Effects of Curvature and Strain
on a Lean Premixed Methane-Hydrogen-Air Flame

by

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S.B., Massachusetts Institute of Technology (2003)

Submitted to the Department of Mechanical Engineering
in partial fulfillment of the requirements for the degree of

Master of Science in Mechanical Engineering

at the

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

February 2006

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Abstract

The elemental flame is a subgrid model for turbulent combustion, parameterized by time-varying strain rate and curvature. This thesis develops the unsteady one-dimensional governing equations for the elemental flame incorporating detailed chemical kinetics and transport and a robust and efficient numerical method for solving the governing equations.

Hydrogen enrichment of some hydrocarbon fuels has been shown to improve stability and extend flammability limits of lean premixed combustion in a number of recent experiments. It is suggested that these trends may be explained by the impact of hydrogen on the flame response to stretch and curvature. The elemental flame model is used to simulate premixed hydrogen-enriched methane flames in positively curved, negatively curved and planar configurations at varying strain rates. Curvature and stretch couple with non-unity species Lewis numbers to affect the burning rates and flame structure. Hydrogen addition is found to increase burning rate and resistance to flame stretch under all conditions. Positive curvature reinforces the effect of hydrogen enrichment, while negative curvature diminishes it. The effects of strong curvature cannot be explained solely in terms of flame stretch. Hydrogen enriched flames display increases in radical concentrations and a broadening of the reaction zone. Detailed analysis of the chemical kinetics shows that high strain rates lead to incomplete oxidation; hydrogen addition tends to mitigate this effect.

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Acknowledgements

My thanks are due first to Professor Ahmed Ghoniem for providing direction and motivation to my research. His guidance has brought depth and clarity to this work and helped me to think more broadly about its significance and context. I would like to thank Youssef Marzouk, whose work forms the basis of this thesis, for introducing me to the elemental flame code, and for our continued enlightening research discussions.

My fellow Reacting Gas Dynamics Lab student Murat Altay deserves my gratitude for his continued optimism and friendship. I would like to acknowledge the other members of the RGD Lab—Daehyun Wee, Jean-Christophe Nave, Fabrice Schlegel and Won yong Lee—for their support as well.

I am enormously thankful to my family for the love and encouragement they have provided me over the years. I would never have made it this far without their unwavering support.

I would like to acknowledge the U.S. Department of Energy, Basic Energy Sciences, MICS for their financial support of this research.
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Chapter 1

Introduction

Accurate simulation of turbulent combustion is a computationally challenging endeavor. Because flame thicknesses are several orders of magnitudes smaller than the overall length scale of typical combustion devices, large numbers of grid points are needed to resolve flame structures. Furthermore, the large separation between fluid mechanic and chemical kinetic time scales dictates the use of time steps that are very short relative to the overall simulation time. Detailed chemical mechanisms for even simple fuels like methane involve dozens of species and hundreds of reactions; for more complex fuels like iso-octane, hundreds of species and thousands of reactions are involved. Because of these requirements, direct simulation of three-dimensional turbulent combustion with detailed chemistry remains computationally intractable for the foreseeable future. Modeling approaches which simplify combustion simulation are therefore of great practical importance.

This thesis is concerned with one such model, the embedded flame. The embedded flame is a subgrid model of combustion, where the computational domain is divided into two parts: an outer non-reacting region in which the only the fluid mechanics are solved, and a thin flame surface where chemistry is important. The flame surface is subdivided into numerous embedded flames, each responding to the locally evolving
flow conditions. Unlike the flamelet approach [25], each embedded flame maintains its own time history and can respond to the full range of boundary conditions imposed upon it.

In the embedded flame model, the short time and length scales which must be resolved to accurately simulate combustion are considered only along the flame surface rather than throughout the entire domain of interest. The computational savings of the embedded flame model are highest when the flame occupies a relatively small portion of the total volume of the flow. The conditions under which the embedded flame is a useful model may be expressed in terms of two nondimensional parameters. The flow time scale is represented by the Damköhler number

\[ Da = \frac{\tau_{flow}}{\tau_{reaction}} \]  

(1.1)

When \( Da \gg 1 \), the chemical time scale is much shorter than the flow time scale and the flame thickness is small. Smaller values of \( Da \) result in distributed reaction zones and conditions resembling those of a well stirred reactor.

The dimensionless flame stretch is the Karlovitz number

\[ Ka = \frac{\kappa}{S_L/\Delta_F} \]  

(1.2)

where \( \kappa \) is the flame stretch, \( S_L \) is the laminar flame speed and \( \Delta_F \) is the flame thickness. Large values of \( Ka \), corresponding to highly stretch rates, may result in flame extinction. Flames which may be modeled with the embedded flame model correspond to the case of \( Da \gg 1 \) and \( Ka \lesssim 1 \). At lower values of \( Da \), the large volume occupied by the reaction zone makes the embedded flame no more efficient than direct simulation. For very large values of \( Da \), the time history captured by the embedded flame is unimportant, and the flamelet approach is sufficient. While these restrictions are important, a wide range of practical combustion processes occur in
the range of validity of the embedded flame model.

1.1 Curvature and Stretch

The stretch of a flame surface element $\delta A$ is defined [3] as

$$\kappa \equiv \frac{1}{\delta A} \frac{d\delta A}{dt} = \nabla \cdot \mathbf{v}_t + (\mathbf{V} \cdot \mathbf{n}) (\nabla \cdot \mathbf{n})$$  \hspace{1cm} (1.3)$$

where $\mathbf{v}_t$ is the flow velocity tangential to the flame surface, $\mathbf{V}$ is the velocity of the flame, and $\mathbf{n}$ is the unit normal vector of the flame surface, pointing toward the reactants. Numerous analytical studies have described the impact of stretch on premixed flames, typically using asymptotic analyses and simplified models of flame structure [1, 7, 16, 19]. These studies yield simple expressions for the variation of burning velocity and flame temperature from their unstretched values, emphasizing the interaction of stretch with preferential diffusion (non-unity Lewis number) effects. In particular, Law [16] gives the following linearized expressions for the burned temperature and flame speed of a stretched flame:

$$\frac{T_b}{T_b^o} = \frac{T_b}{T_{ad}} = 1 + \left( \frac{1}{Le} - 1 \right) Ka$$  \hspace{1cm} (1.4)$$

$$\frac{S_u}{S_u^o} = 1 - \delta_T^o \nabla \cdot \mathbf{n} + \left( \frac{1}{Le} - 1 \right) \frac{Ka}{2T_{ad}/T_a}$$  \hspace{1cm} (1.5)$$

where the Karlovitz number is $Ka = (\delta_T^o/S_u^o) \kappa$. $S_u^o$ and $T_b^o$ are the flame speed and burned temperature of the unstretched flame, respectively. $\delta_T^o$ is the thermal thickness of the unstrained flame, and $T_a$ is the activation temperature for the reaction.

Analytical studies of curvature coupled with stretch have shown that curvature may influence flame speed when stretch is present [20]. Numerical studies with more complete models of kinetics and transport corroborate some of these results [2] and
extend them to wider regimes of stretch rate and to unsteady flow-flame interactions. In addition, detailed experimental and numerical studies of cylindrical laminar flames have described the impact of stretch and curvature on flame structure and extinction characteristics [22]. Experimental and numerical studies of strained flames have also demonstrated the importance of preferential (non-unity Lewis number) and differential (unequal Lewis numbers) diffusion in stretched premixed flames [15, 28].

1.2 Hydrogen Addition

Hydrogen addition has received recent attention as a method for enhancing the performance of lean premixed combustion systems. It is frequently desirable to operate devices such as gas turbines at relatively low flame temperatures to reduce the formation of pollutants, NO\textsubscript{2} in particular. However, low flame speeds, susceptibility to extinction, and combustion-related instabilities restrict the ability to operate near the lean flammability limit.

In the case of unstrained methane–air flames, hydrogen addition has a relatively small impact on the laminar flame speed and the lean flammability limit. For mixtures with 10% fuel volume H\textsubscript{2}, the increase in burning speed is typically 5% over a range of equivalence ratios [29]. In contrast, hydrogen enrichment has been shown to substantially increase burning velocity and to inhibit extinction in turbulent and strained environments [5, 9, 10, 11]. Recent experimental studies have observed a dramatic impact of hydrogen enrichment on turbulent flames that experience vigorous stretch and curvature, improving lean premixed combustion stability and extending flammability limits in a dump combustor [6], suggesting important interactions among strain rate, curvature, and preferential transport in hydrogen-enriched premixed flames.

The embedded flame model developed model used in this thesis is used to investigate the effect of hydrogen enrichment on methane–air flames that are simultaneously
strained and curved.

1.3 Thesis Goals

The goal of this thesis is to develop a one-dimensional model for the embedded flame, which takes into account the effects of strain and curvature. The model developed here responds in an unsteady manner to the time-varying boundary conditions imposed on it. Detailed chemical kinetics and transport models are incorporated, including the Soret (thermal diffusion) and Dufour effects. The governing equations for this model are developed in Chapter 2.

The inclusion of detailed chemistry and transport makes efficient solution of the governing equations challenging. For this reason, the problem is solved numerically on an adaptive, non-uniform grid using a two-part iterative method for non-linear systems. The numerical method is discussed in Chapter 3.

In Chapter 4, the embedded flame model is used to examine the effects of hydrogen addition on curved, strained methane–air flames. Positively curved, negatively curved and planar flames are simulated over a range of strains. Hydrogen concentrations of 0%, 10% and 20% of the fuel by volume are considered. Integral flame properties, species profiles, and detailed kinetics information are used to explain the combined effects of curvature, strain and hydrogen addition.

Conclusions and a discussion of future work are contained in Chapter 5.
Chapter 2

Flame Modelling

The elemental flame model consists of a laminar flame stabilized in a stagnation flow. The parameters of the stagnation flow may be imposed explicitly, or provided through coupling with an outer flow within which the elemental flame is embedded. The kinematics of the coupling between the elemental flame and the outer flow has been described elsewhere [17]. Here, the flame is parameterized by the strain rate and position (radius) of the stagnation point in the non-reacting flow. The stagnation flow models are described in Section 2.1.

The general 3D conservation equations for mass, momentum, energy and chemical species are reduced to one dimension by using a boundary layer approximation across the flame. The derivation of these governing equations is contained in Section 2.2.

The boundary conditions for the elemental flame model are discussed in Section 2.3.
The stretch rate $\kappa$, defined in Equation 1.3, for a flame at radius $R_f$ is

$$\kappa = a + \frac{\alpha}{R_f} \frac{dR_f}{dt}$$  \hspace{1cm} (2.5)$$

When the flame is stationary, the stretch rate reduces to $\kappa = a$ and thus curvature does not contribute to flame stretch for stationary flames in this configuration.

2.2 Governing Equations

The one-dimensional governing equations for the elemental flame are derived in this section. We begin with the general 3D governing equations for reacting flow as given by Kee [12] and reduce them to a single dimension normal to the flame using a boundary layer approximation and solving along the stagnation streamline $z = 0$. Consider the coordinate system $(z, r, \theta)$ with velocity components $(u, v, w)$ and let $\hat{r}$ be the flame normal. We may allow this coordinate system to be either Cartesian or cylindrical through the introduction of a parameter $\alpha$, where $\alpha = 1$ for the cylindrical case and $\alpha = 0$ for the Cartesian case. In making the boundary layer approximation, the tangential variations of all quantities except the pressure $p$ and tangential velocity $u$ are neglected. The velocity and all variations in the $\theta$ direction are zero. For an arbitrary scalar $F$, the gradient and substantial derivative are defined as

$$\nabla F \equiv \frac{\partial F}{\partial z} + r \frac{\partial F}{\partial r}$$  \hspace{1cm} (2.6)$$

$$\frac{DF}{Dt} = \frac{\partial F}{\partial t} + \mathbf{v} \cdot \nabla F = \frac{\partial F}{\partial t} + u \frac{\partial F}{\partial z} + v \frac{\partial F}{\partial r}$$  \hspace{1cm} (2.7)$$

The divergence of a vector $\mathbf{F}$ is defined as

$$\nabla \cdot \mathbf{F} \equiv \frac{\partial F_z}{\partial z} + \frac{1}{r^{\alpha}} \frac{\partial}{\partial r} \left( r^{\alpha} F_r \right)$$  \hspace{1cm} (2.8)$$
where $F_z$ and $F_r$ are respectively the $z$ and $r$ components of $F$.

2.2.1 Momentum Equation

First, we will focus on the momentum equation. In general three-dimensional form, it is

$$ \rho \frac{Dv}{Dt} = f + \nabla \cdot T $$

(2.9)

where $T$ is the stress tensor,

$$ T = \left( \begin{array}{ccc} -p + 2\mu \frac{\partial u}{\partial z} + \kappa \nabla \cdot v & \mu \left( \frac{\partial u}{\partial r} + \frac{\partial v}{\partial z} \right) & \mu \left( \frac{1}{r^2} \frac{\partial u}{\partial \theta} + \frac{\partial w}{\partial z} \right) \\ \mu \left( \frac{\partial u}{\partial r} + \frac{\partial v}{\partial z} \right) & -p + 2\mu \frac{\partial v}{\partial r} + \kappa \nabla \cdot v & \mu \left( \frac{\partial w}{\partial r} - \alpha \frac{\partial v}{r} + \frac{1}{r^2} \frac{\partial w}{\partial \theta} \right) \\ \mu \left( \frac{1}{r^2} \frac{\partial u}{\partial \theta} + \frac{\partial w}{\partial z} \right) & \mu \left( \frac{\partial w}{\partial r} - \alpha \frac{\partial u}{r} + \frac{1}{r^2} \frac{\partial w}{\partial \theta} \right) & -p + 2\mu \left( \frac{1}{r^2} \frac{\partial u}{\partial \theta} + \alpha \frac{\partial u}{z} \right) + \kappa \nabla \cdot v \end{array} \right) $$

(2.10)

and the body force $f = 0$. Here, $p$ is the pressure and $\mu$ is the dynamic viscosity of the mixture. Setting velocities and derivatives in the $\theta$ direction to zero, the $z$-momentum equation is

$$ \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial z} + \rho v \frac{\partial u}{\partial r} = \frac{\partial}{\partial z} \left[ -p + 2\mu \frac{\partial u}{\partial z} + \kappa \nabla \cdot v \right] + \frac{1}{r^2} \frac{\partial}{\partial r} \left[ \tau^\alpha \mu \left( \frac{\partial u}{\partial r} + \frac{\partial v}{\partial z} \right) \right] $$

(2.11)

The term containing the second coefficient of viscosity, $\kappa \nabla \cdot v$, is taken to be zero. Additionally, $\partial v/\partial z$ and $\partial^2 u/\partial z^2$ are neglected by the boundary layer approximation, giving the simplified $z$-momentum equation

$$ \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial z} + \rho v \frac{\partial u}{\partial r} = -\frac{\partial p}{\partial z} + \frac{1}{r^2} \frac{\partial}{\partial r} \left[ \tau^\alpha \mu \frac{\partial u}{\partial r} \right] $$

(2.12)
The pressure gradient outside the boundary layer may be obtained by substituting the potential flow solution for \( u \) and \( v \) into the momentum equation.

\[
\rho_\infty \frac{\partial a}{\partial t} + \rho_\infty a^2 \frac{\partial z}{\partial t} = -\frac{\partial p}{\partial z} \tag{2.13}
\]

where \( \rho_\infty \) is the density of the reactants mixture. By the boundary layer approximation, this must be the pressure gradient inside the boundary layer as well.

The \( z \) dependence of \( u \) may be found similarly. Introducing the notation \( U \equiv u/u_\infty \), where \( u_\infty \) is the velocity outside the boundary layer, we obtain

\[
\rho \left( u_\infty \frac{\partial U}{\partial t} + U \frac{\partial u_\infty}{\partial t} \right) + \rho U u_\infty \left( u_\infty \frac{\partial U}{\partial z} + U \frac{\partial u_\infty}{\partial z} \right) + \rho v \left( u_\infty \frac{\partial U}{\partial r} + U \frac{\partial u_\infty}{\partial r} \right) = \rho_\infty \frac{\partial a}{\partial t} + \rho_\infty a^2 \frac{\partial z}{\partial t} + \frac{1}{r^a} \frac{\partial}{\partial r} \left[ r^a \frac{\partial a}{\partial r} \right] \tag{2.14}
\]

Substituting the potential flow velocity from equation 2.4 for \( u_\infty \), dividing by \( a \), and solving along the stagnation streamline \( z = 0 \), the momentum equation simplifies to

\[
\rho \left( \frac{\partial U}{\partial t} + U \frac{1}{a} \frac{\partial a}{\partial t} \right) + \rho U^2 a + \rho v \frac{\partial U}{\partial r} = \rho_\infty \frac{1}{a} \frac{\partial a}{\partial t} + \rho_\infty a + \frac{1}{r^a} \frac{\partial}{\partial r} \left[ r^a \frac{\partial a}{\partial r} \right] \tag{2.15}
\]

### 2.2.2 Continuity Equation

Now consider the mass conservation equation

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{2.16}
\]

Expanding the divergence using Equation 2.8 gives

\[
\frac{\partial \rho}{\partial t} + \frac{1}{r^a} \frac{\partial}{\partial r} \left( r^a \rho v \right) + \rho \frac{\partial u}{\partial z} = 0 \tag{2.17}
\]
Making the substitution for the similarity variable $U$, the mass conservation equation becomes

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^\alpha} \frac{\partial}{\partial r} (r^\alpha \rho v) + \rho U a = 0 \quad (2.18)$$

### 2.2.3 Species Equation

The general form of the species continuity equation is

$$\frac{\rho}{D} \frac{DY_k}{Dt} = -\nabla \cdot j_k + \dot{\omega}_k W_k \quad (2.19)$$

where $Y_k$ is the mass fraction of species $k$, $\dot{\omega}_k$ is the molar production rate of species $k$, $W_k$ is the molecular weight of species $k$, and the diffusion mass flux $j_k$ is defined as

$$j_k = -\rho D_{km} \frac{W_k}{\bar{W}} \nabla X_k - D_k^T \frac{1}{T} \nabla T \quad (2.20)$$

Here, $X_k$ is the mole fraction of species $k$; $\bar{W}$ is the mixture molecular weight and $T$ is the temperature. $D_{km}$ and $D_k^T$ are respectively the mixture-averaged diffusion coefficient and the thermal diffusion coefficient of species $k$. Note that this definition of the diffusion mass flux includes the thermal diffusion (Soret) effect, which will be discussed in Section 4.1.4. Substituting the gradient, substantial derivative and divergence as defined in equations 2.6, 2.7 and 2.8, respectively, and setting the $z$-derivatives to zero, the species equation becomes

$$\rho \frac{\partial Y_k}{\partial t} + V \frac{\partial Y_k}{\partial r} = -\frac{1}{r^\alpha} \frac{\partial}{\partial r} [r^\alpha j_k] + \dot{\omega}_k W_k \quad (2.21)$$

and the diffusion mass flux is

$$j_k = -\rho D_{km} \frac{W_k}{\bar{W}} \frac{\partial X_k}{\partial r} - D_k^T \frac{1}{T} \frac{\partial T}{\partial r} \quad (2.22)$$
2.2.4 Energy Equation

Finally we turn our attention to the energy conservation equation. The general form of the energy equation, expressed in terms of the enthalpy, is

\[
\frac{Dh}{Dt} = \frac{Dp}{Dt} - \nabla \cdot \mathbf{q} + \Phi
\]  

(2.23)

where \( h \) is the enthalpy, \( q \) is the heat flux and \( \Phi \) is the viscous work. By the zero-Mach-number assumption, we neglect the effect of pressure variations, so \( Dp/Dt = 0 \). The viscous work term is also assumed to be much smaller than the energy released by chemical reactions and is therefore neglected. Expanding the substantial derivative of the enthalpy in terms of \( T, Y_k \) and specific heat capacity \( c_p \) gives

\[
\frac{Dh}{Dt} = \sum_{k=1}^{K} \left( Y_k \frac{Dh_k}{Dt} + h_k \frac{DY_k}{Dt} \right) = c_p \frac{DT}{Dt} + \sum_{k=1}^{K} h_k \frac{DY_k}{Dt}
\]  

(2.24)

The total number of species is \( K \). The substantial derivative of \( Y_k \) is replaced using the species equation 2.19. With these substitutions, the energy equation then becomes

\[
\rho c_p \frac{DT}{Dt} + \sum_{k=1}^{K} h_k \left( -\nabla \cdot \mathbf{j}_k + \omega_k W_k \right) = -\nabla \cdot \mathbf{q}
\]  

(2.25)

The heat flux vector \( \mathbf{q} \) is

\[
\mathbf{q} = -\lambda \nabla T + \sum_{k=1}^{K} h_k j_k + \mathbf{q}_D + \mathbf{q}_r
\]  

(2.26)

where \( \lambda \) is the thermal conductivity of the mixture, the Dufour heat flux \( \mathbf{q}_D \) is defined as

\[
\mathbf{q}_D = \bar{R} T \sum_{k=1}^{K} \sum_{j=1}^{K} \frac{X_j D_k^T}{W_k D_{kj}} \left( \frac{j_k}{\rho Y_k} - \frac{j_j}{\rho Y_j} \right)
\]  

(2.27)
and the radiation heat flux $q_r$ is neglected in the present model. $\bar{R}$ is the universal gas constant and $D_{kj}$ is the binary diffusion coefficient of species $k$ into species $j$ [31]. Substituting the heat flux vector into the energy equation, we obtain

$$\rho c_p \frac{DT}{Dt} + \sum_{k=1}^{K} h_k \dot{\omega}_k W_k - \sum_{k=1}^{K} h_k \nabla \cdot j_k = -\nabla \cdot \left( -\lambda \nabla T + \sum_{k=1}^{K} h_k j_k + q_D \right) \quad (2.28)$$

By expanding the term $\nabla \cdot \left( \sum_{k=1}^{K} h_k j_k \right)$ and performing appropriate cancellations, the energy equation simplifies slightly to

$$\rho c_p \frac{DT}{Dt} + \sum_{k=1}^{K} h_k \dot{\omega}_k W_k + \sum_{k=1}^{K} j_k \nabla \cdot h_k = -\nabla \cdot ( -\lambda \nabla T + q_D ) \quad (2.29)$$

Making the substitutions for the gradient, substantial derivative and divergence, and setting the $z$-derivatives to zero, the one-dimensional form of the energy equation is

$$\rho \frac{\partial T}{\partial t} + \rho \nu \frac{\partial T}{\partial r} + \frac{1}{c_p} \left( \sum_{k=1}^{K} h_k \dot{\omega}_k W_k + \sum_{k=1}^{K} j_k c_{p,k} \frac{\partial T}{\partial r} \right) = \frac{1}{c_p} \frac{r^\alpha}{r} \frac{\partial}{\partial r} \left[ r^\alpha \lambda \frac{\partial T}{\partial r} + r^\alpha q_d \right] \quad (2.30)$$

2.2.5 Summary

Introducing the notation $V \equiv \rho \nu$ for the mass flux and recasting the governing equations in residual form, the final mass, momentum, species, and energy conservation equations are:

$$\frac{\partial \rho}{\partial t} + V \frac{\partial \rho}{\partial r} + \rho U \left( \frac{1}{a} \frac{\partial a}{\partial t} + U a \right) - \rho_{\infty} \left( \frac{1}{a} \frac{\partial a}{\partial t} + a \right) - \frac{1}{r^\alpha} \frac{\partial}{\partial r} \left[ r^\alpha \mu \frac{\partial u}{\partial r} \right] = 0 \quad (2.31)$$

$$\rho \frac{\partial U}{\partial t} + V \frac{\partial U}{\partial r} + \rho \frac{\partial U}{\partial r} \left( \frac{1}{a} \frac{\partial a}{\partial t} + U a \right) - \rho_{\infty} \left( \frac{1}{a} \frac{\partial a}{\partial t} + a \right) - \frac{1}{r^\alpha} \frac{\partial}{\partial r} \left[ r^\alpha \frac{\partial u}{\partial r} \right] = 0 \quad (2.32)$$
\[
\rho \frac{\partial Y_k}{\partial t} + V \frac{\partial Y_k}{\partial r} + \frac{1}{r^\alpha} \frac{\partial}{\partial r} \left[ r^\alpha j_k \right] - \dot{\omega}_k W_k = 0
\]  
(2.33)

\[
\rho \frac{\partial T}{\partial t} + V \frac{\partial T}{\partial r} + \frac{1}{c_p} \left( \sum_{k=1}^{K} h_k \omega_k W_k + \sum_{k=1}^{K} j_k c_{p,k} \frac{\partial T}{\partial r} - \frac{1}{r^\alpha} \frac{\partial}{\partial r} \left[ r^\alpha \lambda \frac{\partial T}{\partial r} + r^\alpha q_d \right] \right) = 0
\]  
(2.34)

where the diffusion mass flux appearing in the species and energy equations is defined as

\[
j_k = -\rho D_{km} \frac{W_k}{W} \frac{\partial X_k}{\partial r} - D_k^T \frac{1}{T} \frac{\partial T}{\partial r}
\]  
(2.35)

### 2.3 Boundary Conditions

Establishing the boundary conditions for the elemental flame requires separate consideration of each of the flame configurations described in Section 2.1.

For the single opposed jet flame, defined in Section 2.1.1, the boundary conditions for the species and energy equations consist of defining the temperature and mass fraction of the two incoming streams. For the momentum equation, \( U = 1 \) by definition on the reactants side of the flame. On the products side, spatial gradients in \( U \) must vanish. For a premixed flame with reactants supplied from \(-\infty\), the boundary conditions for the species, energy, and momentum equations are:

\[
\begin{align*}
  r &= -\infty : \quad Y_k = Y_{k,u} \quad T = T_u \quad U = 1 \\
  r &= +\infty : \quad Y_k = Y_{k,b} \quad T = T_b \quad \frac{\partial U}{\partial r} = 0
\end{align*}
\]  
(2.36)

The boundary condition for the continuity equation defines the stagnation point to be at the origin:

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For the twin opposed jet flame and the curved flame at zero stagnation radius, the boundary conditions are defined at \( r = 0 \) and \( r = \infty \). The mixture temperature and composition are specified explicitly at \( r = \infty \). Unlike the single opposed jet flame, the mixture at \( r = \infty \) is the unburned mixture. At \( r = 0 \), the symmetry condition dictates that gradients of temperature, mass fraction and tangential velocity must vanish. The boundary conditions for the species, energy and momentum equations are then:

\[
\begin{align*}
    r = 0 : & \quad \frac{\partial Y_k}{\partial r} = 0 \quad \frac{\partial T}{\partial r} = 0 \quad \frac{\partial U}{\partial r} = 0 \\
    r = \infty : & \quad Y_k = Y_{k,u} \quad T = T_u \quad U = 1
\end{align*}
\]  

(2.38)

The boundary condition for the continuity equation remains the same as for the single opposed jet flame, as given by Equation 2.37.

For curved flames at finite stagnation radius, or flames specified in terms of the unified formulation given in Section 2.1.5, the \( r = \infty \) boundary condition is the same as for the curved flame at zero stagnation radius. The boundary conditions at \( r = 0 \), however, require special attention. First, the mass flux at the center must be expressed in terms of \( rV \) because \( V \to \infty \) as \( r \to 0 \) in the potential flow solution of Equation 2.3. If we specify the non-reacting stagnation point radius \( R \), then the boundary condition for the continuity equation is

\[
r = 0 : \quad rV = \frac{1}{\alpha + 1} a |R| R
\]  

(2.39)

If the boundary mass flux \( (rV)_0 \) is negative, indicating flow out of the domain, or zero, then the zero-gradient conditions given in Equation 2.38 are used. If, however, the mass flux is positive, indicating the presence of source at the boundary, special
care must be taken in specifying the boundary conditions for the energy, species and momentum equations. While the zero-gradient condition must still hold because of the symmetry at that boundary, it is important to retain the effect of the mixture being introduced, which may not be at the same state as the mixture in the vicinity of \( r = 0 \). To this end, we consider an integral approach to the \( r = 0 \) boundary condition. Beginning with the species conservation equation 2.33, we multiply through by \( r^\alpha \) and integrate from 0 to some small radius \( R_i \).

\[
\int_0^{R_i} r^\alpha \frac{\partial Y_k}{\partial t} + r^\alpha V \frac{\partial Y_k}{\partial r} + \frac{\partial}{\partial r} [r^\alpha j_k] - r^\alpha \dot{\omega}_k W_k \, dr = 0 \tag{2.40}
\]

Because this volume is small, we assume that variations of \( Y_k, \rho \) and \( \dot{\omega}_k \) are negligible, so the unsteady term and the production term may be taken out of the integral.

\[
\frac{r^{\alpha+1}}{\alpha + 1} \left( \rho \frac{\partial Y_k}{\partial t} - \dot{\omega}_k W_k \right) + \int_0^{R_i} r^\alpha V \frac{\partial Y_k}{\partial r} + \frac{\partial}{\partial r} [r^\alpha j_k] \, dr = 0 \tag{2.41}
\]

The convection term may be integrated by noting that variations in \( r^\alpha V \) are negligible across this small distance. Furthermore, we recognize that \( Y_k \rvert_{r=0} = Y_{k,0} \) is the mass fraction corresponding to the inlet mixture. The diffusion term may also be integrated, noting that \( j_k \rvert_{r=0} = 0 \) by the symmetry condition. We now have an ODE for the mass fraction of species \( k \) in the vicinity of the symmetry boundary,

\[
\frac{R_i^{\alpha+1}}{\alpha + 1} \left( \rho \frac{\partial Y_k}{\partial t} - \dot{\omega}_k W_k \right) + (r^\alpha V)_0 (Y_{k,0} - Y_k) + R_t^\alpha j_k \, dr = 0 \tag{2.42}
\]

Similar analyses for the energy and momentum equations yield

\[
\frac{R_i^{\alpha+1}}{\alpha + 1} \left( \rho \frac{\partial T}{\partial t} + \frac{1}{c_p} \sum_{k=1}^K h_k \dot{\omega}_k W_k \right) + (r^\alpha V)_0 (T_0 - T) - R_t^\alpha \left( \lambda \frac{\partial T}{\partial r} + q_\text{d} \right) = 0 \tag{2.43}
\]
\[
\frac{R_{i}^{\alpha+1}}{\alpha + 1} \left( \rho \frac{\partial U}{\partial t} + \rho U \left( \frac{1}{a} \frac{\partial a}{\partial t} + U a \right) - \rho_\infty \left( \frac{1}{a} \frac{\partial a}{\partial t} + a \right) \right) + (r^\alpha V)_0 (U_0 - U) - R_i \mu \frac{\partial U}{\partial r} = 0
\]

(2.44)

### 2.4 Multicomponent Fuel Mixtures

The interest in hydrogen enhanced combustion requires a choice of how to compare fuels with different compositions. The simplest choice would be to fix the equivalence ratio of the fuel mixture. In many practical applications, however, the equivalence ratio is of less importance than the temperature of the burned gas. In gas turbines, for example, the material properties of the turbine blades place limits on the burned gas temperature. Increasing burned gas temperature also increases production of NO\(_x\). For these reasons, we choose to fix the adiabatic flame temperature while varying the fuel composition. For the methane–hydrogen fuel mixtures considered here, the composition of the fuel mixture is determined as follows. The adiabatic flame temperature is determined by solving the energy equation \( h_R = h_P \) where \( h_R \) and \( h_P \) are the enthalpies of the reactants and products mixtures, respectively. For a pure methane flame at equivalence ratio \( \phi \leq 1 \), the chemical reaction for complete combustion is

\[
\phi \text{CH}_4 + 2 (\text{O}_2 + 3.76\text{N}_2) \rightarrow \phi \text{CO}_2 + 2\phi \text{H}_2\text{O} + 2 (1 - \phi) \text{O}_2 + 2 \cdot 3.76\text{N}_2
\]

(2.45)

The adiabatic flame temperature \( T_b \) is found by solving

\[
\sum_R n_R \hat{h}_i (T_u) = \sum_P n_P \hat{h}_i (T_b)
\]

(2.46)
where the $n_i$ are the stoichiometric coefficients of the reaction. For a fuel mixture composed of hydrogen and methane, with hydrogen having a volume fraction of $\xi$, the chemical reaction for complete combustion is

$$
\phi ((1 - \xi) \text{CH}_4 + \xi \text{H}_2) + \left( 2 - \frac{3}{2} \xi \right) (\text{O}_2 + 3.76\text{N}_2) \rightarrow \\
\phi (1 - \xi) \text{CO}_2 + \phi (2 - \xi) \text{H}_2\text{O} + \left( 2 - \frac{3}{2} \xi \right) (1 - \phi) \text{O}_2 + \left( 2 - \frac{3}{2} \xi \right) 3.76\text{N}_2 \quad (2.47)
$$

Given a particular value of $\xi$ and the desired value of $T_0$, Equation 2.46 may then be used to solve for the appropriate value of $\phi$, thus determining the mixture composition.

## 2.5 Chemical Kinetics

In this thesis, a modified version of the GRI-Mech 3.0 chemical kinetic mechanism [27] is used. The standard GRI-Mech 3.0 is a detailed mechanism for methane combustion, comprising 325 reactions among 53 species. The mechanism includes reactions among nitrogen-containing species to allow the calculation of NO$_x$ production. Because we are not particularly interested in the details of NO$_x$ formation in this thesis, we have removed the nitrogen-containing species (except for $\text{N}_2$) and their reactions to reduce computational effort. The resulting mechanism comprises 219 reactions among 36 species.
Chapter 3

Numerical Simulation

The governing equations developed in the previous section are solved numerically using a semi-implicit finite difference method. The equations are discretized spatially on an adaptive non-uniform grid. The discretized equations are solved simultaneously at each timestep using a preconditioned Newton-Krylov method. Thermodynamic and transport properties are evaluated using Sandia’s CHEMKIN [14] and TRANSPORT [13] libraries.

3.1 Finite Difference Discretization

In contrast to the elemental flame formulation on which this work is based [17], which used a fully implicit finite difference method, we now use a semi-implicit method which is a weighted average of implicit and explicit finite difference schemes [21]. We introduce a weighting parameter, $\theta$, which varies between 0 and 1, with $\theta = 0$ corresponding to the explicit method and $\theta = 1$ corresponding to the fully implicit method. When $\theta = \frac{1}{2}$, the Crank-Nicolson scheme is obtained. Unlike the fully implicit scheme, the Crank-Nicolson scheme does not introduce numerical diffusion through the discretization of the convective terms. For this reason, and because the Crank-Nicolson scheme is second-order accurate in time, we use $\theta = \frac{1}{2}$ for the energy,
species and momentum equations. Stability restrictions require the use of the fully implicit method for the continuity equation.

### 3.1.1 Governing Equations

In this section, we will give the finite difference discretization of the species conservation equation; the energy and momentum equations are discretized in essentially the same manner. The unsteady term of the species equation 2.33 is approximated as

$$\left( \rho \frac{\partial Y_k}{\partial t} \right)_j \approx \left( \theta \rho_j^{n+1} + (1 - \theta) \rho_j^n \right) \frac{Y_{k,j}^{n+1} - Y_{k,j}^n}{\Delta t} \quad (3.1)$$

Where the superscript $n$ indicates the time layer, the subscript $j$ indicates the grid point and $\Delta t$ is the timestep. The convective term is discretized using a second-order centered difference approximation

$$\left( V \frac{\partial Y_k}{\partial r} \right)_j \approx \theta V_j^{n+1} \left( \frac{\partial Y_k}{\partial r} \right)_j^{n+1} + (1 - \theta)V_j^n \left( \frac{\partial Y_k}{\partial r} \right)_j^n \quad (3.2)$$

where

$$\left( \frac{\partial Y_k}{\partial r} \right)_j^n = \frac{r_{j+1} - r_j}{(r_{j+1} - r_j)(r_{j+1} - r_{j-1})} Y_{k,j+1}^n + \frac{r_{j+1} - r_j}{(r_{j+1} - r_j)(r_j - r_{j-1})} Y_{k,j}^n - \frac{r_{j+1} - r_j}{(r_j - r_{j-1})(r_{j+1} - r_{j-1})} Y_{k,j-1}^n \quad (3.3)$$

The diffusive term is discretized to second-order accuracy as

$$\left( \frac{1}{r^\alpha} \frac{\partial}{\partial r} (r^\alpha j_k) \right)_j \approx \theta \left[ \frac{1}{r^\alpha} \frac{\partial}{\partial r} (j_k) \right]_j^{n+1} + (1 - \theta) \left[ \frac{1}{r^\alpha} \frac{\partial}{\partial r} (j_k) \right]_j^n \quad (3.4)$$

where

$$\left[ \frac{1}{r^\alpha} \frac{\partial}{\partial r} (j_k) \right]_j^n = \frac{r_{j+1/2}^{\alpha} j_{k,j+1/2}^n - r_{j-1/2}^{\alpha} j_{k,j-1/2}^n}{r_j^\alpha (r_{j+1} - r_{j-1})} \quad (3.5)$$
and the discretized form of the diffusion mass flux is

\[ j_{k,j+1/2}^n = -\frac{W_k}{2} \left( \frac{\rho_j^o D_{km,j}^n}{W_j^n} + \frac{\rho_j^{n+1} D_{km,j+1}^n}{W_{j+1}^n} \right) \frac{X_{k,j+1}^n - X_{k,j}^n}{r_{j+1} - r_j} \]
\[ - \frac{1}{2} \left( \frac{D_{k,j}^T}{T_j^n} + \frac{D_{k,j+1}^T}{T_{j+1}^n} \right) \frac{T_{j+1}^n - T_j^n}{r_{j+1} - r_j} \]  

(3.6)

The chemical production term is simply

\[ \dot{\omega}_k W_k \approx \theta \dot{\omega}_{k,j}^{n+1} W_k + (1 - \theta) \dot{\omega}_{k,j}^n W_k \]  

(3.7)

The derivatives of the momentum and energy equations are discretized in the same manner.

The continuity equation 2.31 is discretized using a first order fully implicit finite difference method. The boundary condition for the mass flux is taken at \( j = 1 \). The discretized form of the continuity equation is

\[ \frac{\rho_j^{n+1} - \rho_j^n}{\Delta t} + \frac{r_j^o V_j^{n+1} - r_j^{n-1} V_j^{n+1}}{r_{j+1/2}^n (r_j - r_{j-1})} + \rho_j^{n+1} U_j^{n+1} a^{n+1} = 0 \]  

(3.8)

### 3.1.2 Boundary Conditions

It is convenient to introduce difference equations for the boundary conditions. The species equation again serves as our example. For a fixed boundary values at \( j = 1 \), we write

\[ \frac{\partial Y_k}{\partial t} \approx \frac{Y_{k,1}^{n+1} - Y_{k,1}^n}{\Delta t} = 0 \]  

(3.9)

Similarly for the zero gradient boundary condition on a floating boundary, we write

\[ \frac{\partial Y_k}{\partial r} \approx \frac{Y_{k,2}^{n+1} - Y_{k,1}^{n+1}}{r_2 - r_1} = 0 \]  

(3.10)
For zero gradient boundary conditions at the centerline, the integrated boundary conditions given by equations 2.42, 2.43, 2.44 are used. When the mass flux at the centerline is zero or negative, \((rV)_o \leq 0\), the term containing \(V\) is eliminated.

### 3.2 Solution of the Discretized Problem

In the previous section, we established a system of nonlinear algebraic equations which approximate the system of partial differential equations modeling the elemental flame. We may write this system of equations generically as

\[
f(x) = 0
\]

(3.11)

where \(f\) is the system of equations and \(x\) is the solution vector. Given the solution vector \(x^n\) at the current time step, the system can be solved for the solution \(x^{n+1}\) at the next time step. The structure of the solution vector is

\[
x = [Y_{1,1}, \ldots, Y_{K,1}, T_1, U_1, V_1, \ldots, Y_{1,J}, \ldots, Y_{K,J}, T_J, U_J, V_J]^T
\]

(3.12)

and the structure of the function \(f\) is

\[
f = [S_{1,1}, \ldots, S_{K,1}, E_1, M_1, C_1, \ldots, S_{1,J}, \ldots, S_{K,J}, E_J, M_J, C_J]^T
\]

(3.13)

where \(S_{k,j}, E_j, M_j\) and \(C_j\) are the respective species, energy, momentum and continuity equations at point \(j\). The total number of grid points is \(J\). For the boundary conditions at \(j = 1\) and \(j = J\), the corresponding boundary equations discussed in section 3.1.2 are used. The inclusion of the trivial boundary conditions as part of the solution vector means that the structure of the solution vector is the same for all flame configurations, which simplifies the computational implementation of the
boundary conditions.

The nonlinear system of governing equations are solved using an inexact Newton's method coupled with an iterative sparse linear solver. Newton's method is a simple method for solving systems of nonlinear equations. Consider the first-order Taylor expansion of $f$ around a point $x_i$:

$$f(x_i + s_i) \approx f(x_i) + J_f(x_i)s_i$$  \hspace{1cm} (3.14)

where $J_f$ is the Jacobian of $f$. To find $x$ such that $f(x) = 0$, let $f(x_i + s_i) = 0$ and solve for $s_i$:

$$s_i = -J_f^{-1}(x_i)f(x_i)$$  \hspace{1cm} (3.15)

This value of $s_i$ is taken as a correction to $x_i$ such that $x_{i+1} = x_i + s_i$. The process may be repeated until the solution converges. Unfortunately, the method may fail if the initial guess $x_0$ is not sufficiently good. Additionally, the repeated evaluations of the Jacobian and the necessary matrix inversions of Newton's method are computationally costly when performed directly. To this end, we use an inexact Newton's method with backtracking where the magnitude of the correction $s_i$ is modified based on the current residual. The use of the inexact Newton condition couples with the use of an iterative linear solver, which will be discussed shortly.

The inexact Newton's method is implemented as follows. The Newton step given in equation 3.15 is replaced by the inexact Newton condition

$$\|f(x_i) + J_f(x_i)s_i\| \leq \eta_i \|f(x_i)\|$$  \hspace{1cm} (3.16)

where $\eta_i$ is the forcing term. An iterative method is used to solve 3.15 approximately, with the tolerance specified by $\eta_i$. Initially, the linearized model of Newton's method may be a poor description of $f$, so $\eta_i$ is chosen close to 1. As $\|f\|$ decreases, the linear
model becomes more accurate, and \( \eta \) is reduced. When \( \eta = 0 \), the Newton step is solved exactly. The forcing term is chosen as

\[
\eta_i = \frac{\|f(x_i)\| - \|f(x_{i-1}) + J_f(x_{i-1})s_{i-1}\|}{\|f(x_{i-1})\|}
\]

(3.17)

Further details on the inexact Newton's method may be found elsewhere [4].

Solution of the linearized system between Newton steps is performed iteratively using a preconditioned Krylov subspace method, Bi-Conjugate Gradients Stabilized (BiCGSTAB) [30]. The inexact Newton and BiCGSTAB algorithms are implemented using the NITSOL package [24]. The convergence of the BiCGSTAB iterations is accelerated using an incomplete LU factorizing preconditioner, ILUTP [26].

### 3.3 Flame Radius Control

To simulate flames at a specific radius of curvature, a mechanism must be implemented to provide control over the flame location. In the elemental flame formulation, the flame radius is controlled by manipulating the mass flux per radian \((rV)_0\) at the \( r = 0 \) boundary. This is expressed in terms of a fictitious non-reacting stagnation point radius \( R \).

\[
(rV)_0 = \frac{a}{2\rho_0} |R| R
\]

(3.18)

The current flame radius is defined as

\[
R_f \equiv \frac{\int_0^\infty q'' r dr}{\int_0^\infty q'' dr}
\]

(3.19)

Given a target flame radius \( R_f^* \), a PI (proportional–integral) control algorithm is applied to the stagnation point radius to determine the value of the centerline mass...
flux.
\[ R = K_1 \left[ (R_f^* - R_f) + K_2 \int (R_f^* - R_f) \, dt \right] \]  \hfill (3.20)

Appropriate values of the controller gains \( K_1 \) and \( K_2 \) depend on the characteristics of the flame being simulated. For the flames presented here, acceptable values of the gains are \( K_1 = 10^4 \, s^{-1}/a \) and \( K_2 = 300 \, s^{-1} \).

### 3.4 Adaptation and Regridding

A number of grid adaptation criteria are applied to ensure accurate solution of the discretized problem with a minimum number of grid points. The following criteria must be met between each pair of grid points. If any of these criteria are not met, a new grid point is introduced midway between the two existing points.

First, the grid must accurately resolve variations in the scalar quantities relative to their respective ranges.

\[ |F_{j+1} - F_j| < \varphi_1 \left( \max_j F - \min_j F \right) \]  \hfill (3.21)

where \( F \) includes each of the dependent variables \( T, Y_k, U, V \) as well as the chemical source term \( \sum h_k \omega_k W_k \), and \( \varphi_1 \) is a tolerance parameter on the order of 0.1. Gradients of the scalar quantities are subject to a similar criterion

\[ \left| \left( \frac{\partial F}{\partial r} \right)_{j+1} - \left( \frac{\partial F}{\partial r} \right)_j \right| < \varphi_2 \left( \max_j \frac{\partial F}{\partial r} - \min_j \frac{\partial F}{\partial r} \right) \]  \hfill (3.22)

where the tolerance parameter \( \varphi_2 \) has a typical value of 0.3. The next criterion ensures that numerical diffusion and dispersion introduced by the discretization of the convection terms in the conservation equations is small compared to the physical diffusion terms

\[ x_{j+1} - x_j < \varphi_3 |d_j| \]  \hfill (3.23)

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where the damping ratio \( d_j \) is \( \rho D_{km}/V \) for the species equation, \( \lambda/c_p V \) for the energy equation and \( \mu/V \) for the momentum equation. The tolerance parameter \( \varphi_3 \) has a typical value of 1.0. The final grid adaptation criterion forces the grid to be relatively uniform.

\[
\varphi_4 < \frac{x_{j+1} - x_j}{x_j - x_{j-1}} < \frac{1}{\varphi_4}
\]

(3.24)

\( \varphi_4 \) has a value of around 2.5. If all of these criteria are met to better than their required tolerance without a particular grid point, then that grid point may be safely removed.

The location of the boundary grid points is also modified dynamically. Because of the inverse dependence on \( V \) contained in Equation 3.23, the spacing between grid points becomes very small far away from the stagnation point. It is therefore important that the computational domain be truncated as close to the flame as possible while still satisfying the boundary conditions. This condition may be written at the right \( (j = J) \) boundary for a scalar \( F \) as

\[
|F_j - F_{j-2}| < \varphi_5 \left( \max_j F - \min_j F \right)
\]

(3.25)

where the tolerance parameter \( \varphi_5 \) is typically chosen on the order of \( 10^{-4} \). Note that the boundary value must be compared with the value two grid points away since the flatness criterion between \( J \) and \( J - 1 \) is frequently satisfied exactly by an imposed zero-gradient boundary condition.

### 3.5 Performance Enhancements

Even with the use of an efficient iterative solver, there are still many opportunities for improving the performance and stability of the elemental flame code. The speed of the code has been increased greatly by implementing a variable time stepping algorithm.
When the time increment is short, on the order of one microsecond, the iterative solver converges quickly and reliably because the solution at the new time step is very similar to that of the previous time step. However, many steps are required to simulate a particular time interval. If fewer, larger steps are taken, then at each time step, the guessed solution, extrapolated from the solution at the previous time layer, is less accurate. This causes the iterative solver to converge more slowly, and can result in failure to converge. Somewhere in between lies an optimal time increment that maximizes the overall simulation speed. Unfortunately, this optimum varies from one flame configuration to another, with faster burning flames typically requiring shorter increments.

We eliminate the need to guess the optimal time increment by dynamically adjusting the time increment based on the rate of convergence of previous time steps. If the weighted sum of the number of linear iterations, the number of nonlinear iterations and the number of backtracking steps drops below a predefined threshold, the time increment is increased. When that same sum is greater that another threshold, the time step is reduced. If the solver fails at any time step, the time increment is reduced and the time step is repeated. Furthermore, the thresholds for increasing and decreasing the timestep are themselves altered over the course of the simulation to avoid spurious changes in the time increment. In many flame configurations, the simulation is able to run with a timestep of 32 microseconds under near-steady conditions, with the timestep dropping automatically to respond to unsteady effects.

Another performance enhancement is achieved by performing selective updates of transport coefficients. Normally, all of the transport properties—diffusion coefficients, thermal conductivity and viscosity—are updated between each step of the Krylov iteration. When using the detailed formulations provided by the TRANSPORT library, these updates become expensive. Because these properties are primarily functions of temperature, depending only weakly on mixture composition, we choose to calcu-
late their values in detail only once per time step. At that time, we also calculate
the derivative with respect to temperature. For each step of the Krylov solver, the
properties are linearly extrapolated as functions of temperature.

While the elemental flame code is fundamentally an unsteady simulation, there
are many times where we are primarily interested in steady-state behavior. To tran-
sition quickly from one steady-state solution to the next, it is sometimes convenient
to temporarily reduce the accuracy of the numerical simulation. The most effective
mechanism for doing this is to increase the termination tolerance for the Newton it-
eration, from a typical value of $10^{-9}$ to a value around $10^{-3}$. This greatly reduces
the effort required for each time step, and also allows the use of larger time incre-
ments. Once the solution approaches the new steady state, the normal value of the
termination tolerance is reinstated to produce accurate steady-state results.
Chapter 4

Results

In this section, we present results obtained for steady planar, positively curved and negatively curved flames over a range of strain rates and a selection of fuel compositions. The baseline case is a methane–air flame at atmospheric pressure with equivalence ratio $\phi = 0.5$ and unburned temperature $T_u = 300$ K. We consider two variations on this baseline case, with $H_2$ comprising either 10% or 20% of the fuel by volume. For each hydrogen-enriched mixture, we adjust the equivalence ratio as described in Section 2.4 so that the burned gas temperature $T_b$ is equal to that of the baseline case.

4.1 Flames at Fixed Radius of Curvature

Here, we compare planar flames and positively and negatively curved flames with a fixed radius of curvature. For the curved flames, the flame radius is held constant at $R_f = 2.5$ mm. This radius is chosen to be comparable to the flame thickness, on the order of 1–2 mm, to highlight the effects of curvature. With each flow configuration and fuel composition, we obtained steady-state integral properties and flame structures at strain rates varying from 10 s$^{-1}$ to 800 s$^{-1}$. Direct simulations [8] and experimental diagnostics of turbulent reacting flows suggest that positively strained
of curvature are diminished. Planar and curved heat release rates then approach each other for each fuel mixture, as do the maximum temperatures. Unlike strain rate, however, the curvature considered here does not affect the flame in two qualitatively separate regimes (i.e., first strengthening it then weakening it). Instead, positive curvature strengthens the flame over the entire parameter range, suggesting that at high strain rates, strain and curvature may influence the flame through different mechanisms.

Curvature has a strong impact on the integral properties as well. Though it does not contribute to stretch in the present configuration, positive curvature strengthens the flame, particularly at low-to-intermediate values of the strain rate. Positive curvature allows a focusing of reactants and a de-focusing of heat across the flame structure [23]. For Lewis numbers less than unity, this process should contribute to both higher heat release rates and higher temperatures within the curved flames, which we indeed observe. The converse is seen in the negatively curved flames, where the curvature inhibits increases in temperature.

4.1.2 Flame Structure

The varied responses to strain rate, curvature, and hydrogen enrichment seen in the preceding figures must reflect changes in the flame structure, and thus we examine profiles of flame temperature, heat release rate, and species concentrations. We compare pure methane and 20% hydrogen enriched flames in planar, positively curved and negatively curved configurations at strain rates of 20 s\(^{-1}\) and 200 s\(^{-1}\). To simplify comparisons, spatial profiles have been shifted by the flame location as defined in Equation 3.19. The coordinate system for each flame has been reoriented as necessary so that reactants are on the right and products are on the left in each case. For each geometry and strain rate, we plot the no-H\(_2\) and 20%-H\(_2\) cases together to highlight the impact of hydrogen on flame structure.
Figure 4-7: Temperature and heat release rate profiles for positively curved, planar, and negatively curved flames ($R_f = 2.5\text{mm}$) at strain rates of $a = 20\text{s}^{-1}$ and $a = 200\text{s}^{-1}$. 
Figure 4-7 shows temperature and heat release rate profiles for each of these cases. As expected, hydrogen-enriched flames exhibit more intense burning. Moving from low \( (a = 20 \text{ s}^{-1}) \) to intermediate \( (a = 200 \text{ s}^{-1}) \) strain rates, the peak value of the heat release rate and the width of the reaction zone both increase, in opposition to the decreasing thermal thickness of the flames. The superadiabatic temperature of the hydrogen-enriched flame is clearly visible at \( a = 200 \text{ s}^{-1} \).

Positive curvature accentuates the impact of strain rate, as evidenced by these changes in the temperature and heat release rate profiles. In the pure methane flame, however, strain rate acts in the opposite manner—narrowing the reaction zone and lowering reaction rates, the latter manifested by a lower heat release rate throughout the flame. Again, this trend is consistent with the integrated heat release rates shown in Figure 4-1. Now, positive curvature slightly raises the peak heat release rate at \( a = 20 \text{ s}^{-1} \), but has a negligible impact at \( a = 200 \text{ s}^{-1} \) as the reaction zone narrows.

Conversely, negative curvature subdues the effects of both strain rate and hydrogen addition. The increases in peak heat release rate with increasing strain rate are less pronounced in the negatively curved flame than in either the positively curved or planar flame. Furthermore, the 0%-H\(_2\) and the 20%-H\(_2\) flames are more similar than the corresponding pairs of positively curved or planar flames.

Major species profiles for the flames are shown in Figure 4-8. The most noticeable feature of these profiles is a shift in products composition between the pure methane and 20% hydrogen flames, due simply to the changing stoichiometry. Gradients are of course steeper for the more highly-strained flames corresponding to the reduced flame thickness, and they are also steeper in each of the hydrogen-enhanced flames. At the higher strain rate, and especially in the 20% hydrogen flames, H\(_2\)O concentrations in excess of the equilibrium and O\(_2\) concentrations below equilibrium are evident on the products side of the flame. Again, these trends are augmented by positive curvature and diminished by negative curvature.
Figure 4-8: Major species profiles for positively curved, planar, and negatively curved flames ($R_f = 2.5\text{ mm}$).
Figure 4-9: Minor species profiles for positively curved, planar, and negatively curved flames ($R_f = 2.5\text{ mm}$).
In Figure 4-9 we show the profiles of the radical species O, H, and OH. The behavior of these profiles coincides with that of the heat release rate profile. Radical concentrations decrease with increasing strain for the pure methane flame, but increase in the case of the 20% hydrogen flame. For both the hydrogen-enriched and pure methane flames, the higher strain rate decreases the width of the radical profiles, particularly on the products side of the flame. For the hydrogen-enriched flames only, positive curvature has a positive effect on radical concentration, as expected from the focusing of H\textsubscript{2} into the reaction zone. Negative curvature results in smaller increases in the radical concentrations as hydrogen is added.

Profiles for carbon monoxide are shown in Figure 4-10. As with the radical profiles, the peak concentration of CO is far more sensitive to strain rate in the pure methane flame than in the hydrogen enriched flame. Indeed, the higher strain rate seems to leave the peak CO concentration unchanged in the H\textsubscript{2} enriched cases. Furthermore, comparing CO profiles in the pure methane and 20%-hydrogen flames shows substantial differences in shape. At low strain rates, the enriched flame has reduced concentrations of CO on its reactants side but similar values in its reaction zone and on its products side. At the higher strain rate, CO concentration on the reactants side is still lower for the hydrogen-enriched flame, but the concentration in the reaction zone and on the products side is substantially higher, despite the lower amount of carbon in the fuel. At higher strain rates, positive curvature again accentuates this effective shift of the CO profile towards the products side of the hydrogen-enriched flame.

Profiles in this section thus demonstrate that hydrogen enrichment increases reaction zone thickness and hence residence time in the flame. Higher radical concentrations are generated within the high temperature zone and diffuse to both sides, increasing the local reaction rates. The impact of increased radical activity is seen most vividly in Figure 4-10, where CO concentrations shift toward higher tempera-
Figure 4-10: Carbon monoxide profiles for positively curved, planar, and negatively curved flames ($R_f = 2.5\, \text{mm}$).
tures with hydrogen addition. Additionally, hydrogen enrichment increases the temperature on the products side of the flame. These effects combine to improve the conversion rate of CO to CO₂, as will be shown in the next section.

4.1.3 Reaction Rates

In addition to species profile information, the results obtained from the elemental flame code contain a wealth of detailed information about the chemical reactions occurring inside the flame. Given a set of elementary reactions that convert species $A$ to species $B$, we sum the rate-of-progress for each of these reactions and integrate this value across the flame, obtaining the total rate at which $A$ is converted to $B$. Since the primary difference in reaction rates among the various flame configurations is correlated to changes in overall burning rate, the values are normalized by the conversion rate of CH₄ $\rightarrow$ CH₃ for each flame. For simplicity, we consider only the planar flames.

One way of displaying this information is a reaction pathway diagram, which shows the conversion rates amongst the reacting species. A reaction pathway diagram for a planar methane–air flame at a strain rate of $a = 20 \text{s}^{-1}$ showing the 20 most active carbon-containing species is contained in Figure 4-11. In this figure, line width and color are used to indicate the magnitude of each conversion rate. Each decrease in line width in the figure indicates a halving of the corresponding conversion rate. Reactions which occur at rates of less that 0.1% of the rate at which methane is consumed are not shown.

The first step in the combustion of the incoming fuel is the conversion of CH₄ $\rightarrow$ CH₃. From there, the CH₃ is converted to a number of other intermediate species, primarily CH₂O, CH₃O, ¹CH₂ and CO. These intermediate species undergo additional reactions until they are converted to CO, with a few reactions leading directly to CO₂. Finally, the CO is oxidized to CO₂.
Figure 4-11: The reaction pathway graph of doom.
The impact of hydrogen enrichment on CO profiles seen in Section 4.1.2 motivates a more detailed examination of the role H₂ plays in CH₄ oxidation. We show conversion rates for the most important carbon-containing species in Fig. 4-12. A larger subset of the reactions (though by no means complete) at $a = 200 \text{s}^{-1}$ is shown in Figure 4-13.

At the low strain rate, there is very little difference between the pure methane and 20% hydrogen flames. Between the two pathways $^3\text{CH}_2 \rightarrow \text{CO}_2$ and $\text{CO} \rightarrow \text{CO}_2$, 95% of the CH₄ is ultimately converted to CO₂ in the pure methane flame, slightly more with H₂ enrichment. At the higher strain rate, the conversion rate to CO₂ drops substantially, to 73% for the hydrogen enriched flame and 62% for the pure methane flame. At the same time, conversion to CO, through the pathways CH₃ → CO, HCO → CO and $^3\text{CH}_2 \rightarrow \text{CO}$, is only slightly reduced by the increase in strain rate.
Figure 4-13: Detailed reaction rate diagram for planar flames at $a = 200 \text{s}^{-1}$.
There are a few other noticeable changes in the hydrogen enriched flame at the higher strain rate. More CH$_3$ is directly converted to CH$_2$O, rather than being converted to CH$_3$O first. Less CH$_5$ is converted to C$_2$H$_6$, and more is converted directly to CO. The presence of hydrogen thus alters the route by which methane is oxidized, and its effect is magnified as strain rate increases.

### 4.1.4 Soret and Dufour Effects

It is worth taking a moment to evaluate the impact of including the Soret and Dufour effects in the elemental flame model. Figure 4-14 shows the components of the diffusion mass flux for H and H$_2$ for pure methane and 20%-H$_2$ enriched flames at a strain rate of $a = 200 \text{ s}^{-1}$. The Fick component of the diffusion mass flux is

\[
j_{k,Fick} = -\rho D_{km} \frac{W_k}{W} \frac{\partial X_k}{\partial r}
\]

The Soret component of the diffusion mass flux is

\[
j_{k,Soret} = -D_k \frac{1}{T} \frac{\partial T}{\partial r}
\]

For the pure methane flame, the Soret contribution to the diffusion mass flux is quite small for both H and H$_2$. For other species, the contribution of thermal diffusion to the diffusion mass flux is even smaller. In the hydrogen-enriched flame, however, the Soret effect diffusion of H$_2$ is substantial, with the Soret component representing nearly half of the total diffusion mass flux at some locations. Ignoring the contribution of the Soret effect in hydrogen-enriched flames results in measurable reductions in the computed burning rate and other flame properties.

The Fourier and Dufour contributions to the heat flux are shown in Figure 4-15 for planar flames with 0% and 20% hydrogen enrichment at a strain rate of $a = 200 \text{ s}^{-1}$. 
The Fourier heat flux is

\[ q_F = -\lambda \frac{\partial T}{\partial r} \]  

(4.6)

The Dufour heat flux is

\[ q_D = \bar{R} T \sum_{k=1}^{K} \sum_{j=1}^{K} \frac{X_j D_k^T}{W_k D_{kj}} \left( \frac{j_k}{\rho Y_k} - \frac{j_j}{\rho Y_j} \right) \]  

(4.7)

Similar to what is seen with Soret effect, hydrogen enrichment increases the magnitude of the Dufour heat flux. However, the most important thing to note about the Dufour heat flux is how small it is. The peak value of the Dufour heat flux for the hydrogen-enriched flame is nearly four orders of magnitude smaller than the peak value of the Fourier heat flux. Thus, it is entirely acceptable to neglect the Dufour effect even in hydrogen-enriched flames.

### 4.2 Flames at Zero Stagnation Radius

In this section, results for flames at zero stagnation radius are shown. This boundary condition permits positively curved flames (Section 2.1.3) and planar twin flames (Section 2.1.2), but not negatively curved flames. Unlike the flames at fixed flame radius presented in Section 4.1, the products composition is not imposed on the flow, thus allowing extinction to be observed in these flames.

#### 4.2.1 Integral Properties

To compare the effects of strain rate on each flame configuration, we establish flames at a relatively weak strain rate \(a = 10 \text{s}^{-1}\) and incrementally raise the strain rate until the flame is extinguished. The total heat release rate for each case is shown in Figure 4-16, and the maximum flame temperature, which occurs at the symmetry axis or plane, is shown in Figure 4-17.
Figure 4-14: Mass fluxes due to the Soret effect

In all cases, the heat release rate initially rises with increasing strain rate, which is expected since the Lewis number is less than unity in each case. Furthermore, the hydrogen enhanced flames exhibit a larger increase in heat release rate than the unenriched flames, which is related to the lower effective Lewis number of the hydrogen enriched flames. Near extinction, the heat release rate of the planar twin-flames drops, while the heat release rate of the tubular flame continues to rise up until extinction. This behavior is partially an artifact of the method used to determine the heat release rate per unit area (see Equation 4.1) and the validity of the definition of the flame radius as $R_f \to 0$. If we instead examine the heat release rate per unit
Figure 4-15: Heat flux due to the Dufour effect

length for the positively curved flame,

\[ q' = 2\pi \int_0^\infty q''r \, dr \]  \hspace{1cm} (4.8)

we see that the change in the heat release rate is dominated by the change in the total surface area of the flame. This heat release rate per unit length is shown as a function of flame radius in Figure 4-18. In this figure it is relatively difficult to see that functions shown are not in fact straight lines. By dividing by the flame radius, we obtain a more meaningful picture of how the burning rate is changing, obtaining
Hydrogen addition has a large impact on extinction strain rate. For the planar flame, 20% hydrogen addition increases the extinction strain rate from $167 \text{ s}^{-1}$ to $367 \text{ s}^{-1}$, a 120% increase. For the positively curved flame, 20% hydrogen addition increase the extinction rate by 210%, from $90 \text{ s}^{-1}$ to $281 \text{ s}^{-1}$.

The maximum flame temperature deviates from the adiabatic flame temperature because of non-unity Lewis number effects and confinement of reaction products near the symmetry plane or axis of symmetry. Confinement keeps radical concentrations high by preventing diffusion of radical species into the reaction products. For the tubular flames, the maximum temperature rises starting at low strain rates, and then falls prior to extinction. The initial increase in temperature is related to the non-
unity Lewis number effect predicted by Equation 1.4. The decrease in temperature as the flame approaches extinction is caused by confinement of the flame at the axis of symmetry. The maximum departure from the equilibrium temperature \( T_\text{b} = 1482 \text{ K} \) is 45 K for the unenriched flame and 95 K for the 20% hydrogen-enriched flame, corresponding to the lower effective Lewis number of the hydrogen enriched flame. In both tubular cases, the flame temperature remains above the adiabatic value over the entire range of strain rates covered here.

The planar twin-flame is located closer to the symmetry plane at all strain rates, and confinement begins to affect the flame even at low strain rates. At low strain rates, \( T_{\text{max}} \) rises above the adiabatic flame temperature by as much as 25 K for the unenriched flame and 50 K for the 20% hydrogen-enriched flame. For the planar flames,
Figure 4-18: Heat release rate as a function of flame position for flames at zero stagnation radius.

$T_{max}$ drops to 70 K below the adiabatic flame temperature as the flame approaches extinction for the unenriched flame and 55 K below the adiabatic flame temperature for 20% hydrogen-enriched flame.

Change in the strain rate causes the flame to translate with respect to the hydrodynamic flow field, seeking a position where the flame's burning speed matches the flow velocity. The strain rate also affects flame thickness, with higher strain rates generating thinner flames. The flame thickness and position as a function of strain rate for each of the cases considered are shown in Figures 4-19 and 4-20 respectively. The flame thermal thickness is defined by Equation 4.3 and the flame position is defined by Equation 3.19. At equal strain rates, the tubular flame stabilizes farther from the symmetry boundary than the planar twin flame because the flow velocity normal to
the flame varies faster in the planar case. This effect may be seen by comparing the potential-flow velocity solutions for the two flame geometries, given in Equations 2.1 and 2.2. At high strain rates, all of the flames come to within one flame thickness of the symmetry boundary, and the effects of confinement at the symmetry boundary play an important role in determining the flame behavior near extinction. The planar twin-flames survive until they are much closer to the plane of symmetry than the tubular flames.

4.2.2 Flame Structure

To better understand the response of tubular and planar flames to stretch, we now look how the scalar structure of these flames changes as they are stretched. The most
visible changes in the flame scalar profiles are translation of the flame with respect to the imposed flow, and thinning of the flame at higher strain. These effects are quantified in Figures 4-20 and 4-19. Since the flame radius does not directly influence the burning characteristics of the flame, the profiles in this section are shifted by flame radius.

Three strain rates are compared in each profile figure. Subfigures (a) and (b) compare positively curved and planar flames at a strain rate of \( a = 20 \text{s}^{-1} \), with 0%-H\(_2\) and 20%-H\(_2\) cases compared within each subfigure. Subfigures (c) and (d) compare the same flames at \( a = 90 \text{s}^{-1} \). Subfigures (e) and (f) compare each flame at the highest strain rate where a stable flame could be obtained for that particular flame configuration and fuel composition. In each case, only the portion of the flame
to the right of the symmetry boundary is shown.

Temperature and heat release rate profiles are shown in Figure 4-21.

Hydrogen addition visibly reduces the flame thickness for both tubular and planar flames at all strain rates. The temperature on the products side of the flame is increased by hydrogen addition. At low strain rates, the positively curved and planar flames are nearly identical because the curved flame is at a large flame radius ($R_f \gg \Delta r$) and curvature effects are therefore negligible. Hydrogen addition results in a modest increase in the peak heat release rate, and a small increase in the burned gas temperature.

At intermediate strain rates, the flame is much closer to the axis or plane of symmetry, and the burned gas properties deviate substantially from their equilibrium values. The heat release rate for the unenriched flames begins to have a finite value at the symmetry boundary.

Near the extinction strain rate, the flame is pushed onto the symmetry boundary. The reaction zone for both tubular and planar flames extends onto the boundary. Tubular flames near extinction remain substantially farther away from the symmetry boundary than planar flames near extinction. Here, the effect of hydrogen addition is quite pronounced. Despite the fact that these flames are near extinction, the peak heat release rate for the hydrogen enriched flames is two to three times higher than at low strain rates. For the unenriched flames, the peak heat release rate is only slightly higher than at low strain rates.

The profiles of the major chemical species—CH$_4$, O$_2$, H$_2$O and CO$_2$—are shown in Figure 4-22. Similar to the temperature profiles, the most notable effects are the changes in the composition of the burned mixture. While the burned gas composition of the planar flame is relatively constant, the tubular flame exhibits a substantial increase in the CO$_2$ mole fraction and a corresponding drop in the O$_2$ mole fraction at high strain rates.
Figure 4-21: Heat release rate and temperature profiles for flames at zero stagnation radius.
Figure 4-22: Major species profiles for flames at zero stagnation radius.
Figure 4-23: Minor species profiles for flames at zero stagnation radius.
The most dramatic effects of strain are seen in the profiles of radical species—OH, H and O—which are shown in Figure 4-23. The peak radical concentration for each of these radicals occurs on the products side of the reaction zone, closer to the symmetry boundary than the reaction zone itself. As the flame is strained and pushed against the symmetry boundary, these radical species are among the first to interact with the boundary. Confinement of the radicals at the symmetry boundary causes their concentrations to increase, since there is no longer any loss due to diffusion into the reaction products. At high strain rates, the maximum radical concentrations are 50–100% greater than at low strain rates, and the radical concentrations in the reaction zone also rise substantially. The addition of hydrogen also increases the radical concentrations in the reaction zone, especially the H radical, between the unenriched and enriched flames at high strain rates. The increase in radical concentration in the reaction zone is responsible for the large increase in heat release rate observed for the highly strained flames, and for the burning enhancement in the hydrogen enriched flames.

Profiles for carbon monoxide are shown in Figure 4-24. As strain rate increases, there is a small increase in carbon monoxide concentrations within the flame. Hydrogen enrichment has an interesting effect on the carbon monoxide profiles within the flame. As strain rate increases, the presence of hydrogen tends to shift the peak carbon monoxide concentration towards the products side of the flame. This results in higher consumption rates for CO since the radicals required to oxidize CO are also present in higher concentrations on the products side of the flame. The improved burning of CO is partly responsible for the increased heat release rates seen in the hydrogen-enriched flames at higher strain rates.
Figure 4-24: Carbon monoxide profiles for flames at zero stagnation radius.
Chapter 5

Conclusions

This thesis has developed a fully unsteady subgrid combustion model incorporating the effects of strain and curvature on a elemental flame. Using detailed kinetics and transport, the elemental flame model was used to examine the combined effects of curvature and strain rate on hydrogen enriched lean methane flames in a variety of configurations. It was found that curvature exerts an influence on flame structure and burning rate that cannot be captured by stretch alone.

Hydrogen addition amplifies flame response to strain rate and positive curvature through non-unity Lewis number effects and differential diffusion. Compared to pure methane flames, hydrogen-enriched flames exhibit a stronger positive response of heat release to low values of the strain rate, consistent with reduction of the Lewis number of the mixture. Hydrogen enrichment also renders flames more robust, shifting their peak heat release to higher strain rates and slowing their eventual decay at even stronger strains. Positive curvature further increases the heat release rate for both methane-only and hydrogen-enriched flames over a broad range of strain rates.

These behaviors are reflected in changes in the flame structure and reaction pathways. The introduction of hydrogen increases superadiabatic flame temperatures through non-unity Lewis number effects active in stretched and curved flames. Hy-
drogen addition also results in higher radical concentrations, a widening of the reaction zone, and shifted CO profiles, particularly at higher strain rates. These changes in flame structure alter the fuel oxidation process, increasing the amount of CH$_4$ that is oxidized completely and contributing to the robustness of hydrogen-enriched flames.
Bibliography


