered thermally thick. Substituting in property values for PMMA of $T_g = 380^\circ C$, $k_s = 0.19 W/m - K$ and assuming an average heat flux of $25 kW/m^2$ results in $l_{\text{trans}} = 2.3 mm$. For this study, $l > l_{\text{trans}}$, therefore a thermally thick assumption of the solid phase is deemed acceptable.
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