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THE INFLUENCE OF EQUIVALENCE RATIO AND WALL TEMPERATURE ON THE IGNITION OF H$_2$/AIR MIXTURES IN HYPERSONIC FLOW BOUNDARY LAYERS

by

Darien Sussman

A thesis submitted in conformity with the requirements for the Degree of Master of Applied Science
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The Influence of Equivalence Ratio and Wall Temperature On the Ignition of \( \text{H}_2/\text{Air} \)
Mixtures in Hypersonic Flow Boundary Layers
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Abstract

The ignition of \( \text{H}_2 \) in air in the boundary layers of high-enthalpy hypersonic flows was numerically solved for a flat plate geometry using the Thin-Layer Navier-Stokes equations coupled with a complex thirteen species chemical solver. The Mach number range of study was between 2 and 17. Four different constant wall temperatures and three equivalence ratios were implemented. The heat transfer rate along the wall was studied and the solutions compared to each other. For higher Mach number flows (approximately greater than Mach 9), the heat transfer rate to the wall becomes largely independent of the inflow Mach number. The heat generation within the flow was analyzed at various transversal sections along the flat plate. As the inflow Mach number is increased, the presence of \( \text{H}_2 \) originally in the flow eventually result in endothermic reactions which cause the heat produced in the boundary layer to be less than that of a chemically frozen flow.
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# Contents

Abstract ii

1 Introduction 1
  1.1 Motivation ................................................. 1
  1.2 Previous work ............................................. 2
  1.3 Scope of Present Study .................................... 5
  1.4 Overview .................................................. 6

2 Solution Method 8
  2.1 Background ................................................ 8
  2.2 Governing Equations ....................................... 9
  2.3 Numerical Method .......................................... 11
    2.3.1 Discretizing the Fluxes .............................. 11
    2.3.2 Solving the Governing Equations ....................... 16
  2.4 Thermodynamic and Chemical Models ....................... 20
    2.4.1 Thermodynamic Data .................................. 20
    2.4.2 Chemical Model ....................................... 20
  2.5 Physical Domain and Gridding ................................ 23
    2.5.1 Physical Domain ...................................... 23
    2.5.2 Gridding ............................................... 24
  2.6 Validation .................................................. 24
    2.6.1 Comparison of Different Chemical Solvers ............... 24
    2.6.2 Validation of Numerical Method Using Heat Transfer Rates .... 28

3 Results 30
  3.1 Heat Transfer to the Wall .................................. 30
    3.1.1 Background ............................................ 30
    3.1.2 Comparison of Results ................................ 31
  3.2 Heat Generation Within the Flow ............................ 41
3.2.1 Background ................................................. 41
3.2.2 Analysis .................................................. 44

4 Conclusion .................................................. 68
  4.1 Conclusions Drawn From Current Research Effort ................. 68
  4.1.1 Heat Transfer to the Wall ................................ 68
  4.1.2 Heat Generation Within the Flow .......................... 69
  4.2 Possible Future Work and Recommendations ....................... 70
# List of Figures

1.1 Schematic of mixed compression scramjet ........................................ 1
1.2 Ignition process in the boundary layer ........................................... 4

2.1 Schematic of hypersonic flow of air over a flat plate ........................ 8
2.2 Schematic of cells to discretize $\delta_z G$ ..................................... 13
2.3 Schematic of cells used to discretize $\delta_y F$ ................................. 14
2.4 Computational domain and subsequent boundary conditions ............... 16
2.5 Cells to discretize near wall nodes (left), and wall nodes (right) ........ 16
2.6 Grid used for Mach 7 case ......................................................... 25
2.7 Magnified view of grid in pseudo-laminar and combustion regions ....... 25
2.8 Comparison at Mach 5.5, $T_\infty = 700$ K ................................. 27
2.9 Comparison at Mach 6, $T_\infty = 700$ K .................................. 27
2.10 Comparison of Heat Transfer Rates to the Wall ............................... 29

3.1 Heat transfer to wall, $T_W = 300$ K, $T_\infty = 700$ K ....................... 32
3.2 Heat transfer to wall, $T_W = 500$ K, $T_\infty = 700$ K ....................... 33
3.3 Heat transfer to wall, $T_W = 700$ K, $T_\infty = 700$ K ....................... 34
3.4 Heat transfer to wall, $T_W = 1000$ K, $T_\infty = 700$ K .................... 34
3.5 Heat transfer to wall, Mach 2, $T_\infty = 700$ K ............................. 35
3.6 Heat transfer to wall, Mach 5, $T_\infty = 700$ K ............................. 36
3.7 Heat transfer to wall, Mach 7, $T_\infty = 700$ K ............................. 36
3.8 Heat transfer to wall, Mach 10, $T_\infty = 700$ K ........................... 37
3.9 Heat transfer to wall, Mach 13, $T_\infty = 700$ K ........................... 37
3.10 Heat transfer to wall, Mach 15, $T_\infty = 700$ K .......................... 38
3.11 Heat transfer to wall, Mach 7, $T_\infty = 300$ K, $T_\infty = 700$ K .......... 39
3.12 Heat transfer to wall, Mach 7, $T_W = 1000$ K, $T_\infty = 700$ K .......... 39
3.13 Heat transfer to wall, Mach 10, $T_W = 300$ K, $T_\infty = 700$ K .......... 40
3.14 Heat transfer to wall, Mach 10, $T_W = 1000$ K, $T_\infty = 700$ K .......... 40
3.15 Heat of reaction and temperature at 60 cm transversal cut ................. 43
3.16 Heat of combustion at 60 cm transversal cut, $T_\infty = 700$ K ............ 44
3.17 Heat of reaction at 60 cm transversal cut, $T_W = 700$ K .......... 44
3.18 Mass fraction of H$_2$O at 60 cm transversal cut, $T_W = 700$ K .......... 47
3.19 Mass fraction of H at 60 cm transversal cut, $T_W = 700$ K .......... 47
3.20 Mass fraction of O at 60 cm transversal cut, $T_W = 700$ K .......... 48
3.21 Mass fraction of N at 60 cm transversal cut, $T_W = 700$ K .......... 49
3.22 Temperature profile at 60 cm transversal cut, $T_W = 700$ K .......... 50
3.23 2-D profile of H$_2$O mass fraction at 60 cm transversal cut, Mach 7 ...... 50
3.24 2-D profile of H$_2$O mass fraction at 60 cm transversal cut, Mach 10 ...... 51
3.25 2-D profile of H$_2$O mass fraction at 60 cm transversal cut, Mach 13 ...... 52
3.26 2-D profile of OH mass fraction at 60 cm transversal cut, Mach 13 ...... 52
3.27 2-D profile of H mass fraction at 60 cm transversal cut, Mach 7 ...... 53
3.28 2-D profile of H mass fraction at 60 cm transversal cut, Mach 10 ...... 53
3.29 2-D profile of H mass fraction at 60 cm transversal cut, Mach 13 ...... 54
3.30 2-D profile of O mass fraction at 60 cm transversal cut, Mach 7 ...... 55
3.31 2-D profile of O mass fraction at 60 cm transversal cut, Mach 10 ...... 55
3.32 2-D profile of O mass fraction at 60 cm transversal cut, Mach 13 ...... 56
3.33 Heat of reaction at 60 cm transversal cut, Mach 10 ............... 56
3.34 Mass fraction of H$_2$O at 60 cm transversal cut, Mach 10 ............... 57
3.35 Mass fraction of H at 60 cm transversal cut, Mach 10 ............... 57
3.36 Mass fraction of O at 60 cm transversal cut, Mach 10 ............... 58
3.37 Temperature at 60 cm transversal cut, Mach 10 .................. 58
3.38 Heat of reaction at 60 cm transversal cut, $T_W = 300$ K, Mach 10 .......... 59
3.39 Mass fraction of H$_2$O at 60 cm transversal cut, $T_W = 300$ K, Mach 10 ...... 60
3.40 Mass fraction of H at 60 cm transversal cut, $T_W = 300$ K, Mach 10 ...... 61
3.41 2-D profile of H mass fraction at 60 cm transversal cut, Mach 10, $T_W = 300$ K 62
3.42 Mass fraction of O at 60 cm transversal cut, $T_W = 300$ K, Mach 10 ...... 62
3.43 Heat of reaction at 60 cm and 90 cm transversal cut, $T_W = 700$ K ...... 63
3.44 Mass fraction of H$_2$O at 60 cm and 90 cm transversal cut, $T_W = 700$ K ...... 64
3.45 Mass fraction of H at 60 cm and 90 cm transversal cut, $T_W = 700$ K ...... 65
3.46 Mass fraction of O at 60 cm and 90 cm transversal cut, $T_W = 700$ K ...... 66
Nomenclature

Roman Symbols

\( a \) acoustic speed [m/s]
\( A \) convective \( x \) jacobian
\( B \) convective \( y \) jacobian
\( C_2 \) diffusive \( y \) jacobian
\( c_k \) mass fraction of species \( k \)
\( D \) source term jacobian
\( E \) total energy [J]
\( F \) convective flux in \( x \)-direction
\( G \) Gibbs free energy [J/kg]
\( G \) convective flux in \( y \)-direction
\( h_k \) enthalpy for species \( k \) [J/kg]
\( h_{PR} \) heat of reaction [J/kg]
\( I \) identity matrix
\( k_b \) backward reaction rate coefficient
\( K_e \) equilibrium constant
\( k_f \) forward reaction rate coefficient
\( M \) mach number
\( \mathcal{M}_k \) molecular weight of species \( k \)
\( n_i \) mass-specific mole number of species \( i \) [kg-moles k/kg]
\( P \) pressure [Pa]
\( Q \) vector of conservative variables
\( \dot{Q}_w \) heat transfer rate to the wall [W/m²]
\( R \) residual
\( \mathcal{R} \) universal gas constant [J/kg-K]
\( S \) diffusive flux in \( y \)-direction
\( t \) time [s]
\( T \) temperature [K]
$u$ longitudinal velocity component [m/s]
$v$ transverse velocity component [m/s]
$W$ vector of species production source terms
$x$ longitudinal coordinate of physical reference frame [m]
$y$ transverse coordinate of physical reference frame [m]

Greek Symbols

$\alpha$ angle of attack
$\gamma$ specific heat ratio
$\kappa^*$ thermal conductivity [W/m-K]
$\lambda_k^*$ mass diffusion coefficient for species $k$ [m$^2$/s]
$\mu^*$ viscosity [N-s/m$^2$]
$\nu$ stoichiometric coefficient
$\rho$ density [kg/m$^3$]
$\phi$ equivalence ratio
$\chi_i$ concentration of species $i$
$\omega$ pressure correction term
Chapter 1

Introduction

1.1 Motivation

Hypersonic flight has been an area of increased research effort in recent years. Of particular interest, studies of air-breathing engines operating within a wide Mach number range is being performed. The desired goal is to expand the Mach range and altitudes for which these engines can operate efficiently.

Conventional air-breathing engines (e.g., turbojets, turbofans) used for commercial and most military applications cannot traverse the high velocities required for hypersonic flight. However, one class of air-breathing propulsion systems called ramjets might operate effectively and efficiently for these higher Mach number flows. An engine that can reach orbiting velocities is desired.

One type of ramjet under consideration is a shcramjet (SHock-induced Combustion RAMJET), as shown in Figure 1.1. This engine is designed to operate with supersonic flow conditions present throughout the flow domain. The main distinguishing feature of the shcramjet is its combustor. Premixed fuel (H₂) and air enter the combustor with a temperature just below that required for the ignition of the fuel (approximately 900 K). A wedge is placed

![Figure 1.1: Schematic of mixed compression shcramjet](image_url)
in the combustor such that as the fuel/air mixture enters into the combustor and flows over the wedge a oblique shock is formed which causes the ignition of the fuel. If the flame front is coupled with the shock wave a detonation wave is produced.

As mentioned previously, the scramjet’s design requires that the fuel and air be premixed before entering the combustor. This implies that the fuel enters the flow from the inlet. Indeed, this is the case for all scramjet designs. As the air passes through the inlet the flow is compressed through equal strength shocks (to minimize entropy production). Jets along the walls of the inlet inject fuel into the flow. As can be expected, as the flow passes through the shocks the temperature of the fuel/air mixture increases. In previous inviscid studies of scramjet performance, it is shown that the inlet is designed such that premature ignition of the fuel does not happen: Dudebout (1995). As the fuel/air enters the combustor the temperature is just below that required for ignition of the fuel.

As indicated above, the assumption that premature ignition will not take place is only valid for an inviscid flow field. In reality, viscous dissipation along the walls of the inlet will most likely create enough heat to cause ignition of the fuel in the boundary layer. This phenomenon is an undesirable effect and will lead to many complications in the design of the scramjet.

One potential problem that premature ignition in the boundary layer will produce is that fuel will be wasted before entering the combustor. However, the increased cooling requirements and/or material selection placed on the scramjet will be an even greater design problem caused by premature ignition of the fuel.

To approximately gauge the scope of the premature ignition problem it is useful to consider an adiabatic wall scenario. When no external cooling is applied to the walls of the inlet, the inlet wall temperature can reach in excess of 3000 K. These expected temperatures are far in excess of the limits nearly all materials can endure. Clearly, some system of cooling the walls of the inlet is required. However, it should also be noted that the more energy taken out of the flow the less efficient the compression process becomes. Further, mere cooling of the walls of the scramjet may not be enough to hinder ignition of fuel in the boundary layer. Perhaps additional cooling strategies might need to be adopted.

1.2 Previous work

The phenomenon of ignition of fuel in the boundary layer is an area with surprisingly only a small amount of research devoted to it. All of the papers researched for this thesis involved a numerical study of the phenomenon of ignition of the fuel. No experimental studies could be found to correlate with numerical solutions obtained.

One numerical study performed by Treviño and Méndez (1991) examined the ignition of
hydrogen by a hot plate. Depending on the initial pressure and temperature of the hot plate, three different regimes can be identified in the ignition process. The regimes are identified relative to a critical temperature. The critical temperature is the temperature in which the reaction rates of the chain branching reaction $\text{H} + \text{O}_2 \rightarrow \text{OH} + \text{O}$ and the chain terminating reaction $\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M}$ are equal in magnitude. Therefore, the three regimes are classified into plate temperatures, (1) higher, (2) nearly equal, and (3) lower than the critical temperature. For the first regime, essentially no heat is released in the ignition process to a first approximation. The ignition process in the first regime is typified by a chain branching explosion. For the second regime, a heat release is present to improve the ignition time. Lastly, for the third regime, ignition is controlled mainly by intermediate species evolution. A thermal runaway zone is present for this regime. For the purposes of this thesis, the second and third regimes are of key importance.

As is shown by Treviño and Méndez (1991), for subsonic boundary layers, if the initial temperature of the flow is lower than that required for ignition of the fuel, ignition will not take place unless the plate is heated. However, with supersonic flows, for an adiabatic wall condition the fuel will ignite solely by the effect of viscous dissipation at the wall. Moreover, for supersonic flows, the fuel will ignite due to viscous dissipation even if the temperature of the flow and plate is less than that required for ignition of the fuel.

Only two papers could be found dealing with ignition of fuel in supersonic flow along a flat plate, namely Da Silva et al. (1993), and Da Silva and Deshaies (1994). Essentially, these papers dealt with examining the effects various inflow Mach numbers, equivalence ratios, and wall conditions has on the ignition process of H₂/air mixtures.

Using classical boundary layer assumptions, Da Silva et al. (1993) examined laminar flows within the Mach range of two to six. Three different nine species (H₂, O₂, H, O, OH, H₂O, HO₂, H₂O₂, and N₂) chemical solvers were used to capture the combustion characteristics. Of particular note, N₂ is considered inert for these studies. A verification of this assumption is done by Da Silva et al. (1993). It is shown that for temperatures below about 3000 K the N₂ inert assumption is valid to a good approximation.

The combustion process for these types of supersonic flows can be characterized by three zones. In progressive order they are the induction zone, thermal runaway zone, and flame zone (see Figure 1.2). In the induction zone, the temperature in the boundary layer is mainly controlled by viscous dissipation. For this zone, convective forces are larger than the chemical kinetic influences. Further, molecular transport leads to transverse smoothing. The induction zone is identified by an induction length. Although there are a few quantitative ways to characterize the induction length (e.g., distance at which the mass fraction of H₂O reaches 50% of its maximum value, or the distance in which the mass fraction of H₂O reaches 10% of its final equilibrium value), however for lower Mach number flows (approx. below
Mach 10) the induction length is usually physically apparent. More accurately, the start of the thermal runaway zone is obvious enough that an approximate induction length can be gauged. The second zone (i.e., the thermal runaway zone), is marked by a sharp increase in the thermal boundary layer. In this zone a heat release is present as chain-branching reactions with large activation energies become more pronounced. It is this heat release that is responsible for the thickening of the boundary layer. The third zone (i.e., flame zone), is where a strongly oblique flame is present. The flame zone is controlled by a balance between convection, chemistry, and transverse molecular transport. This region typically contains a high HO2 mass fraction at the outer edge of the boundary layer. This layer separates the unburned gases in the outer flow from the burned gases in the boundary layer.

Although the above description is accurate for a large Mach number range, the individual zones become less apparent at higher Mach numbers. Specifically, as the inlet Mach number increases the induction length decreases. Eventually, it appears as though combustion takes place almost immediately as the flow hits the flat plate. Further, as the Mach number increases the temperatures in the stagnation region at the leading edge increases as well. With these increased temperatures at the leading edge, dissociation of some of the species present in the flow (endothermic reactions) will become more apparent thus further skewing the concept of an induction length.

Wall conditions also have an effect on the combustion process. Da Silva et al. (1993) studied two different wall conditions, adiabatic wall and constant wall temperature. As expected the adiabatic wall assumption yields much higher temperatures in the boundary layer.

The equivalence ratio (fuel to air mass ratio related to that of a stoichiometric mixture) has an important effect on the ignition process. In general, a fuel rich mixture will have a longer induction length and a fuel lean mixture will have a shorter induction length compared to a stoichiometric (ϕ = 1) mixture. The reason for this trend in induction lengths due to varying equivalence ratios is related to the specific heat of the mixture. A lean fuel mixture
will have a smaller specific heat value compared to the stoichiometric mixture. Even though the total heat released will be less for the lean fuel mixture the initial heating due to viscous dissipation will be more intense, thus yielding a shorter induction length.

Although the presence of an exothermically combustible fuel such as H\textsubscript{2} will in general add heat to the flow, this is not always true. In fact, in some higher Mach number flows the flow behaves endothermically. Less heat is produced compared to a chemically frozen flow for some inflow conditions. This phenomenon is very important when considering any future thermal protection systems to a hypersonic vehicle.

1.3 Scope of Present Study

The research performed by Da Silva et al. (1993) explored the ignition process for the Mach range of two to six. The goal of this current research effort is to expand the Mach range in which the combustion process is known. However, even though this present study is more of a fundamental investigation into ignition in the boundary layer, the parameters of the simulations should conform closely with conditions that will most likely be seen by the scramjet.

The geometry of the simulations consists of a flat plate with pre-mixed fuel (H\textsubscript{2}) and air flowing over it. For all the simulations only laminar flow will be considered. It is important to examine laminar flow before turbulence can be considered. However, the modeling of laminar flow first is a good strategy because the addition of turbulence will most likely result in only quantitative differences for the flow geometry under consideration. This study is numerical and involves solving the Thin-Layer Navier-Stokes (TLNS) equations coupled with a complex chemical solver. Since the Mach number range under investigation is to be increased compared to current known ranges it is likely that temperatures in excess of 3000 K will be realized in the flow. Therefore, for the purposes of this area of research N\textsubscript{2} will not be considered inert.

The specific flow constants are as follows: \( T_\infty = 700 \) K  
\( P_\infty = 15000 \) Pa  
1 m long flat plate  
\( \alpha = 0 \), angle of attack

The inflow temperature \( T_\infty \) is held at value close to, but less than that required for igniting the fuel (approx. 900 K). This is done to approximate the conditions along the wall of the scramjet's inlet. As the flow passes through the equal strength shocks the temperature of the flow will increase. As indicated previously, the scramjet is designed
such that for \textit{inviscid} flow the fuel/air mixture will be slightly less than that required for ignition of the fuel when it enters the combustor. Along the latter part of the inlet it is likely that the flow temperature will be in the 700 K range.

To further approximate the conditions likely seen by the shcramjet the inflow pressure $P_\infty$ is set to 15000 Pa. Since the shcramjet is designed to operate at high altitudes it is unlikely that the local pressure seen by the shcramjet will be standard pressure (approx. 0.1 MPa). Therefore, the inflow pressure is set to a lower value for the simulations.

This study into the phenomenon of ignition in the boundary layer explores the effect such things as Mach number, wall temperature, and equivalence ratio has on the combustion process. The Mach range studied is set by the upper temperature limit of the chemical solver (approx. 5000 K). A constant wall temperature requirement gives a much better approximation to a real shcramjet than an adiabatic wall assumption gives. Any hypersonic vehicle is going to require some thermal protection system as no known material can sustain the high thermal load that will most likely will be placed upon it in a hypersonic environment. The wall temperatures studied are 300 K, 500 K, 700 K, and 1000 K. Essentially, the 300 K wall temperature lower limit is set to simulate a very aggressive heat transfer requirement. In fact, setting a wall temperature to 300 K for a real situation is most likely unrealizable. However, it is interesting to investigate if it is even possible to curtail ignition of fuel in the boundary layer over the domain studied with an overly optimistic thermal protection requirement. The upper wall temperature limit is set to 1000 K as an approximation to not only a realizable heat transfer requirement, but also to the upper limit most materials can endure for any length of time. Two additional wall temperatures are studied, namely 500 and 700 K. This is done to establish the trends of the changing heat transfer requirements has on the ignition process between the upper and lower wall temperature limits. One final variable under investigation is the effect different equivalence ratios has on the combustion process. It is highly unlikely that in the shcramjet inlet a constant equivalence ratio can be maintained. Therefore, it is important to understand the possible effects this non-homogeneous fuel/air mixture will have on the combustion process. Also, it may be seen in some situations that having a fuel lean or rich mixture might be beneficial. If this is the case, this knowledge could effect the rate at which the jets in the inlet pump fuel into the flow.

It is hoped that through this study an understanding of the possible thermal protection systems required for the shcramjet will be obtained.

1.4 Overview

The following is a brief overview of the subsequent chapters in this thesis. Chapter two deals with the methods and processes performed to complete the specified area of research. An
explanation of the numerical method and the chemical solver used is explained. Further, a brief validation of the code is performed. A more in depth validation can be found in a paper by Parent (1998). Also, a description of how the specific simulations were obtained is covered (e.g., gridding, flow domains). The third chapter deal with the results of the simulations. First a description of how the flows were analyzed and subsequently the results of this analysis. The fourth and final chapter details conclusions that can be made from the research performed. Also, recommendations are made for possible future work in the area of ignition of fuel in the boundary layer.
Chapter 2

Solution Method

2.1 Background

As mentioned in section 1.2, in order to solve the problem of fuel ignition in boundary layers Da Silva et al. (1993) solved the classical boundary layer equations. One of the major assumptions made by the boundary layer equations is that the pressure gradients in the transverse direction to the flow is zero (i.e., \( \frac{\partial p}{\partial y} = 0 \)). This assumption can no longer be considered accurate for higher Mach number flows, as will be explained later. Therefore, to expand the Mach number range for which the phenomenon of ignition of fuel in the boundary layer is understood, the boundary layer equations will not be used.

To further grasp the scope of the problem with using the boundary layer equations for higher Mach number flows, consider the schematic in Figure 2.1. This figure depicts hypersonic air flow over a flat plate. A shock forms from the leading edge and near this region the shock interacts with the boundary layer. In the region of shock-boundary layer interaction, the boundary layer equations cannot be used. In order for the boundary layer equation to be used there must be a clear distinction between the inviscid and viscous parts of the flow. This inviscid/viscous distinction cannot be made for the situation in Figure 2.1. However,

Figure 2.1: Schematic of hypersonic flow of air over a flat plate
the Navier-Stokes (NS) equations are appropriate to solve such problems: (Anderson, Tannehill, and Pletcher 1984). Although the NS equations can be used without restrictions as posed by the shock-boundary layer interactions, there are parts of the flow in Figure 2.1 in which the NS equations cannot really be considered accurate or valid. At the leading edge, the flow is a non-continuum or rarefied flow. Under those types of flows, the NS equations cannot be used: (Anderson, Tannehill, and Pletcher 1984). However, usually this portion is small and these restrictions are neglected to simplify the computation involved.

Although the Navier-Stokes equations are robust, they are also computationally expensive. It is possible to use a simplified version of the NS equations for the types of flows investigated in the present: the Thin-Layer Navier-Stokes (TLNS) equations. The TLNS equations differ from the NS equations in that all the viscous terms with derivatives parallel to the flow direction are neglected. For solutions in which there is a preferred flow direction, the TLNS equations are quite well suited for these types of cases. The two main advantages of using the TLNS equations over the NS equations are that first, solving the TLNS equations is considerably less computationally expensive, and second, removing terms from the equations changes the mathematical character of the equations: (Anderson, Tannehill, and Pletcher 1984). The TLNS equations are "parabolized" in the streamwise direction. This "parabolized" character lends well to a space-marching technique. When most of the flow is supersonic (as is the case with this current area of research) a space-marching scheme is ideal as information only travels upstream in a supersonic flowfield. Also, as mentioned, a space-marching approach decreases the computation needed as one less dimension is involved.

### 2.2 Governing Equations

As indicated in the previous section, the two dimensional unsteady laminar Thin-Layer Navier-Stokes equations are to be solved. Written in the conservation form:

$$\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = \frac{\partial S}{\partial y} + W$$

(2.1)

The matrices of $Q, F, G, S$ and $W$ can be seen below. The first thirteen are for the conservation of mass for each of the thirteen species (at least for the chemical solver used for this study). The remaining three are for the conservation of $x$ and $y$ momentum, respectively, and the conservation of energy equations.

The $Q$ represents the conservative variables. The $F$ and $G$ are designating the $x$ and $y$ convective fluxes, respectively. The $W$ is the source term as the flow will be considered chemically reactive. The last matrix is the $S$, which represents the $y$-direction viscous fluxes.
To clarify some of the non-obvious notation, the following is detailed. In matrix $S$, $\lambda_\ell$ is the mass diffusion coefficient for species $k$, $\mu^*$ the viscosity of the mixture, $\kappa^*$ the thermal conductivity of the mixture, and $h_k$ the enthalpy for species $k$.

A $\omega$ term is present in the fourteenth line in the $F$ matrix. This $\omega$ term is tied to the streamwise pressure gradient. The $\omega$ acts as a pressure correction. For most of the domain in question supersonic conditions will be present, however for small regions near the wall in the boundary layer the flow will be subsonic. For subsonic regions, the $\omega$ termed allows information to travel upstream. If the flow is subsonic $\omega$ is calculated using Equation 2.4, otherwise $\omega$ is set to a value of one.

\[
Q = \begin{bmatrix}
\rho_{CH_2} \\
\rho_{CO_2} \\
\rho_{CH} \\
\rho_{CO} \\
\rho_{COH} \\
\rho_{H_2O} \\
\rho_{HCO_2} \\
\rho_{CN} \\
\rho_{NO} \\
\rho_{NNO} \\
\rho_{N_2} \\
\rho_{NO_2} \\
\rho_\nu \\
\rho_{\nu v} \\
\rho_\nu E \\
\end{bmatrix}, \quad F = \begin{bmatrix}
\rho u_{CH_2} \\
\rho u_{CO_2} \\
\rho u_{CH} \\
\rho u_{CO} \\
\rho u_{COH} \\
\rho u_{H_2O} \\
\rho u_{HCO_2} \\
\rho u_{CN} \\
\rho u_{NO} \\
\rho u_{NNO} \\
\rho u_{N_2} \\
\rho u_{NO_2} \\
\rho u^2 + \omega P \\
\rho u_{\nu v} \\
\rho u_{\nu E} + uP \\
\end{bmatrix}, \quad G = \begin{bmatrix}
\rho u_{CH_2} \\
\rho u_{CO_2} \\
\rho u_{CH} \\
\rho u_{CO} \\
\rho u_{COH} \\
\rho u_{H_2O} \\
\rho u_{HCO_2} \\
\rho u_{CN} \\
\rho u_{NO} \\
\rho u_{NNO} \\
\rho u_{N_2} \\
\rho u_{NO_2} \\
\rho u^2 + \omega P \\
\rho u_{\nu v} \\
\rho u_{\nu E} + vP \\
\end{bmatrix}
\]
2.3 Numerical Method

2.3.1 Discretizing the Fluxes

The governing equations listed in Section 2.2 must now be solved in an efficient manner. Taking advantage of the mathematical qualities of the Thin-Layer Navier-Stokes equations, a space-marching scheme was developed by Parent (1998) and further refined by the present author for this current area of research. The space-marching code is referred to by Parent as “LAD”. Any further reference to LAD will indicate the space-marching code. Of special note, LAD has no artificial dissipation added to it. It is found by Parent (1998) that when artificial dissipation is added to the code too much fictitious viscosity is seen in the boundary layer. Obviously, since the current area of research focuses on boundary layer phenomenon, this is an undesirable effect. LAD is written in orthogonal coordinates, although it can be easily be transformed to use curvilinear coordinates. For the flows solved in this study

\[
\begin{bmatrix}
W_{H_2} \\
W_{O_2} \\
W_H \\
W_O \\
W_{OH} \\
W_{H_2O} \\
W_{H_2O_2} \\
W_N \\
W_{NO} \\
W_{HNO} \\
W_{N_2} \\
W_{NO_2} \\
0 \\
0
\end{bmatrix}
= \begin{bmatrix}
\frac{\partial c_{H_2}}{\partial y} \\
\frac{\partial c_{O_2}}{\partial y} \\
\frac{\partial c_H}{\partial y} \\
\frac{\partial c_O}{\partial y} \\
\frac{\partial c_{OH}}{\partial y} \\
\frac{\partial c_{H_2O}}{\partial y} \\
\frac{\partial c_{H_2O_2}}{\partial y} \\
\frac{\partial c_N}{\partial y} \\
\frac{\partial c_NO}{\partial y} \\
\frac{\partial c_{HNO}}{\partial y} \\
\frac{\partial c_{N_2}}{\partial y} \\
\frac{\partial c_{NO_2}}{\partial y}
\end{bmatrix}
\]  

\[
\omega = \frac{\gamma M_x^2}{1 + (\gamma - 1)M_x^2} \text{ if } M_x < 1
\]  

\[
\omega = 1 \text{ otherwise}
\]
curvilinear coordinates were not necessary.

Since LAD is a space-marching code, each x-station (i.e., direction of marching) is converged to steady-state (steady-state reached when the residual equals zero). The equation for calculating the residual \( R \) is as follows:

\[
R = \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} - \frac{\partial S}{\partial y} - W
\]  

Of course, the residual will never reach exactly zero, however some small number approximation can be assumed to be essentially zero. With the way the residual is calculated from all the fluxes (see Equation 2.7) machine zero is reached when the Root-Mean-Square (RMS) is about \( 10^{-9} \).

\[
RMS = \frac{\sum_{k=1}^{nf} \left( \sum_{j=1}^{nn} \left( \frac{R_{j,k} \Delta t_{REF}}{q_{j,k}} \right)^2 \right)^{1/2}}{nf}
\]  

(2.7)

Where \( nf \) and \( nn \) designate the number of fluxes (16 for this current area of research) and the number of nodes in the y-direction (dependent upon the grid). \( \Delta t_{REF} \) is described in Section 2.3.2.

Obviously, since the exact value of the partial derivatives in Equation 2.6 cannot be found an approximation to the partial derivatives must be used. Expressed in the delta form the expression for the residual now becomes:

\[
R_{\Delta} = \delta_x F + \delta_y G - \delta_y S - W
\]  

(2.8)

The \( \delta \) term is not stating that all the fluxes are discretized the same way, only that it is a general discretization notation. The specifics of the discretization is described below.

Discretizing the y-convective fluxes, \( G \)

If a simple 2nd-order central difference approximation to the \( G \) and \( F \) convective fluxes were performed, this could lead to non-physical oscillations (Parent 1998). To avoid the discoupling of even/odd nodes special averaging is performed across the nodes.

Consider Figure 2.2, where a schematic of the nodes involved in the discretization of the
Figure 2.2: Schematic of cells to discretize $\delta_z G$

$G$ fluxes can be seen. Noting that for simplicity, the nodes will be referenced by a north-south-east-west (NSEW) process instead of an i-j method. Further, in general the spacing between the nodes are not equidistant.

As indirectly stated above, more than three nodes are needed to discretize the convective terms. A five point stencil is used to define the fictitious fluxes $G'_p, G'_N,$ and $G'_S$. By using these fictitious fluxes discoupling can be avoided. However, first the cell boundary fluxes must be found which are defined by the following:

\[
\begin{align*}
G_{nn} &= \frac{1}{2} (G_{NN} + G_N) \quad G_n = \frac{1}{2} (G_N + G_P) \\
G_s &= \frac{1}{2} (G_P + G_S) \quad G_{ss} = \frac{1}{2} (G_S + G_{SS})
\end{align*}
\]  \hspace{1cm} (2.9)

For simplicity, this description of discretizing the $G$ fluxes will consider all the nodes equidistant. The non-equidistant expression for the discretization of the $G$ fluxes is given at the end of this section. From the above notation, the fictitious fluxes are written as follows:

\[
\begin{align*}
G'_p &= \frac{G_n + G_s}{2} = \frac{G_N + G_P + G_S}{4} \\
G'_N &= \frac{G_{nn} + G_s}{2} = \frac{G_{NN} + 2G_N + G_P}{4} \\
G'_S &= \frac{G_s + G_{ss}}{2} = \frac{G_P + 2G_S + G_{SS}}{4}
\end{align*}
\]  \hspace{1cm} (2.10)

Therefore, the discretization of the $G$ fluxes with constant $\Delta y$ is given by:

\[
\delta_y G = \frac{G'_N - G'_S}{2\Delta y} = \frac{G_{NN} + 2G_N - 2G_S - G_{SS}}{8\Delta y}
\]  \hspace{1cm} (2.11)
Figure 2.3: Schematic of cells used to discretize \( \delta_y F \)

Or more realistically, with non-equidistant nodes:

\[
\delta_y G = \frac{1}{2} \left[ G_{NN} \left( \frac{c_{11}}{\Delta y_N} \right) + G_N \left( \frac{c_{11} - c_{11}}{\Delta y_N} + \frac{c_{13}}{\Delta y_S} \right) \right] \\
+ G_P \left( \frac{c_{21} - c_{11}}{\Delta y_N} + \frac{c_{11} - c_{31}}{\Delta y_S} \right) \\
+ G_S \left( -\frac{c_{11} - c_{31}}{\Delta y_N} + \frac{c_{13} - c_{33}}{\Delta y_S} \right) + G_{SS} \left( \frac{c_{33}}{\Delta y_S} \right)
\]  

(2.12)

| \( c_{11} \) | \( c_{12} = \frac{\Delta y_N}{2(\Delta y_N + \Delta y_S)} \) | \( c_{13} = \frac{\Delta y_S}{2(\Delta y_N + \Delta y_S)} \) |
| \( c_{21} = \frac{\Delta y_N}{2(\Delta y_N + \Delta y_W)} \) | \( c_{22} = \frac{\Delta y_W}{2(\Delta y_N + \Delta y_W)} \) | \( c_{23} = \frac{\Delta y_N}{2(\Delta y_N + \Delta y_W)} \) |
| \( c_{31} = \frac{\Delta y_S}{2(\Delta y_S + \Delta y_W)} \) | \( c_{32} = \frac{\Delta y_W}{2(\Delta y_S + \Delta y_W)} \) | \( c_{33} = \frac{\Delta y_S}{2(\Delta y_S + \Delta y_W)} \) |

Discretizing the \( x \)-convective fluxes, \( F \)

The \( x \)-convective fluxes are discretized with a first order backward difference. This backward discretization takes advantage of the space-marching scheme in the flow direction. Although a backward second-order scheme is possible it is noted by Parent (1998) that convergence problems were present when this type of discretization is used. See Figure 2.3 for schematic of the discretization of the \( F \) fluxes.

Similar to the \( G \) fluxes, fictitious fluxes are defined by \( F' P \) and \( F' W \). Although the actual fluxes \( F_P \) and \( F_W \) could be used it is also noted by Parent (1998) than even when the solution is fully converged, protuberances were present near strong shocks. The fictitious fluxes are defined by:

\[
F' P = F_P \quad F' W = \frac{1}{4} (F_{SW} + 2F_W + F_{NW})
\]  

(2.13)

Therefore, the discretization of the \( F \) fluxes is given below:
\[
\delta_z F = \frac{F'_p - F'_w}{\Delta x_w} = \frac{F_p - \frac{1}{4}(F_{SW} + 2F_W + F_{NW})}{\Delta x_w}
\] (2.14)

**Discretizing the y-diffusive Fluxes, S**

The S fluxes will be discretized in a slightly different manner than the F and G fluxes were. The S fluxes will be defined as:

\[
S_j = \sum_{i=1}^{n} \overline{s}_i \quad \text{where} \quad \overline{s}_i = \xi_i \frac{\partial \phi_i}{\partial y}
\] (2.15)

To further clarify this notation consider the following example. When \( n=1 \), \( S_j = \lambda_{H_2} \frac{\partial c_{H_2}}{\partial y} \) where \( \xi_1 = \lambda_{H_2} \) and \( \phi_1 = c_{H_2} \).

Discretizing \( \frac{\partial S}{\partial y} \) is tantamount to discretizing \( \frac{\partial \overline{s}}{\partial y} \). Therefore, the discretization of \( \overline{S} \) is given by:

\[
\delta_y \overline{S} = \frac{\left( \xi_{N+1} \phi_{N+1} \right) \left( \phi_{N+1} - \phi_{N} \right)}{\Delta y_N + \Delta y_{N+1}} - \frac{\left( \xi_{N} \phi_{N} \right) \left( \phi_{N} - \phi_{N-1} \right)}{\Delta y_N + \Delta y_N} \] (2.16)

And, with reference to S:

\[
\delta_y S = \sum_{i=1}^{n} \delta_y \overline{s}_i
\] (2.17)

**Boundary Conditions**

When numerically solving partial differential equations, boundary conditions must be specified. There are four boundary conditions that are imposed in the present problem. Referring to Figure 2.4 the four conditions can be seen. For the computational domain in question the right boundary is the outflow and the left the inflow. A wall condition is imposed on the lower boundary. For the simulations conducted in this paper, the wall has a constant temperature. However, an adiabatic or constant heat flux wall condition could be used. The upper boundary must conform to free stream values. Although with the space-marching code used it is possible to impose an axisymmetric boundary on the upper boundary, this was not implemented for this investigation.
There are two cases of discretizing the nodes in which the boundary conditions must be considered carefully. A schematic of the two cases can be seen in Figure 2.5.

Consider the case in which the central node (i.e., P) is right at the wall. As required by a viscous solution, the velocity of the flow right at the wall must be zero. The temperature is set by the wall condition, but the pressure and mass fractions are not as clear. It is found by Parent (1998) that the approximation to the pressure \( P_P = \frac{5}{4}P_N - \frac{1}{4}P_{NN} \) yield good results. For the mass fractions, to satisfy the requirement that \( \frac{\partial c}{\partial y} = 0 \) at the wall, \( c_P = c_N \).

For the second case, the central node is one node up from the wall. Obviously, a five-point stencil averaging cannot be done. In this case the \( G \) fluxes are discretized as follows:

\[
\delta_y G = \frac{\overline{G}_N - \overline{G}_S}{2\Delta y}
\]

where \( \overline{G} = [\rho v_c H_2, \ldots, \rho v c_{NO_2}, \rho c_{uv}, 0, \rho c_{vE} + v P] \) (2.18)

Also, to avoid oscillations the assumption \( v_P = \frac{v}{2} \) is made one node up from the wall.

### 2.3.2 Solving the Governing Equations

Now that the discretization procedure has been established, the method of solving the TLNS equations will be described. As a starting point the equations to be solved are shown again in the conservation form:
\[
\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = \frac{\partial S}{\partial y} + W
\]  
(2.19)

The solution will follow an implicit Euler time-marching scheme, which is shown in Equation 2.20.

\[
\frac{\Delta Q^n}{\Delta t} + \delta_x F^{n+1} + \delta_y G^{n+1} - \delta_y S^{n+1} - W^{n+1} = 0
\]  
(2.20)

Where \( \Delta Q^n = Q^{n+1} - Q^n \).

Adding \( \delta_y S^n + W^n - \delta_y F^n - \delta_y G^n \) to both sides results in the following:

\[
\frac{\Delta Q^n}{\Delta t} + (\delta_x F^{n+1} - \delta_x F^n) + (\delta_y G^{n+1} - \delta_y G^n) \\
- (\delta_y S^{n+1} - \delta_y S^n) - (W^{n+1} - W^n) \\
= \delta_y S^n + W^n - \delta_x F^n - \delta_y G^n
\]  
(2.21)

Written in the more compact delta form, Equation 2.21 becomes:

\[
\frac{\Delta Q^n}{\Delta t} + \delta_x (\Delta F^n) + \delta_y (\Delta G^n) - \delta_y (\Delta S^n) - \Delta W^n = -R_\Delta^n
\]  
(2.22)

Where the \( R_\Delta \) term is as described in Equation 2.8.

To linearize Equation 2.22, the following is performed.

\[
\Delta F = A\Delta Q \quad \Delta G = B\Delta Q \quad \Delta W = D\Delta Q
\]

with \( A = \frac{\partial F}{\partial Q} \) \( B = \frac{\partial G}{\partial Q} \) \( D = \frac{\partial W}{\partial Q} \)  
(2.23)

Where A and B are the convective x and y jacobians, respectively, and D is the source term jacobian. To linearize the y-diffusive flux \( S \), a technique described by Chang and Merkle (1989) is used.

\[
S = C_1 \frac{\partial Q}{\partial y} = C_1 \frac{\partial (C_2 Q)}{\partial y}
\]

with \( C_2 = \frac{\partial \hat{Q}}{\partial Q} \)  
(2.24)

With \( C_1 \) a multiplication factor, \( C_2 \) the diffusion jacobian, and \( \hat{Q} \) a fictitious flux. \( C_1 \) and \( \hat{Q} \) are explicitly shown below.
Now linearized, the equation is again shown in the delta form.

$$\Delta Q^n + \delta_x (A^n \Delta Q^n) + \delta_y (B^n \Delta Q^n) - \delta_y (C^n \delta_y (C^n \Delta Q^n)) - D^n \Delta Q^n = - R^n_\Delta$$

(2.27)

Written in a more practical form, Equation 2.27 is transformed into readily discretizable form. The $\xi$ in this case represents a general discretization. Of course, depending on the particular flux these terms will be discretized differently from each other.

$$\Delta Q^n_{P} + \frac{\Delta Q^n_{P}}{\Delta t_P} + \xi_B^n A^n_{P} \Delta Q^n_{P} + \xi_{NN}^B B^n_{NN} \Delta Q^n_{NN} + \xi_{N}^B B^n_{N} \Delta Q^n_{N} + \xi_B^n B^n_{P} \Delta Q^n_{P}$$

$$+ \xi_S^n B^n_{S} \Delta Q^n_{S} + \xi_{SS}^B B^n_{SS} \Delta Q^n_{SS} + D^n \Delta Q^n_{P}$$

(2.28)

$$= - R^n_\Delta$$

Note that $\Delta Q$'s west of point P are omitted. Due to the space marching scheme, all fluxes upstream are already converged (i.e., $\Delta Q^n = 0$).

Re-writing Equation 2.28 in a more compact form:

$$\sigma^n_{SS} \Delta Q^n_{SS} + \sigma^n_{S} \Delta Q^n_{S} + \sigma^n_{P} \Delta Q^n_{P} + \sigma^n_{N} \Delta Q^n_{N} + \sigma^n_{NN} \Delta Q^n_{NN} = - R^n_\Delta$$

(2.29)
Where the $\sigma$'s represent the following:

\[
\begin{align*}
\sigma_P^n &= \frac{1}{\Delta t_P} + \xi_P^A P + \xi_P^B P + \frac{(C_{T_N}^p + C_{T_P}^p)C_{T_P}^p}{2\Delta y_N\Delta y_P} + \frac{(C_{T_P}^p + C_{T_S}^p)C_{T_S}^p}{2\Delta y_S\Delta y_P} \\
\sigma_N^n &= \xi_N^B N - \frac{(C_{T_N}^p + C_{T_P}^p)C_{T_N}^p}{2\Delta y_N\Delta y_P} \\
\sigma_{NN}^n &= \xi_{NN}^B B_{NN} \\
\sigma_S^n &= \xi_S^B S - \frac{(C_{T_P}^p + C_{T_S}^p)C_{T_S}^p}{2\Delta y_S\Delta y_P} \\
\sigma_{SS}^n &= \xi_{SS}^B B_{SS}
\end{align*}
\] (2.30)

Finally, the equations are placed in a penta-diagonal matrix. Then to obtain a solution the following matrix is inverted.

\[
\begin{bmatrix}
I & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
\sigma_{N,2} & \sigma_{P,2} & \sigma_{S,2} & 0 & 0 & 0 & 0 & \cdots & -R_{N,2} \\
\sigma_{NN,3} & \sigma_{N,3} & \sigma_{P,3} & \sigma_{S,3} & \sigma_{SS,3} & 0 & 0 & \cdots & -R_{N,3} \\
\vdots & \vdots & \sigma_{N,4} & \sigma_{P,4} & \sigma_{S,4} & \sigma_{SS,4} & 0 & \cdots & -R_{N,4} \\
\cdots & \cdots & \sigma_{NN,5} & \sigma_{N,5} & \sigma_{P,5} & \sigma_{S,5} & \sigma_{SS,5} & 0 & \cdots & -R_{N,5} \\
\cdots & \cdots & \sigma_{NN,6} & \sigma_{N,6} & \sigma_{P,6} & \sigma_{S,6} & \sigma_{SS,6} & \cdots & \cdots & -R_{N,6}
\end{bmatrix}
\] (2.31)

**Local Time Stepping**

Since the solutions to ignition of fuel in the boundary layer are not time-accurate some more efficient solution methods can be employed. One such modification is using local time stepping. The equation for local time stepping can be seen in the following equation:

\[
\Delta t_P = \frac{C_{CFL}\Delta y_P}{v_P + a_P}
\] (2.32)

The $C_{CFL}$ is related to the magnitude of the time-stepping process and is a user-inputed value, and $a_P$ is the local speed of sound. For an implicit method such as LAD, the restrictions on the $C_{CFL}$ are not as strict as for an explicit approach. However, if the $C_{CFL}$ is initially set too high, the residual may diverge.

It was noticed by Parent (1998) than when the above time-stepping equation is used, for large variations in grid spacing in the marching direction (i.e., $x$-direction), as the method was space-marched, different values of the $C_{CFL}$ had to be implemented. To counteract this variation an empirically determined modification to the above equation is determined. This modified equation is as follows:
\[ \Delta t_p = \left( \frac{C_{FL} \Delta y_p}{|v_p| + a_P} \right) \left( \frac{\Delta x_p}{0.01} \right)^{\frac{1}{2}} \]  

(2.33)

2.4 Thermodynamic and Chemical Models

2.4.1 Thermodynamic Data

As mentioned previously, to study the ignition of fuel in the boundary layer it is necessary to include as many relevant species in the solution so as to properly represent the chemical process. However, with each species considered in the chemical scheme its corresponding physical and thermodynamic properties must be included into the solution method.

With any hypersonic flow and especially exothermically reacting flows, great variations in temperature are expected. To more accurately capture the flow characteristics the thermodynamic properties of the species considered cannot be assumed to be constant. To approximate the thermodynamics expected in the flow pre-determined polynomials are used to calculate the specific heats and any subsequent thermodynamic variable derived from these (e.g., enthalpy, free energy). The coefficients for these polynomials were obtained from McBride et al. (1993). These polynomials are accurate up to 5000 K.

The transport properties (i.e., viscosity, mass diffusion, and thermal conductivity) are calculated from a method described by Dixon-Lewis (1984). Each species present in the chemical solver has its own Lennard-Jones 12-6 potential parameters. From these values, polynomial fits of collision integrals \( \Omega^{(1,1)} \), \( A^* \), and \( A^*_{H_2O} \) are used to calculate the transport properties.

2.4.2 Chemical Model

The chemical solver used consists of 13 species and 33 reactions (Jachimowsky 1988). A hydrogen/air system is used.

For finite rate chemistry (i.e., involving one step) the law of mass action is used to determine the rate of production from species \( k \).

\[
\sum_{i=1}^{N_i} \nu'_i \chi_i \overset{k_f}{\Rightarrow} \sum_{i=1}^{N_i} \nu''_i \chi_i
\]  

(2.34)

Where, \( N_i \) is the number of species, and \( \nu'_i \) and \( \nu''_i \) are the stoichiometric coefficients for the reactants and products, respectively. Also, \( \chi_i \) is the concentration of species \( i \). \( k_f \) and
are the forward and backward reaction rate constants, respectively.

The forward reaction rate constant is determined as follows:

\[ k_f = AT^m \exp(-E/RT) \] (2.35)

\( \mathcal{R} \) is the universal gas constant and the values for \( A, E, \) and \( n \) can be found in Table 2.1. The forward and backward rate constants are related by the equilibrium constant.

\[ \frac{k_f}{k_b} = K_e \] (2.36)

Noting that Gibbs free energy is calculated from \( G_i = H_i - TS_i \). The equilibrium constant can be found from the following equation:

\[ K_e = (\mathcal{RT})^{-\Delta \nu} \exp \left( \frac{-\Delta G^0}{\mathcal{RT}} \right) \] (2.37)

where,

\[ \Delta \nu = \sum_{i=1}^{N_i} (\nu''_i - \nu'_i) \] (2.38)

The change in Gibbs free energy can be seen in Equation 2.39. \( h_i^0 \) is the molar enthalpy and \( s_i^0 \) is the molar entropy, each calculated at standard pressure (i.e., one atmosphere).

\[ \Delta G^0 = \sum_{i=1}^{N_i} (\nu''_i - \nu'_i) (h_i^0 - Ts_i^0) \] (2.39)

Now the species production term \( w_k \) must be determined for all the species considered in the chemical solver. Given in kg/s, essentially the species production terms are the source terms seen in matrix \( \mathbf{W} \) in Section 2.2.

\[ w_k = \mathcal{M}_k \sum_{i=1}^{N_e} (\nu''_{i,k} - \nu'_{i,k}) \left[ k_f \prod_{m=1}^{N_i} [X_m]^{\nu'^{i,m}} - k_b \prod_{m=1}^{N_i} [X_m]^{\nu''^{i,m}} \right] \] (2.40)

Where, \( N_e \) is the number of elementary reactions involving species \( k \), \( N_i \) is the number
of species involved in the reaction, \( x_m \) the concentration of species \( m \), \( M_k \) is the molecular weight (kg/kg mole) of species \( k \), and \( \nu_{i,m} \) and \( \nu_{i,m}'' \) are the stoichiometric coefficients for the reactants and products, respectively, for reaction \( i \).

Table 2.1 shows all the 33 reactions considered in the chemical solver (Jachimowsky 1998). This chemical solver was designed for scramjet combustor flowfields.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>A</th>
<th>n</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>( H_2 + O_2 \rightarrow OH + OH )</td>
<td>( 1.70 \times 10^{13} )</td>
<td>0</td>
</tr>
<tr>
<td>(2)</td>
<td>( H + O_2 \rightarrow OH + O )</td>
<td>( 2.60 \times 10^{14} )</td>
<td>0</td>
</tr>
<tr>
<td>(3)</td>
<td>( O + H_2 \rightarrow OH + H )</td>
<td>( 1.80 \times 10^{10} )</td>
<td>1.00</td>
</tr>
<tr>
<td>(4)</td>
<td>( OH + H_2 \rightarrow H_2O + H )</td>
<td>( 2.20 \times 10^{13} )</td>
<td>0</td>
</tr>
<tr>
<td>(5)</td>
<td>( OH + OH \rightarrow H_2O + O )</td>
<td>( 6.30 \times 10^{12} )</td>
<td>0</td>
</tr>
<tr>
<td>(6)</td>
<td>( H + OH + M \rightarrow H_2O + M )</td>
<td>( 2.20 \times 10^{22} )</td>
<td>-2.00</td>
</tr>
<tr>
<td>(7)</td>
<td>( H + H + M \rightarrow H_2 + M )</td>
<td>( 6.40 \times 10^{17} )</td>
<td>-1.00</td>
</tr>
<tr>
<td>(8)</td>
<td>( H + O + M \rightarrow OH + M )</td>
<td>( 6.00 \times 10^{16} )</td>
<td>-0.60</td>
</tr>
<tr>
<td>(9)</td>
<td>( H + O_2 + M \rightarrow HO_2 + M )</td>
<td>( 2.10 \times 10^{15} )</td>
<td>0</td>
</tr>
<tr>
<td>(10)</td>
<td>( HO_2 + H \rightarrow H_2 + O_2 )</td>
<td>( 1.30 \times 10^{13} )</td>
<td>0</td>
</tr>
<tr>
<td>(11)</td>
<td>( HO_2 + H \rightarrow OH + OH )</td>
<td>( 1.40 \times 10^{14} )</td>
<td>0</td>
</tr>
<tr>
<td>(12)</td>
<td>( HO_2 + H \rightarrow H_2O + O )</td>
<td>( 1.00 \times 10^{13} )</td>
<td>0</td>
</tr>
<tr>
<td>(13)</td>
<td>( HO_2 + O \rightarrow O_2 + OH )</td>
<td>( 1.50 \times 10^{13} )</td>
<td>0</td>
</tr>
<tr>
<td>(14)</td>
<td>( HO_2 + OH \rightarrow H_2O + O_2 )</td>
<td>( 8.00 \times 10^{12} )</td>
<td>0</td>
</tr>
<tr>
<td>(15)</td>
<td>( HO_2 + HO_2 \rightarrow H_2O_2 + O_2 )</td>
<td>( 2.00 \times 10^{12} )</td>
<td>0</td>
</tr>
<tr>
<td>(16)</td>
<td>( H + H_2O_2 \rightarrow H_2 + HO_2 )</td>
<td>( 1.40 \times 10^{12} )</td>
<td>0</td>
</tr>
<tr>
<td>(17)</td>
<td>( O + H_2O_2 \rightarrow OH + HO_2 )</td>
<td>( 1.40 \times 10^{13} )</td>
<td>0</td>
</tr>
<tr>
<td>(18)</td>
<td>( OH + H_2O_2 \rightarrow H_2O + HO_2 )</td>
<td>( 6.10 \times 10^{11} )</td>
<td>0</td>
</tr>
<tr>
<td>(19)</td>
<td>( M + H_2O_2 \rightarrow OH + OH + M )</td>
<td>( 1.20 \times 10^{17} )</td>
<td>0</td>
</tr>
<tr>
<td>(20)</td>
<td>( O + O + M \rightarrow O_2 + M )</td>
<td>( 6.00 \times 10^{17} )</td>
<td>0</td>
</tr>
<tr>
<td>(21)</td>
<td>( N + N + M \rightarrow N_2 + M )</td>
<td>( 2.80 \times 10^{17} )</td>
<td>-0.75</td>
</tr>
<tr>
<td>(22)</td>
<td>( N + O_2 \rightarrow NO + O )</td>
<td>( 6.40 \times 10^{9} )</td>
<td>1.00</td>
</tr>
<tr>
<td>(23)</td>
<td>( N + NO \rightarrow N_2 + O )</td>
<td>( 1.60 \times 10^{13} )</td>
<td>0</td>
</tr>
<tr>
<td>(24)</td>
<td>( N + OH \rightarrow NO + H )</td>
<td>( 6.30 \times 10^{11} )</td>
<td>0.50</td>
</tr>
<tr>
<td>(25)</td>
<td>( H + NO + M \rightarrow HNO + M )</td>
<td>( 5.40 \times 10^{15} )</td>
<td>0</td>
</tr>
<tr>
<td>(26)</td>
<td>( H + HNO \rightarrow NO + H_2 )</td>
<td>( 4.80 \times 10^{12} )</td>
<td>0</td>
</tr>
<tr>
<td>(27)</td>
<td>( O + HNO \rightarrow NO + OH )</td>
<td>( 5.00 \times 10^{11} )</td>
<td>0.50</td>
</tr>
<tr>
<td>(28)</td>
<td>( OH + HNO \rightarrow NO + H_2O )</td>
<td>( 3.60 \times 10^{13} )</td>
<td>0</td>
</tr>
<tr>
<td>(29)</td>
<td>( HO_2 + HNO \rightarrow NO + H_2O_2 )</td>
<td>( 2.00 \times 10^{12} )</td>
<td>0</td>
</tr>
<tr>
<td>(30)</td>
<td>( HO_2 + NO \rightarrow NO_2 + OH )</td>
<td>( 3.40 \times 10^{12} )</td>
<td>0</td>
</tr>
<tr>
<td>(31)</td>
<td>( H + NO_2 \rightarrow NO + OH )</td>
<td>( 3.50 \times 10^{14} )</td>
<td>0</td>
</tr>
<tr>
<td>(32)</td>
<td>( O + NO_2 \rightarrow NO + O_2 )</td>
<td>( 1.00 \times 10^{13} )</td>
<td>0</td>
</tr>
<tr>
<td>(33)</td>
<td>( M + NO_2 \rightarrow NO + O + M )</td>
<td>( 1.16 \times 10^{12} )</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 2.1 Reactions described by Jachimowsky.

Note the M terms in some of the reactions (e.g., reactions 6, 7, and 8). These terms
are called third-bodies, and they act only as catalysts to the reactions. The third-body concentrations can be found by the following equation:

\[ \chi_M = \sum_{k=1}^{n_s} \eta_k \chi_k \]  

(2.41)

\( \eta_k \) is the third-body efficiency and has a value of one except in the following reactions given in Table 2.2.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>third body efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>(6) ( \text{H} + \text{OH} + \text{M} \rightarrow \text{H}_2\text{O} + \text{M} )</td>
<td>( \text{H}_2 ) 1.0 ( \text{H}_2\text{O} ) 6.0</td>
</tr>
<tr>
<td>(7) ( \text{H} + \text{H} + \text{M} \rightarrow \text{H}_2 + \text{M} )</td>
<td>( \text{H}_2 ) 2.0 ( \text{H}_2\text{O} ) 6.0</td>
</tr>
<tr>
<td>(8) ( \text{H} + \text{O} + \text{M} \rightarrow \text{OH} + \text{M} )</td>
<td>( \text{H}_2 ) 1.0 ( \text{H}_2\text{O} ) 5.0</td>
</tr>
<tr>
<td>(9) ( \text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M} )</td>
<td>( \text{H}_2 ) 2.0 ( \text{H}_2\text{O} ) 16.0</td>
</tr>
<tr>
<td>(19) ( \text{M} + \text{H}_2\text{O}_2 \rightarrow \text{OH} + \text{OH} + \text{M} )</td>
<td>( \text{H}_2 ) 1.0 ( \text{H}_2\text{O} ) 15.0</td>
</tr>
</tbody>
</table>

Table 2.2 Reactions with third-body efficiencies other than one.

### 2.5 Physical Domain and Gridding

#### 2.5.1 Physical Domain

The physical domain of the simulations varies with the inflow Mach number. The length of the flat plate (i.e., the x-direction) is set to 1 m. The flat plate should be as long as necessary so as to capture the salient features of fuel ignition in the boundary layer. However, the length of the physical domain in the direction normal to the flow (i.e., the y-direction) is not held constant for all simulations. As mentioned previously in Section 2.3.1, for LAD the flow in the upper boundary must reach approximately free stream values. Specifically, the physical domain should be such that the bow shock formed at the leading edge should exit out of the right (i.e. downstream) boundary. Therefore, the y-range will be determined for each simulation as it is largely dependent upon the inflow Mach number and the plate length. This y domain is approximated from an equation in which inflow Mach number and flat plate length are the only unknowns. This equation is as follows:

\[ y \approx x \frac{1}{M - 1} \]  

(2.42)

Where \( M \) is the inflow Mach number, \( x \) the length of the flat plate, and \( y \) the height of the domain above the flat plate.
2.5.2 Gridding

Once the physical domain is set, a gridding strategy can be applied. Obviously, since the scope of the present study deals with analysis of a reacting boundary layer the boundary layer needs to be resolved adequately. The actual gridding is divided up into three regions. The three regions are the pseudo-laminar layer, pseudo-combustion layer, and the free stream region. The description of these regions is as follows. When combustion occurs in the boundary layer there is an increase in the boundary layer thickness. It can be hypothesized that there are two regions in the boundary layer. For a non-reacting flow, the boundary develops to some extent (i.e., the actual laminar boundary layer). When combustion occurs the increase in the boundary layer thickness can be termed the pseudo-combustion layer. Of course, the word pseudo must be stressed as there is no clear distinction between these two regions, chemical reactions are present throughout the boundary layer. It is only for gridding purposes that these regions are defined. The third region, (i.e., free stream region) is the remainder of the flow above the pseudo-combustion layer where the physical properties of the flow are close to free stream or inflow values. Obviously, the flow does not need to be as well resolved in this region compared to the other two.

An example of one of the grids created for a simulation can be seen in Figure 2.6. The inflow Mach number for this grid is 7. Calculated from Equation 2.42 plus a small safety factor, the y-range is 0.23 m. Note that the y-spacing is not equidistant but increases in the direction of the top boundary. The x-range is set slightly greater than one meter so that there is no ambiguity at the one meter mark due to outflow boundary definitions. Viewing the grid under closer magnification Figure 2.7 shows the divisions of the pseudo-laminar and combustion layers more clearly. The y-range for the pseudo-laminar layer is 0.0015 m and contains 50 nodes. The y-range for the pseudo-combustion layer is 0.0065 m and contains 100 nodes. The remaining free stream region contains 50 nodes.

For all of the simulations there are 100 nodes in the x-range. To help convergence of the initial x-stations (recall space-marching scheme), 2 nodes are placed in the first millimeter. After these first two nodes the node spacing gradually increases. It is important to have a sufficient number of nodes in the x-direction, because unlike in non-reacting flat plate flows, large gradients in the x-direction can occur at initially unknown locations (e.g., combustion).

2.6 Validation

2.6.1 Comparison of Different Chemical Solvers

The space-marching Thin-Layer Navier-Stokes code (LAD) has been thoroughly validated in a paper by Parent (1998). However, most of these validations were performed on non-
Figure 2.6: Grid used for Mach 7 case

Figure 2.7: Magnified view of grid in pseudo-laminar and combustion regions
reacting flows. A complex chemical solver is required of the space-marching code to capture combustion flow characteristics. To this end, a 13 species chemical solver involving H₂ and air is applied to the code. The chemical solver to be considered is described by Jachimowsky (1988). This chemical solver contains 33 reactions, in which N₂ is not considered inert.

A particular chemical solver cannot be validated against another. For even small differences in the thermodynamic data of a chemical solver compared to that of another, the resultant flows can differ significantly. However, it is important to check that any differences in the resultant flows are largely due to the chemical solver and not the method of the solution (i.e., the space-marching TLNS code).

There are very few simple test cases available to compare chemical solvers. However, one particular study performed by Da Silva et al. (1993) is considered. In this study the ignition of a combustible mixture (H₂/air) is analyzed over a flat plate at supersonic speeds. Viscous dissipation at the wall can produce enough energy to cause ignition of the fuel in the boundary layer. One such case, is a stoichiometric mixture of fuel and air flowing over a flat plate at an inlet temperature of 700 K and a pressure of 0.1 MPa. Two different Mach numbers are studied, 5.5 and 6. A transversal cut at 2 and 10 cm is taken along the flat plate for both cases. A plot of \( T / T_\infty \) versus \( \eta = y \sqrt{\frac{u_0}{\chi_{\infty} T_\infty}} \) is produced from the transversal cuts. The location of the cuts are defined such that even with a slight increase in Mach number (e.g., 5.5 to 6) the induction length of the combustion process changes. The end of the induction length is realized by an important heat release, which sharply raises the temperature in the boundary layer.

There are three different solution methods which will be compared. The first one is the solutions obtained by Da Silva et al. (1993). The second is performed using LAD coupled with a chemical solver described by Maas and Warnatz (1988). And the third, LAD will be used again, however, the chemical solver implemented will be one described by Jachimowsky (1988).

The Jachimowsky chemical solver has been used from many previous scramjet studies: (Dudebout 1995). However, the Maas-Warnatz chemical solver is not arbitrarily chosen. In the paper by Da Silva et al. (1993), three different chemical solvers are used. For the simulations to be compared, Da Silva does not specify which of the three chemical solvers are used. However, a comparison study of the three chemical solvers used by Da Silva et al. (1993) was performed in the paper in question. It was shown that all three chemical solvers give close agreement with each other. Since the specific chemical solver used by Da Silva et al. (1993) for the current simulations to be compared is not known, one of the solvers was assumed to be the one used. The chemical solver chosen was the one by Maas and Warnatz (1988). Therefore, the hypothesis being made is that if LAD used the same chemical solver as da Silva uses, then the results of the simulations should be closer than those given by
LAD with the Jachimowsky chemical solver.

The Maas-Warnatz chemical solver is a H$_2$/air 9 species, 19 reaction chemical solver and does consider N$_2$ inert.

The results of the three solutions can be seen for the Mach 5.5 case in Figure 2.8 and Mach 6 case in Figure 2.9. In Figure 2.8 the temperature ratio agrees well with all the solutions at the 2 cm transversal cut. In this region the effect of chemistry remains small and viscous dissipation dominates the temperature increase. However, at the 10 cm cut the
temperature ratio curve for the TLNS code with Jachimowsky chemical solver differs greatly from the other two solutions. This difference in temperature ratio curves is due to variations in induction length for different chemical solvers. The Jachimowsky chemical solver yields a shorter induction length, hence the temperature increase caused by combustion is seen earlier. Of note, the temperature ratio curves for the TLNS with Maas-Warnatz chemical solver and the boundary layer code are similar to each other. This similarity is strong evidence that differences in solutions are largely due to the chemical solver used and not the solution method.

To further show that the main difference in solutions is due to the chemical solver, Figure 2.9 shows the same comparison as Figure 2.8 except for an inlet Mach number of 6. As before, the 2 cm transversal cut agrees well for all the solution methods. However, for the 10 cm cut the Jachimowsky chemical solver yields varying results from the other two. The main difference between the Mach 5.5 and Mach 6 cases is that at the 10 cm cut ignition takes place for all the solutions but only for the Jachimowsky chemical solver in the Mach 5.5 case. Also, it is noted by Da Silva et al. (1993) that the Maas-Warnatz solver has a shorter induction length that the other two chemical solvers used in the paper. This fact indicates that for this test case, da Silva et al. did not use the Maas-Warnatz chemical solver but one of the other two specified. If this is true, the non-Jachimowsky results would most likely agree even better with the da Silva results.

To summarize, it is shown that different chemical solvers do indeed yield different solutions. However, it is also shown that the differences resulting from using different chemical solvers is for the most part not due to using different solution methods for the cases studied above.

2.6.2 Validation of Numerical Method Using Heat Transfer Rates

When studying hypersonic flow over a body, viscous dissipation along the body surface will produce an enormous amount of heat. Even if the body is made out of materials with very high thermal tolerances, there will still be some limit in which the material cannot survive. One way to maintain the integrity of the body is to cool the surface continuously. If a surface is to be cooled, the cooling requirements must be quantified. By setting a constant wall temperature to the surface of the body and studying the flow as it passes over it, heat transfer rates to the wall may be obtained.

Further validation of the TLNS code produced by Parent (1998) is accomplished by comparing the heat transfer rate for a particular case with another solution method. A test case is described by Pratt and Heiser (1994) in which air flows over a flat plate. The specifics of the flow are as follows: \( M_0 = 10.0, q_0 = 47.88 \text{ kN/m}^2, \gamma_0 = 1.40, T_w = 1111 \text{ K}, x = \)
Pratt and Heiser (1994) solves the flows with a computer program called HAP (Air). Further, the convective heat transfer rate is calculated using the Eckert reference enthalpy method. This method assumes the boundary layer flow is laminar.

To calculate the heat transfer to the wall see Section 3.1.1.

As can be seen from Figure 2.10, the two methods agree quite well with each other with respect to heat transfer rate to the wall. There is about a 13 percent difference between the two values at $x = 0.3048$ m.
Chapter 3

Results

3.1 Heat Transfer to the Wall

3.1.1 Background

Most hypersonic vehicles will need some form of thermal protection system. Even considering
the flow of air over a body traveling at hypersonic velocities, viscous dissipation will produce
an enormous amount of heat. Now, if the flow of a exothermically combustible mixture is
considered (like in this current area of research) the heat generated will most likely increase
compared to that of the flow of only air. The materials needed to withstand such thermal
constraints either do not exist, or are too impractical to use.

The design of a shcramjet will require that its cooling requirements be determined (see
Section 1.1). Although an actual shcramjet is not modeled in this paper, a good approxima-
tion of the scope of its cooling requirements are obtained.

For all the simulations performed, a constant wall temperature is assumed. Using the
heat conduction equation (see Figure 3.1) the heat transfer rate can be determined all along
the flat plate (see Section 1.3).

\[ \dot{Q}_w = -\kappa^* \frac{\partial T}{\partial y} \] (3.1)

Where \( \kappa^* \) is the thermal conductivity of the flow at the central discretization point (i.e.,
reference coordinate P).

The partial derivative in Equation 3.1 is approximated using a second-order forward
difference form as seen by the following equation:
\[
\frac{\partial T}{\partial y} \approx \frac{3T_P - 4T_N + T_{NN}}{y_{NN} - y_P}
\] (3.2)

Remembering that, in general, the node spacing is non-equidistant so the above equation is not truly second-order accurate. However, even if the partial derivative is close to second-order accuracy, the value of \( \dot{Q}_w \) is still only first-order accurate because of the initial discretization of the governing equations.

To analyze the effect of varying the value of the wall temperature, Mach number, and equivalence ratio has on heat transfer rates, the following is presented.

Thirty different simulations were produced for this thesis. The simulations spanned the Mach numbers from 2 to as high as 17. Four different wall temperature were used (i.e., 300, 500, 700, and 1000 K). Also, three different equivalence ratios were compared (i.e., \( \phi = 0.5, 1, 2 \)). The following is a summation of all the simulations performed.

<table>
<thead>
<tr>
<th>Wall Temp.</th>
<th>( \phi=1 )</th>
<th>( \phi=0.5 )</th>
<th>( \phi=2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T_w=300 ) K</td>
<td>Mach 2,5,7,10,13,15,17</td>
<td>Mach 7,10</td>
<td>Mach 7,10</td>
</tr>
<tr>
<td>( T_w=500 ) K</td>
<td>Mach 2,5,7,10,13,15</td>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td>( T_w=700 ) K</td>
<td>Mach 2,5,7,10,13</td>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td>( T_w=1000 ) K</td>
<td>Mach 2,5,7,10</td>
<td>Mach 7,10</td>
<td>Mach 7,10</td>
</tr>
</tbody>
</table>

Table 3.1 Summation of numerical simulations performed

Essentially, the upper Mach limit for constant wall temperature for an equivalence ratio of one (\( \phi=1 \)) is determined mainly from the temperature limit of the chemical solver. This upper temperature limit is 5000 K for the Jachimowsky chemical model.

### 3.1.1 Comparison of Results

#### Constant Wall Temperature

As mentioned in section 1.3, having a wall temperature range of 300 K to 1000 K gives a good representation of an overly optimistic wall temperature (i.e., 300 K) and a realistic wall temperature (i.e., 1000 K). Also, the 500 K and 700 K wall temperatures are used to track the trends between the two wall temperature limits.

The following is a graphical comparison of the heat transfer rates to the wall as the inflow Mach number is increased, but the wall temperature is held constant.

Figure 3.1 displays the heat transfer rate \( \dot{Q}_w \) with a wall temperature of 300 K. The larger the absolute value of \( \dot{Q}_w \), the greater the heat transfer rate. The negative sign attached to
\( \dot{Q}_w \) indicates that the direction of net-heat movement is to the plate. Note that, at the leading edge the heat transfer rate is at its greatest. This is because the stagnation point temperatures present at the leading edge are relatively large. A large temperature gradient is present which would account for the \( \dot{Q}_w \) drop seen in this region. The most striking attribute seen on Figure 3.1 is the sharp increase in \( \dot{Q}_w \) for the Mach 7 case at about 0.5 m. This increase is due to combustion taking place in the boundary layer. As predicted, the end of the induction length (or the beginning of the thermal runaway zone) is marked by an important heat release. With this result it can be seen that indeed combustion of fuel in the boundary layer does increase the heat transfer rate to the wall. Also of note, looking at the Mach 2 and 5 cases, no sudden increase is seen along the flat plate like the Mach 7 case. The explanation for this is that combustion has not taken place in these two (Mach 2 and 5) cases. That is not to say that combustion will never take place, only that for the flat plate domain studied the induction lengths for the Mach 2 and 5 simulations are probably longer than the flat plate. This statement can be verified by noting that an increase in the mass fraction of \( \text{H}_2\text{O} \) (the main product in the combustion of \( \text{H}_2 \) in air) is seen at the trailing edge of the Mach 2 and 5 simulations. Looking at the Mach numbers greater than 7, deceivingly enough there is no sharp \( \dot{Q}_w \) spike for these cases. This result does not suggest that combustion does not take place for these Mach numbers only that the induction lengths for these cases are so small that ignition takes place almost as soon as the flow hits the flat plate leading edge. This conclusion can be supported by looking at the Mach 10 case at a distance down the flat plate of about 0.05 to 0.1 m. In this region a
slight change in slope can be seen. This change in slope is due to ignition of the fuel. Since the induction length decreases with increasing Mach number, this change in slope is not as pronounced for the higher Mach numbers. As a final and important note about the Mach 10 and higher cases, the heat transfer rates of the cases vary only slightly with each other. This is an important result, as it is intuitively thought that the heat transfer rate should increase with an increasing Mach number. However, this is not the case as seen in Figure 3.1. The reason for this will be shown in Section 3.2, however a brief explanation to this phenomenon is related to endothermic reactions taking place in the flow.

Figure 3.2 shows a little more clearly compared to Figure 3.1 that \( \dot{Q}_w \) increases with increasing Mach number. Similar to the previous graph, the Mach 7 case has a thermal spike; however, note that the location of the spike is closer to the leading edge for the 500 K wall temperature compared to that of the 300 K wall temperature. Further comparing the two cases, ignition of the fuel does not take place for the Mach 2 and 5 cases. A similar profile is also seen for the Mach numbers higher than 7.

Referring to Figure 3.3, a few changes can be seen compared to the 300 K, and 500 K wall temperature cases. First, with a wall temperature of 700 K the induction length for the Mach 5 cases has decreased enough that it can now be seen in the domain studied. Also, the induction length of the Mach 7 case continues to decrease and the size of thermal spike is decreasing. This latter result indicated that the heat release due to combustion is decreasing as the wall temperature increases.

The last constant wall temperature case studied (i.e., \( T_W = 1000 \) K) can be seen in
Figure 3.3: Heat transfer to wall, $T_W = 700$ K, $T_\infty = 700$ K

Figure 3.4: Heat transfer to wall, $T_W = 1000$ K, $T_\infty = 700$ K
Figure 3.5: Heat transfer to wall, Mach 2, $T_\infty = 700$ K

Figure 3.4. In this figure, all of the Mach numbers produced show ignition of the fuel within the domain studied. Further, the heat release decreases as the Mach number is increased. This is an interesting graph as this shows that even with a more physically realistic wall temperature, ignition of fuel in the boundary layer will occur over the entire Mach range studied for the plate domain studied.

Constant Mach Number

All of the data in this section can be seen in the previous one. However, the data is arranged in this section so that greater insight can be made into the effect of varying the wall temperature has on the ignition process.

Figure 3.5 shows the heat transfer rate with a constant Mach number of 2, but varying the wall temperature. Note, that $\dot{Q}_w$ decreases with decreasing wall temperature, except for the $T_W = 1000$ K. For the Mach 2 simulations, only a wall temperature of 1000 K caused ignition of the fuel in the boundary layer. This result can be seen by the large thermal spike in the graph. However, interestingly enough even though ignition took place for the 1000 K wall temperature, the heat transfer rate is still lower than that for the 300 K wall temperature case.

For a constant Mach number of 5, Figure 3.6 shows that ignition takes place for 700 K and 1000 K wall temperatures. However, it should be noted that a higher wall temperature yields a shorter induction length. This results can be seen more clearly in the Figure 3.7.

For the Mach 7 case, ignition takes place for all of the wall temperatures (see Figure 3.7).
Figure 3.6: Heat transfer to wall, Mach 5, $T_\infty = 700$ K

Figure 3.7: Heat transfer to wall, Mach 7, $T_\infty = 700$ K
It can be seen more clearly in this graph that, in general, a higher wall temperature results in a shorter induction length. Further, a higher wall temperature also results in a small heat release when combustion occurs.

For Figures 3.8, 3.9, and 3.10 the induction lengths are not that apparent. Also, near the leading edge it is not clear as to which wall temperature values yield greater or less heat transfer rates. However, the expected patterns of heat transfer rates with reference to
Figure 3.10: Heat transfer to wall, Mach 15, $T_\infty = 700$ K

Wall temperature can be seen further down the flat plate. Of special note, above a Mach number of about 7, the heat transfer rate curves do not vary significantly with each other for a combustible H$_2$/air mixture. This is a positive result, as the thermal protection requirements need only to be designed up to the Mach range of about 8 or 9.

**Constant Wall Temperature and Mach Number**

It is highly unlikely in a hypersonic engine that when the fuel is injected into the flow that a stoichiometric mixture will exist throughout the flow. This is especially true for regions close to the wall where the fuel will most likely will be injected from. Therefore, it is important to study what effects an equivalence ratio other than a stoichiometric one has on the phenomenon of ignition of fuel in the boundary layer. To examine the effect of just varying the equivalence ratio, the Mach number and wall temperature are held constant. The varying equivalence ratio simulations are done examining the two wall temperature limits (i.e., 300 K and 1000 K). With these two wall temperature conditions, Mach 7 and Mach 10 cases are performed. The Mach 7 number is chosen so that the induction length can clearly be seen and the Mach 10 is used so that the effects of increasing the inflow Mach number can be seen.

Referring to Figure 3.11, three different equivalence ratios are studied ($\phi = 1, 0.5, \text{ and } 2$). The wall temperature is held constant at 300 K and the Mach number is also held constant at 7. As expected, the leaner the equivalence ratio the shorter the induction length. The reason for this trend is explained in Section 1.2. However, briefly stated, the leaner fuel mixture
experiences a greater initial heating due to a lower specific heat. This causes ignition to take place first in this leaner mixture, however also note that the thermal spike is the smallest for this mixture. This result is expected as well because the stoichiometric mixture should produce a greater amount of heat compared to the leaner mixture.

Figure 3.12 shows a similar result to the previous graph. However, although the Mach number is held constant at 7, now the wall temperature is raised to 1000 K. The main differences other than the shorter induction lengths, is that the thermal spike and the overall
Figure 3.13: Heat transfer to wall, Mach 10, $T_W = 300$ K, $T_\infty = 700$ K

Figure 3.14: Heat transfer to wall, Mach 10, $T_W = 1000$ K, $T_\infty = 700$ K

heat transfer rates are smaller for this higher wall temperature compared to that of the 300 K wall temperature cases.

Figure 3.13 and Figure 3.14 are both Mach 10 simulations with a wall temperature of 300 K and 1000 K, respectively. Similar to the previous graphs, the same heat transfer rate pattern is seen.
3.2 Heat Generation Within the Flow

3.2.1 Background

When studying ignition of fuel in the boundary layer for hypersonic flows, there is a complex interplay between aggressive viscous dissipation effects and chemical reactions. Some method of determining how much heat is actually produced in the flow is needed to quantify these results.

One method of examining the heat produced in the flow is described by Pratt and Heiser (1994). The analysis of the heat produced within the flow is performed by the following. By assuming that the fuel/air mixture is initially at a reference temperature of 298 K, the combustion process takes place. Now, the products are cooled at a constant pressure until the mixture reaches the initial reference temperature of 298 K. The amount of heat removed from this process is called the heating value or the heat of reaction $h_{PR}$. The heat of reaction is calculated as follows:

$$ h_{PR} = (h_R)_{298} - (h_P)_{298} = \sum_{i=1}^{NS} (n_i)^R (\Delta h_i^0)_{298} - \sum_{i=1}^{NS} (n_i)^P (\Delta h_i^0)_{298} \quad (3.3) $$

$(n_i)^R$ and $(n_i)^P$ are the mass-specific mole numbers of species $i$ for the reactants and products, respectively. The mass-specific mole numbers is given in units of kg-moles k/kg mixture. $(\Delta h_i^0)_{298}$ is the enthalpy of formation of species $i$. The values of $(\Delta h_i^0)_{298}$ are given in Table 3.2 for each species present in the chemical solver.

Noticing that for all the simulations performed in this thesis, the initial reactants are $H_2$, $O_2$, and $N_2$. Keeping that in mind that by definition, the enthalpy of formation of all elements are zero at the reference temperature (i.e., 298 K). This fact will reduce the heat of reaction equation to that seen in Equation 3.4.

$$ h_{PR} = -\sum_{i=1}^{NS} (n_i)^P (\Delta h_i^0)_{298} \quad (3.4) $$

Noting that,

$$ (n_i) = \frac{c_i}{M_{w_i}} \quad (3.5) $$

Where, $c_i$ and $M_{w_i}$ are the mass fraction and molecular weight, respectively, for species
Referring to Table 3.2, noting that the enthalpy of formation of most of the species are positive (especially dissociated species H, O, and N). Also, the main combustion product (namely H₂O) has a negative enthalpy of formation. These facts in conjunction with Equation 3.4 indicate that if the flow is tending towards exothermicity (i.e., net heat production), \( h_{PR} \) will be positive. Conversely, if the flow tends toward endothermicity (i.e., net heat removal), \( h_{PR} \) will be negative. Also, considering just the magnitude of the enthalpy of formation values, the production of H, O, N, H₂O, and H₂O₂ will remove an enormous amount of heat from the flow. Of course, the magnitude of this effect is also largely dependent upon the relative species mass fractions and molecular weights.

Looking at just a brief analysis using the heat of reaction equation, many insights can be made about the flow. A transversal cut 60 cm down the flat plate is taken using one of the simulations. Specifically, the simulation parameters are, a Mach number of 7, \( T_W = 700 \) K, and \( \phi = 1 \). Figure 3.15 shows the heat of reaction, \( h_{PR} \) and the temperature profile plotted against the transversal flow direction (i.e., y-direction). As can be seen, the maximum temperature in the transverse direction coincides with the slope change in the heat of reaction curve (approximately at 0.0012 m). The heat of reaction equation (Equation 3.4) is mainly based upon the mass fraction of the species present in the flow. Therefore, the trend in the heat of reaction curve gives a good indication of what is chemically happening in the flow. These results will be better shown in the subsequent analysis.

### Table 3.2 Enthalpy of formation values for species present in chemical solver

<table>
<thead>
<tr>
<th>Name</th>
<th>Symbol</th>
<th>( (\Delta h_{f_i}^0)_{298} ) (kJ/kmol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atomic hydrogen</td>
<td>H</td>
<td>217 999</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>H₂</td>
<td>0</td>
</tr>
<tr>
<td>Water vapour</td>
<td>H₂O</td>
<td>-241 826</td>
</tr>
<tr>
<td>Hydrogen peroxide</td>
<td>H₂O₂</td>
<td>-136 106</td>
</tr>
<tr>
<td>Hydrogen peroxyl</td>
<td>HO₂</td>
<td>2 090</td>
</tr>
<tr>
<td>Atomic oxygen</td>
<td>O</td>
<td>249 170</td>
</tr>
<tr>
<td>Oxygen</td>
<td>O₂</td>
<td>0</td>
</tr>
<tr>
<td>Hydroxyl</td>
<td>OH</td>
<td>38 987</td>
</tr>
<tr>
<td>Atomic nitrogen</td>
<td>N</td>
<td>472 680</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>N₂</td>
<td>0</td>
</tr>
<tr>
<td>Hydrogen nitric oxide</td>
<td>HNO</td>
<td>99 579</td>
</tr>
<tr>
<td>Nitric oxide</td>
<td>NO</td>
<td>90 291</td>
</tr>
<tr>
<td>Nitrogen dioxide</td>
<td>NO₂</td>
<td>33 100</td>
</tr>
</tbody>
</table>
Figure 3.15: Heat of reaction and temperature at 60 cm transversal cut

Note in Figure 3.15 that near the edge of the boundary layer the heat of reaction is slightly negative. An investigation was performed to determine if this anomaly was physical or a deficiency in using Equation 3.4 to calculate the heat generation within the flow. Two adiabatic wall simulations were carried out each with an inflow Mach number of 7 and an inflow temperature of 700 K. One of the simulations allowed combustion of the fuel (H₂) to take place and the other was considered chemically frozen. At a transversal cut of 60 cm down the flat plate the temperature profile of the chemically frozen flow was used with the combustion case to calculate the heat of combustion $\Delta H_{abTR}$ through the 60 cm cut. Equation 3.6 was used to calculate the heat of combustion. The resultant heat of combustion profile can be seen in Figure 3.16. The purpose of such a calculation is to decrease the effect viscous dissipation has on the heat generation calculation. As can be seen in Figure 3.16 the same sign change as seen for the heat of reaction calculations can be seen in the region near the edge of the boundary layer. Therefore, it can be concluded that the sign change noticed when using Equation 3.4 is not a characteristic solely of this this equation.

$$\Delta H_{abTR} = \sum_{i=1}^{13} c_{Pi} h_{Pi}(T_R) - \sum_{i=1}^{3} c_{Ri} h_{Ri}(T_R)$$  \hspace{1cm} (3.6)
3.2.2 Analysis

Constant Wall Temperature

As the inflow Mach number of the fuel and air mixture is increased, there will be a subsequent change to the heat generated within the flow. By keeping a constant wall temperature and studying the ignition of fuel in the boundary layer as the inflow Mach number is increased, this change can be seen.
Referring to Figure 3.17, the heat of reaction is plotted for the Mach range of 5 to 13. A transversal cut is taken at 60 cm down the flat plate. A constant wall temperature of 700 K is held for this comparison as the Mach number is increased. There are a few points of interest in the heat of reaction plotting that stand out. First, the heat of reaction for the Mach 5 case is significantly less than those of the other Mach numbers. The reason for this variance is simply that for the simulation the curve is taken from, combustion has not fully developed at the 60 cm transversal cut. As explained previously, the induction length decreases with increasing Mach number. However, the most striking feature of this Mach number comparison is that as the Mach number increases, the slope of the heat of reaction curves increase in the region where the maximum temperature can be found (approximately 0.001 m). In fact, at some point above Mach 7 the slope actually becomes inverted. This change in slope is indicating that in this region the flow is becoming increasingly endothermic. These results will be shown more clearly later in this section. The third region of interest in Figure 3.17 is between 0.003 m and 0.005 m in the y-domain. This region is near the outer edge of the boundary layer. Noting that for most of the boundary layer the heat of reaction has a positive value. These results are consistent with an exothermically reacting flow as is the case with a H2/air reacting system. Further, as the heat of reaction is calculated in the free stream, $h_{PR}$ should approach zero as the composition of the free stream consists mainly of H2, O2, and N2 (recall by definition, elements have an enthalpy of formation of zero at 298 K). However, for the region near the edge of the boundary layer the value for the heat of reaction is slightly negative. This might indicate that endothermic reactions are dominating the chemistry in this region. This assumption cannot be considered correct as the temperature in this region is too small (approximately 800-900 K) for a H2/air system to tend towards endothermicity. This statement can be proven by examining the flow in the largest negative $h_{PR}$ point in the Mach 13 simulation (at about $y = 0.0032$ m) at the 60 cm cut. An analysis of the mass fractions of the species present in the flow reveal that the mass fraction of H is high enough and for H2O, low enough that the heat of reaction will be negative in this region. Looking at the species production term for H2O and H in this region: $w_{H_2O} = 11.8$ kg/s, and $w_H = 0.11$ kg/s. These results account for the presence of H2O, but not H. More concisely, the dominant reactions in the production or destruction of H and H2O are as follows. However, first an explanation is given on how the importance of the reactions are ranked.

Written in decreasing dominance, where the "order" expression indicates that the reactions are within the same order of magnitude. The higher the order of the reaction, the less importance the reaction carries to the net species production term.
\( \text{H}_2\text{O}, \text{Mach} 13, y = 0.0032 \text{ m} \):

\[
\begin{align*}
\text{OH} + \text{H}_2 & \rightarrow \text{H}_2\text{O} + \text{H} \quad \{ \text{order 3} \\
\text{HO}_2 + \text{H} & \rightarrow \text{H}_2\text{O} + \text{O} \quad \{ \text{order 4} \\
\end{align*}
\]

\( \text{H}, \text{Mach} 13, y = 0.0032 \text{ m} \):

\[
\begin{align*}
\text{OH} + \text{H}_2 & \rightarrow \text{H}_2\text{O} + \text{H} \\
\text{H} + \text{O}_2 + \text{M} & \rightarrow \text{HO}_2 + \text{M} \\
\text{HO}_2 + \text{H} & \rightarrow \text{OH} + \text{O} \\
\text{H} + \text{O}_2 & \rightarrow \text{OH} + \text{O} \\
\text{O} + \text{H}_2 & \rightarrow \text{OH} + \text{H} \quad \{ \text{order 3} \\
\end{align*}
\]

These results explain the production of \( \text{H}_2\text{O} \) as the two most dominant reactions involved with the \( \text{H}_2\text{O} \) species production term show a net increase in \( \text{H}_2\text{O} \) production. Also, although the most dominant reaction for the \( \text{H} \) reactions shows \( \text{H} \) being produced, the next three reactions show the destruction of \( \text{H} \). This results explains the small species production of \( \text{H} \).

It has been proven that endothermic reactions are not responsible for the negative heat of reaction in the above mentioned Mach 13 simulation. Therefore, it can be concluded that the most likely explanation for this negative heat of reaction is that mass diffusion is responsible. Since atomic hydrogen is the lightest species present in the chemical solver it seems likely that \( \text{H} \) should diffuse faster to the edge of the boundary layer than \( \text{H}_2\text{O} \) would. This verbose explanation is only meant to show that this negative heat of reaction is not some new phenomenon, but only just a characteristic of the heat of reaction calculations.

As mentioned previously, the heat of reaction results give useful insight into what is chemically happening in the flow. Referring to Figure 3.18, the mass fraction of \( \text{H}_2\text{O} \) is given for the along the 60 cm transversal cut for the Mach numbers shown in Figure 3.17. The main point of interest in Figure 3.18 is that a decreases in the mass fraction of \( \text{H}_2\text{O} \) is seen in the same region as the slope change for the heat of reaction curves for the same Mach numbers. The reason for these slope changes can be seen by analyzing the dominant reactions involved with the production or destruction of \( \text{H}_2\text{O} \) for the Mach 13 case.

\( \text{H}_2\text{O}, \text{Mach} 13, y = 0.00077 \text{ m} \):

\[
\begin{align*}
\text{H}_2\text{O} + \text{H} & \rightarrow \text{OH} + \text{H}_2 \quad \{ \text{order 2} \\
\text{H}_2\text{O} + \text{O} & \rightarrow \text{OH} + \text{OH} \quad \{ \text{order 3} \\
\text{H}_2\text{O} + \text{M} & \rightarrow \text{H} + \text{OH} + \text{M} \quad \{ \text{order 4} \\
\end{align*}
\]

As can be seen in the reactions in Equation 3.9, \( \text{H}_2\text{O} \) is being destroyed by combining with \( \text{H} \) and \( \text{O} \).
Looking at Figures 3.19, 3.20, and 3.21 the mass fractions of H, O, and N can be seen. There are significant variations in the mass fractions for all these species in the region mentioned in the heat of reaction curves.

Clearly, Figure 3.19 shows that atomic hydrogen is being produced in the boundary layer. However, at approximately 0.00077 m above the flat plate there is a decrease in the H mass fraction. The explanation for this phenomenon can be seen by looking at the dominant reactions involved with H.
Figure 3.20: Mass fraction of O at 60 cm transversal cut, $T_W = 700$ K

H, Mach 13, $y = 0.00077$ m:

$$
\begin{array}{l}
H_2O + H \rightarrow OH + H_2 \quad \text{order 2} \\
OH + O \rightarrow H + O_2 \quad \text{order 3} \\
H_2O + M \rightarrow H + OH + M \\
HO_2 + M \rightarrow H + O_2 + M \quad \text{order 4}
\end{array}
$$

(3.10)

As expected from the previous results, H is combining with $H_2O$. This would account for the decrease in the mass fraction of H in the region approximately 0.00077 m above the flat plate.

Also, Figure 3.20 shows that atomic oxygen is being produced in the same region as the decrease in atomic hydrogen. However, as the Mach number is increased, the mass fraction of atomic oxygen increase appears to be localized to only the hottest part of the flow (see Figure 3.22). Looking at the dominant reactions involved with O, the reason for the increase in O in the hottest part of the flow is shown.

O, Mach 13, $y = 0.00077$ m:

$$
\begin{array}{l}
O_2 + M \rightarrow O + O + M \quad \text{order 2} \\
O + H_2O \rightarrow OH + OH \\
H + O_2 \rightarrow OH + O \quad \text{order 3}
\end{array}
$$

(3.11)

Although for the most part O is being formed by the interaction with a third body, to a smaller extent, O is reacting with $H_2O$ to form OH. This latter result was indicated in the
dominant H₂O reactions as well.

Looking at Figure 3.21 it can be seen that nitrogen dissociation does not become apparent except at higher Mach numbers (e.g., Mach 13). Also, the location of N production appears to be confined to the hottest part of the flow. Looking at the dominant reactions involved with N.

N, Mach 13, y = 0.00077 m:

\[
\begin{align*}
N₂ + O &\rightarrow N + NO \quad \text{order 5} \\
N + OH &\rightarrow NO + H \\
N + O₂ &\rightarrow NO + O \quad \text{order 6}
\end{align*}
\]

The most dominant reaction has N₂ combining with O to form N and NO. Interesting that the mass fraction of O is decreasing as a result of the formation of N. The production of both O and N are confined to the hottest part of the flow. It is hypothesized that for larger Mach numbers than the range currently studied, the formation of N could be achieved increasingly at the detriment of O.

Referring to Figure 3.22, the temperature profiles can be seen for the Mach inflow numbers of 7 to 13 at the 60 cm transversal section. It appears from the results presented so far that the formation of the dissociated species H, O, and N appear to be confined to a specific temperature range. The formation of H seems prevalent in the 1000 to 2500 K range. Also, the formation of O doesn't seem to become important until temperatures reach above approximately 2500 K. The formation of N also doesn't seem to be involved until
temperatures reach over approximately 3000 K.

The above results give a good indication as to what the effects of increasing the Mach number has on the ignition process. However, an examination of the mass fractions of some of the more important species depicted in a two dimensional representation better relay the general trends.

The shading in the 2-D mass fraction profiles can be interpreted as such. The darker shades in the boundary layer indicate a higher mass fraction of the particular species. The
Figure 3.24: 2-D profile of H$_2$O mass fraction at 60 cm transversal cut. Mach 10

near free stream shading outside of the boundary layer appears simply as black.

Figures 3.23, 3.24, and 3.25 show how the H$_2$O mass fraction profile changes as the inflow Mach number is increased. At an inflow Mach number of 7, Figure 3.23 depicts combustion taking place at approximately 20 cm down the flat plate. This phenomenon can be seen by the sharp increase in the mass fraction of H$_2$O. The mass fraction profile for this Mach number is fairly steady. A large H$_2$O mass fraction near the wall and steadily decreasing as it approaches free stream values. However, one region of note is between about 50 cm and 70 cm down the flat plate. The mass fraction profile can be seen to skew a little at a distance of about 0.0013 m above the flat plate at this plate region.

Figures 3.24 and 3.25 show the phenomenon mentioned in the Mach 7 case, but now for a Mach number of 10 and 13. The small perturbation seen in Figure 3.23 appears to be more developed for these higher Mach number flow. Clearly seen in these Mach number 10 and 13 cases, the mass fraction of H$_2$O appears to be decreasing in the hottest part of the flow. The explanation for this can be seen in Equation 3.9, which are the dominant reactions involved in the species production term for H$_2$O. Recalling that the reactions are taken for the flow region 60 cm down the flat plate at about 0.0032 m above the flat plate. The net effect of these equations shows that H$_2$O is being destroyed in large quantities and OH and to a lesser extent H$_2$ are being created from this H$_2$O destruction.

The mass fraction profile of OH can be seen in Figure 3.26. The mass fraction of OH can be seen to be the largest down a thin strip restricted to the hottest part of the flow. For completion, this region is approximately where the H$_2$O mass fraction decreases in the Mach 13 case.
Figure 3.25: 2-D profile of H$_2$O mass fraction at 60 cm transversal cut, Mach 13

Figure 3.26: 2-D profile of OH mass fraction at 60 cm transversal cut, Mach 13
Figure 3.27: 2-D profile of H mass fraction at 60 cm transversal cut, Mach 7

Figure 3.28: 2-D profile of H mass fraction at 60 cm transversal cut, Mach 10
Figures 3.27, 3.28, and 3.29 show the mass fraction profile for atomic hydrogen (H) in the same region as the mass fractions of H₂O profiles were. In all the H profiles, it can be seen that the mass fraction of H is greatest near the wall and at the outer edge of the boundary layer. In the hottest part of the flow there is a noticeable decrease in the mass fraction of H. This decreased region coincides with the H₂O mass fraction decrease. These results agree with the dominating reactions involved with the species production term seen in Equation 3.10 for H. The reactions show that there is a net decrease in H, and H₂O, and a net increase in OH, and H₂.

Figures 3.30, 3.31, and 3.32 show the mass fraction profiles for atomic oxygen (O). As indicated in Figure 3.20, as the inflow Mach number increases, the region of the largest O mass fraction is localized to the hottest part of the flow. The dominating reactions of the species production term for O in Equation 3.11 show that atomic oxygen and H₂O are being created at the expense of O₂ and H₂O.

To summarize, when a H₂/air mixture flows over a flat plate at hypersonic velocities, combustion will usually occur and increase the heat generated within the flow compared to viscous dissipation alone. However, as the inflow Mach number is increased and temperatures in the boundary layer reach values higher than the adiabatic flame temperature of the fuel (i.e., H₂) the presence of the H₂ in the flow will result in endothermic reactions. In fact, these endothermic reactions will eventually result in less heat being produced in the boundary layer compared to that of a chemically frozen flow.
Figure 3.30: 2-D profile of O mass fraction at 60 cm transversal cut. Mach 7

Figure 3.31: 2-D profile of O mass fraction at 60 cm transversal cut, Mach 10
Figure 3.32: 2-D profile of O mass fraction at 60 cm transversal cut, Mach 13

Figure 3.33: Heat of reaction at 60 cm transversal cut, Mach 10

**Constant Mach Number**

By keeping a constant inflow Mach number it is possible to see the direct effect that the wall temperature has on the heat generated in the flow due to the combustion and viscous effects. Simulations with a constant Mach number of 10 are compared as the wall temperature is increased for each case. Figure 3.33 shows the heat of reaction taken at 60 cm down the flat plate. As can be seen, it appears that wall temperature has only a small effect on the heat
Figure 3.34: Mass fraction of H\textsubscript{2}O at 60 cm transversal cut, Mach 10

Figure 3.35: Mass fraction of H at 60 cm transversal cut, Mach 10

generated within the flow. Only for regions near the wall does h\textsubscript{PR} vary to any degree.

Figures 3.34, 3.35, and 3.36 are the mass fractions of H\textsubscript{2}O, H, and O respectively, at the same 60 cm cut that the heat of reaction is taken at. As can be seen, the mass fractions do not vary greatly when the wall temperature is increased. Essentially, by increasing the wall temperature the temperature of the flow itself increases only slightly. This results can be seen in Figure 3.37. A 700 K increase in wall temperature results in only a approximately 300 K increase at the hottest part of the flow.
Figure 3.36: Mass fraction of O at 60 cm transversal cut, Mach 10

Figure 3.37: Temperature at 60 cm transversal cut, Mach 10
Figure 3.38: Heat of reaction at 60 cm transversal cut, $T_W = 300$ K. Mach 10

**Constant Wall Temperature and Mach Number**

As mentioned in Section 1.3, it is unlikely that if fuel is injected into the flow (e.g., in a scramjet inlet) that a uniform fuel/air distribution will exist throughout the entire flow domain. Also, it might be beneficial to purposely use an equivalence ratio different from a stoichiometric value. Therefore, it is important to study the heat generation in a non-stoichiometric fuel/air environment and compare it to a stoichiometric scenario.

Figure 3.38 depicts the heat of reaction for three different equivalence ratios. For all three cases the inflow Mach number is 10 and the wall temperature is 300 K. As expected, the greatest heat released is in the stoichiometric case. Also, for most of the boundary layer the fuel-rich case has a greater heat of reaction value than the fuel-lean case.

Recall in the subsection, “Constant Wall Temperature” it is noted that near the edge of the boundary layer the heat of reaction values is slightly negative. Figure 3.38 in conjunction with figure 3.40 shows more clearly the effect that the presence of H in the flow has on the heat of reaction calculations. In the region in question (approximately $y = 0.003-0.005$ m) the mass fraction of H increases with the equivalence ratio. This fact is played out in the heat of reaction graph. The curve that goes the most negative is the fuel-rich one, and conversely the curve that goes the least negative is the fuel-lean curve.

The mass fraction of $H_2O$ at the 60 cm cut for the three equivalence ratios can be seen in Figure 3.39. The slopes of the curves start to reach a local maximum at about 0.002 m and a local minimum at about 0.001 m. Further, as the equivalence ratio increases the local minimum correspondingly decreases. An analysis of the dominant reaction in these two
regions is required to determine the cause of these extrema points.

Referring to the fuel-rich curve (i.e., $\phi = 2$), and comparing the species production terms at the points $y = 0.002$ m and $y = 0.001$ m above the flat plate. At $y = 0.002$ m, $w_{H_2O} = 24.69$ kg/s, and at $y = 0.001$ m, $w_{H_2O} = -5.13$ kg/s. The dominant reactions are as follows: $H_2O$, $\phi = 2$, $y = 0.002$ m:

\[
\begin{align*}
OH + H_2 &\rightarrow H_2O + H \quad \text{order 2} \\
H_2O + O &\rightarrow OH + OH \\
H + OH + M &\rightarrow H_2O + M
\end{align*}
\]

(3.13)

$H_2O$, $\phi = 2$, $y = 0.001$ m:

\[
\begin{align*}
H_2O + H &\rightarrow OH + H_2 \quad \text{order 3} \\
H + OH + M &\rightarrow H_2O + M \quad \text{order 5}
\end{align*}
\]

(3.14)

Note that in the $y = 0.001$ m point of the curve the drastic reduction in the $H_2O$ species production term is due to the reaction of $H_2O$ with $H$. The hottest part of the flow is approximately in this $y = 0.001$ m region, and as will be shown shortly, this region has a great deal of dissociated hydrogen. The presence of excess hydrogen in a fuel-rich mixture increases the $H_2O$ destruction. In the $y = 0.001$ m region the species production term goes from $w_{H_2O} = -0.136$ kg/s in the fuel-lean mixture, $w_{H_2O} = -4.83$ kg/s for the stoichiometric case, and $w_{H_2O} = -5.13$ kg/s in the fuel-rich mixture. The reaction $H_2O + H \rightarrow OH + H_2$ increases in importance as the equivalence ratio increases.
Figure 3.40: Mass fraction of H at 60 cm transversal cut, $T_W = 300$ K. Mach 10

Figure 3.40 shows that there is a large increase in the mass fraction of H at $y = 0.002$ m in the $\phi = 2$ curve compared to the other two curves. This result can be accounted for due to the initially high H$_2$ mass fraction. Since not all of the H$_2$ will react with O$_2$, the excess H$_2$ will dissociate at elevated temperatures like those seen in the boundary layer. The dominant reactions involved in the production of H are as follows:

\begin{align*}
OH + H_2 &\rightarrow H_2O + H \quad \text{order 2} \\
O + H_2 &\rightarrow OH + H \\
H + O_2 &\rightarrow OH + O \quad \text{order 3}
\end{align*}

A 2-D profile of the mass fraction of H can be seen in Figure 3.41 for the $\phi = 2$ case. The decrease in the mass fraction of H near the wall agrees with the results in Figure 3.40.

Figure 3.42 shows the mass fraction of O for the 60 cm transversal cut for the three different equivalence ratios. The most prominent feature of this graph is that for the $\phi = 2$ case the mass fraction of O decreases significantly at about $y = 0.002$ m, then increases again to a local maximum at about $y = 0.002$ m. At the $y = 0.002$ m section O is being destroyed, and then being created closer to the wall. To confirm this statement, the species production term for O is $w_{H_2O} = -2.52$ kg/s at $y = 0.002$ m, and $w_{H_2O} = 0.85$ kg/s at $y = 0.001$ m. The dominant reactions for these two regions are as follows:
Figure 3.41: 2-D profile of H mass fraction at 60 cm transversal cut. Mach 10, $T_W = 300$ K

Figure 3.42: Mass fraction of O at 60 cm transversal cut, $T_W = 300$ K, Mach 10
Figure 3.43: Heat of reaction at 60 cm and 90 cm transversal cut, $T_W = 700$ K

O, $\phi = 2$, $y = 0.002$ m:

\[
\begin{align*}
O + H_2 &\rightarrow OH + H \\
H + O_2 &\rightarrow OH + O \\
O + H_2O &\rightarrow OH + OH
\end{align*}
\]

order 3

(3.16)

O, $\phi = 2$, $y = 0.001$ m:

\[
\begin{align*}
OH + H &\rightarrow O + H_2 \\
O + O + M &\rightarrow O_2 + M \\
H + O_2 &\rightarrow OH + O
\end{align*}
\]

order 4

(3.17)

At the $y = 0.002$ m region O is largely combining with H$_2$ and to a smaller extent H$_2$O to form OH. This accounts for the destruction of O in this region. However, at $y = 0.001$ m OH is combining with H (which is in abundance in this region) to form O.

**Two Different Transversal Sections**

Up until now, a transversal cut was taken down the flat plate at one location. This transversal cut was then subsequently compared to cuts taken at the same location for different inflow and boundary conditions. However, the heat generated within the flow is not expected to be constant throughout the length of the flat plate. Therefore, it is useful to compare the heat of reaction at two different sections along the flat plate.

Figure 3.43 shows the heat of reaction taken at sections 60 cm and 90 cm down the
Figure 3.44: Mass fraction of H$_2$O at 60 cm and 90 cm transversal cut, T$_W$ = 700 K

flat plate. A Mach 7, 10, and 13 case with a wall temperature of 700 K are shown on the graph. The 90 cm curves return to free stream values higher above the flat plate because the boundary layer continues to grow as the flow travels down the flat plate. Self-similar solutions (i.e., changing coordinates to be independent of x location) are not possible to produce in these cases as the presence of combustion alters the boundary layer development. Earlier in this section (see subsection, "Constant Wall Temperature") an analysis was performed on the Mach 13, 60 cm transversal cut curve. Specifically, at a value 0.00077 m above the flat plate. For completion, this same case and approximate region will be compared to the Mach 13 case except now at a distance 90 cm down the flat plate.

Figure 3.44 depicts the mass fraction of H$_2$O for the same transversal cuts and cases as given in the heat of reaction graph. Looking at the Mach 13 curves in the region in question above the flat plate the species production terms for H$_2$O in the two transverse sections are $w_{H_2O} = -30.06$ kg/s and $w_{H_2O} = -19.75$ kg/s for the 60 and 90 cm cuts, respectively. The dominant reactions for the two cuts are as follows:

H$_2$O, Mach 13, 60 cm transv. cut:

\[
\begin{align*}
H_2O + H & \rightarrow OH + H_2 \quad \text{order 2} \\
H_2O + O & \rightarrow OH + OH \quad \text{order 3} \\
H_2O + M & \rightarrow H + OH + M \quad \text{order 4}
\end{align*}
\]  

(3.18)
As can be seen by the above reactions, the three most dominant reactions are the same for both transverse sections, but the order of the equations has shifted slightly. The three dominant reactions in the 90 cm cut are not as important as in the 60 cm case. These results account for the increase in the species production term for the 90 cm cut compared to the 60 cm cut as H$_2$O is not being destroyed with the same intensity.

Now examining the mass fraction of H (see Figure 3.45), it can be seen that the mass fraction is greater in the 60 cm cut compared to the 90 cm cut. The species production term for H bears this out as $w_H = -0.77$ kg/s and $w_H = -0.32$ kg/s at the 60 and 90 cm cuts, respectively. The dominant reactions for these two cuts are as follows:

**H$_2$O, Mach 13, 90 cm transv. cut:**

$$
\begin{align*}
    H_2O + H &\rightarrow OH + H_2 \\
    H_2O + O &\rightarrow OH + OH \\
    H_2O + M &\rightarrow H + OH + M
\end{align*}
$$

(order 3) \hfill (3.19)

(order 4)

As can be seen by the above reactions, the three most dominant reactions are the same for both transverse sections, but the order of the equations has shifted slightly. The three dominant reactions in the 90 cm cut are not as important as in the 60 cm case. These results account for the increase in the species production term for the 90 cm cut compared to the 60 cm cut as H$_2$O is not being destroyed with the same intensity.

Now examining the mass fraction of H (see Figure 3.45), it can be seen that the mass fraction is greater in the 60 cm cut compared to the 90 cm cut. The species production term for H bears this out as $w_H = -0.77$ kg/s and $w_H = -0.32$ kg/s at the 60 and 90 cm cuts, respectively. The dominant reactions for these two cuts are as follows:

**H, Mach 13, 60 cm transv. cut:**

$$
\begin{align*}
    H_2O + H &\rightarrow OH + H_2 \\
    OH + O &\rightarrow H + O_2 \\
    H_2O + M &\rightarrow H + OH + M \\
    HO_2 + M &\rightarrow H + O_2 + M
\end{align*}
$$

(order 2) \hfill (3.20)
Figure 3.46: Mass fraction of O at 60 cm and 90 cm transversal cut. $T_W = 700$ K

H, Mach13, 90 cm transv. cut:

$$
\begin{align*}
H_2O + H &\rightarrow OH + H_2 \\
OH + O &\rightarrow H + O_2 \\
O + H_2 &\rightarrow OH + H \\
H_2O + M &\rightarrow H + OH + M
\end{align*}
$$

The first two reactions are the same, however their orders differ. The changing order of the first reaction (which consumes H) accounts for the increase in the production of H for the 90 cm cut compared to the 60 cm cut.

Referring to Figure 3.46, the mass fraction of O can be seen for the two transversal cuts. Again, looking at the Mach 13 case in the region in question above the flat plate, it can be seen that there is a decrease in the mass fraction of O when comparing the 90 cm cut to the 60 cm cut. The species production term for O at the specified cuts are $w_O = 10.21$ kg/s and $w_O = 6.002$ kg/s at the 60 and 90 cm cuts, respectively. The dominant reactions involved with the production of O are as follows:

O, Mach 13, 60 cm transv. cut:

$$
\begin{align*}
O_2 + M &\rightarrow O + O + M \\
O + H_2O &\rightarrow OH + OH \\
H + O_2 &\rightarrow OH + O
\end{align*}
$$
O, Mach 13, 90 cm transv. cut:

\[
\begin{align*}
O_2 + M & \rightarrow O + O + M \ \{ \text{order 2} \} \\
OH + O & \rightarrow H + O_2 \\
H_2O + O & \rightarrow OH + OH \ \{ \text{order 3} \}
\end{align*}
\] (3.23)

Although the first reaction is the same for both the 60 and 90 cut, the second and third dominant reactions differ. Note that although the second reactions are different, O is consumed for both cases. However, only for the 90 cm cut does the third reaction consume O as opposed to create it as is the case for the 60 cm cut.
Chapter 4

Conclusion

4.1 Conclusions Drawn From Current Research Effort

Although a flat plate does not properly represent a typical supersonic inlet geometry, it is a useful first approximation. As mentioned previously, in any scramjet design it is almost a certainty that if fuel is injected into the flow from injectors along the inlet wall, viscous dissipation will ignite the fuel in the boundary layer.

In this current area of research, the phenomenon of ignition of fuel in the boundary layer has been studied over a wide Mach range. The Mach range studied is in excess of the total Mach range expected for a scramjet inlet to be subjected to. Therefore, for a simplified geometry (i.e., a flat plate) the phenomenon of ignition of fuel in boundary layers is better understood for a wider Mach range.

The following section is a summary of the results discussed in this research effort.

4.1.1 Heat Transfer to the Wall

Constant Wall Temperature

As the inflow Mach number was increased and an equal constant wall temperature used for all the Mach numbers plotted their heat transfer rates were compared. The heat transfer rate to the wall has been studied from the Mach range of 2 to as high as 17. Interestingly enough, for Mach numbers larger than about 9 or 10 the heat transfer rates along the flat plate do not vary greatly as the inflow Mach number was increased. The reason for this lack of variation in heat transfer rate is because as the inflow Mach number is increased endothermic reactions become more dominant. Once the adiabatic flame temperature is exceeded in the flow, the flow becomes increasingly endothermic. These endothermic reactions result in less heat being produced compared to a chemically frozen scenario. Also, for inflow velocities within the Mach range of 10 or higher no clear induction length is seen. This is because ignition takes
place within the stagnation region at the leading edge. However, for lower Mach numbers, the induction length can clearly be seen by a sharp increase in the heat transfer rate. In general, this sharp increase in the heat transfer rate decreases in intensity as the inflow Mach number increases.

**Constant Mach Number**

Constant inflow Mach number and varying constant wall temperature simulations were plotted against each other. In general, a higher wall temperature will result in a shorter induction length. Since the heat transfer rate increases when combustion occurs, the comparison of heat transfer rates with reference to different wall temperature is dependent on whether combustion occurs for a particular wall temperature. Also, when comparing two or more wall temperatures in which combustion does occur along the domain of the flat plate studied, the sharp heat transfer rate increase seen as combustion occurs decreases with increasing wall temperature. The reason for this decreased in the heat transfer rate is that since the wall temperature is held constant for each case, when combustion does occur and a heat increase is realized as the wall temperature approaches the combustion temperature, a smaller temperature differential (between the wall temperature and the combustion temperature) is seen which will result in a smaller heat transfer rate increase.

**Constant Wall Temperature and Mach Number**

The heat transfer rates for simulations in which the inflow Mach number and wall temperature are held constant and the equivalence ratio is varied were compared. The fuel-lean mixtures had shorter induction lengths and smaller heat transfer rate increases seen at the onset of combustion compared to the stoichiometric and the fuel-rich mixtures. Also, the fuel-rich mixture had a larger induction length compared to the stoichiometric mixture.

**4.1.2 Heat Generation Within the Flow**

**Constant Wall Temperature**

As the inflow Mach number increases the heat generated within the flow increases as well. However, as temperatures within the boundary layer increase to values above the adiabatic flame temperature of the fuel (H₂), endothermic reactions result in a decreases in the heat generated within certain parts of the boundary layer instead of an expected increase even as the inflow Mach number is raised. This is an interesting result as the presence of the fuel in the flow will at first increase the heat generated within the flow for one Mach regime,
however the fuel will actually decrease the heat generated within the flow in another Mach regime compared to a chemically frozen flow.

Constant Mach Number

For this analysis the heat generated within the flow was performed for a constant Mach number comparing the effect of varying the constant wall temperature. By increasing the wall temperature only minor heat generation changes are seen in the boundary layer. Most of these changes are seen close to the wall.

Constant Wall Temperature and Mach Number

A comparison on the heat generated within the flow with different equivalence ratios was performed. As expected, the stoichiometric case produced the largest amount of heat. However, for the fuel-rich case, the excess H\textsubscript{2} absorbed a significant amount of heat by dissociating into atomic hydrogen (H). The presence of this excess H staved off the destruction of H\textsubscript{2}O in the hottest part of the flow.

Two Different Transversal Sections

The heat generated within the flow is not constant along the flat plate. An analysis of the heat generated at 60 cm and 90 cm down the flat plate was performed. It can be concluded that once combustion has occurred in the boundary layer, the heat generated within the boundary layer will increase in the downstream direction.

4.2 Possible Future Work and Recommendations

For all of the simulations performed for this current area of research a constant wall temperature condition was imposed. This constant wall temperature assumption more closely simulates a real scramjet inlet thermal protection system compared to an adiabatic wall assumption. However, an equally or perhaps more valid wall condition could be a constant heat flux requirement. It is hypothesized that the main difference in the results of this constant heat flux boundary condition would be that the induction lengths for similar inflow conditions would be smaller compared to a constant wall temperature condition. The reason for this expected result is that, with the exception of a overly optimistic heat flux requirement, the stagnation region near the leading edge will most likely experience larger temperature values. With these larger temperatures the induction length should be smaller. This result was seen when for the constant wall temperature cases, as the wall temperature was increased for the same Mach number, the subsequent induction lengths decreased.
Another proposed future investigation might be adding turbulence terms to the governing equations. For all the simulations in this current research effort only laminar flow was considered. Although in a real scramjet inlet, turbulent flow conditions would most likely be present, but for a flat plate geometry only quantitative changes are expected by adding a turbulence model to the solution.
Bibliography


