Abstract

KEISLTER, PATRICK G. Simulation of Supersonic Combustion Using Variable Turbulent Prandtl/Schmidt Numbers Formulation. (Under the direction of Dr. Hassan A. Hassan.)

A turbulence model that allows for the calculation of the variable turbulent Prandtl ($\text{Pr}_t$) and Schmidt ($\text{Sc}_t$) numbers as part of the solution is presented. The model also accounts for the interactions between turbulence and chemistry by modeling the corresponding terms. Four equations are added to the baseline $k-\zeta$ turbulence model: two equations for enthalpy variance and its dissipation rate to calculate the turbulent diffusivity, and two equations for the concentrations variance and its dissipation rate to calculate the turbulent diffusion coefficient. The variable $\text{Pr}_t/\text{Sc}_t$ turbulence model is used to simulate the SCHOLAR supersonic combustion experiments. The experiments include one model with normal hydrogen injection into a vitiated airstream at Mach 2.0, while the other injects hydrogen at Mach 2.5 and an angle of 30° to the vitiated airstream. Two sets of calculations are presented for each experiment, one where the turbulent Prandtl and Schmidt numbers are constant and one where they are allowed to vary. Two chemical kinetic models are employed for each calculation: a seven species/seven reaction model where the reaction rates are temperature dependent and a nine species/nineteen reaction model where the reaction rates are dependent on both pressure and temperature.

The simulation of the vectored injection experiment predicts an earlier ignition than what is suggested by the experimental data. Also, the downstream pressure is underpredicted. The temperature distribution in the downstream portion of the combustor is higher with the variable $\text{Pr}_t/\text{Sc}_t$ model than with the constant model, which places it within the experimental scatter. When the computed temperature profiles are subjected to the same curve fit as the experimental scatter, very good agreement is observed. The simulation of the normal injection experiment showed similar results, with underprediction of downstream pressures and less overall combustion. However, the variable $\text{Pr}_t/\text{Sc}_t$ model does show improved results over the constant model. The variable
model shows a complex shock-boundary layer interaction that extends upstream of the backward facing step. The pressure distribution along the bottom wall is very closely matched in this region, but downstream, the pressures are still underpredicted. A pressure “plateau” effect that is seen in the experimental data suggests that an area of large separation or intense combustion exists in the region immediately below the hydrogen injector. This is not reproduced in any of the simulations. In general the two chemical kinetic mechanisms provide nearly identical results. Finally, it is shown that the computed results are highly dependent on the compressibility correction for the turbulence model. When this term is neglected, unstart conditions result for both the vectored injection experiment and the normal injection experiment.
Simulation of Supersonic Combustion Using Variable Turbulent Prandtl / Schmidt Numbers Formulation

by

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Approved by:

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Biography

Patrick Garrett Keistler was born in Concord, North Carolina on May 1st, 1982. One of the major influences on his educational choices was his participation in the Air Force Junior ROTC at Central Cabarrus High School. During this time his interest in aviation was sparked. With this and an interest in physics and mathematics, the obvious choice was to study aerospace engineering at North Carolina State University. It was not until his senior year that an interest in computational fluid dynamics developed, but that was enough time to decide that it was what he wanted to pursue. Patrick plans to continue his education in the pursuit of a Ph.D. at NC State.
**Acknowledgements**

There are a number of people I would like to thank for their support through the course of this work. First is my thesis advisor Dr. Hassan A. Hassan, who has taught me many valuable lessons, and provided excellent guidance. Another individual who has been an invaluable source of information and assistance is Dr. Xudong Xiao. I would not be to this point without his expertise and knowledge. Also, I would like to thank my parents, Max and Kristy Keistler for their continued motivation and support throughout my college career. The interest they show in my work is very encouraging. Finally, I would like to thank Mr. George Rumford, the program manager of the Defense Test Resource Management Center’s Test and Evaluation/Science and Technology program for funding this effort under the Hypersonic Test focus area.
Table of Contents

List of Figures .................................................................................................................... vi
List of Tables .................................................................................................................... viii
List of Symbols ................................................................................................................ ix
1 Introduction .................................................................................................................. 1
2 Governing Equations .................................................................................................. 5
  2.1 Reacting Gas Equation Set ..................................................................................... 5
    2.1.1 Navier-Stokes Equations ............................................................................. 5
    2.1.2 Thermodynamic Relations .......................................................................... 7
  2.2 Governing Equations in Vector Form ..................................................................... 8
  2.3 Reynolds and Favre Averaging .............................................................................. 9
2.4 Chemical Kinetics .................................................................................................... 11
  2.4.1 Jachimowski Chemical Mechanism .............................................................. 13
  2.4.2 Connaire et al. Chemical Mechanism ............................................................ 13
  2.5 Turbulence Closure .............................................................................................. 15
    2.5.1 k-ζ Model .................................................................................................. 16
    2.5.2 Variable Turbulent Prandtl Number Model ............................................... 19
    2.5.3 Variable Turbulent Schmidt Number Model .............................................. 22
    2.5.4 Turbulence / Chemistry Interactions ......................................................... 25
  2.6 Complete Equation Set ......................................................................................... 26
    2.6.1 Solution Methods ...................................................................................... 26
3 Experimental Overview ............................................................................................... 27
  3.1 The SCHOLAR Experiments ............................................................................... 27
    3.1.1 Vectored Injection Case ............................................................................... 28
    3.1.2 Normal Injection Case ................................................................................ 30
  3.2 CARS Measurement Techniques .......................................................................... 32
  3.3 Experimental Data Fitting .................................................................................... 33
4 Implementation ........................................................................................................... 35
  4.1 Multiblock Parallel Approach .............................................................................. 35
4.2 Computational Geometry ................................................................. 35
4.3 Wall and Inlet Boundary Conditions .................................................. 39
  4.3.1 Wall Boundaries ........................................................................ 39
  4.3.2 Inflow and Outflow Boundaries .................................................. 41
5 Results and Discussion ........................................................................ 42
  5.1 General Results ............................................................................. 42
  5.2 Vectored Injection Model ............................................................... 47
    5.2.1 Variable Prt / Sc Run .............................................................. 47
    5.2.2 Constant Prt / Sc Run .............................................................. 56
  5.3 Normal Injection Model ................................................................. 60
    5.3.1 Constant Prt / Sc Run .............................................................. 61
    5.3.2 Variable Prt / Sc Run .............................................................. 64
6 Conclusions ....................................................................................... 71
References ............................................................................................ 73
Appendix A: Governing Equations Vectors ............................................ 78
Appendix B: Transformation to Generalized Coordinates ....................... 80
Appendix C: Chemical Kinetic Mechanism Parameters ........................... 84
Appendix D: Complete Equation Set in Vector Form ............................... 88
Appendix E: Numerical Formulation ...................................................... 92
List of Figures

Figure 3.1: Schematic of Vectored Injection SCHOLAR Experiment ........................................ 28
Figure 3.2: Detail of Vectored Hydrogen Injector ..................................................................... 29
Figure 3.3: Schematic of Normal Injection SCHOLAR Experiment .......................................... 30
Figure 3.4: Detail of Normal Hydrogen Injector ....................................................................... 31
Figure 3.5: Example of CARS Measurements and Curve Fit (Plane 6, y = 18.2 mm) .......... 34
Figure 4.1: Block Layout and H₂ Injector Detail for Vectored Injection ................................. 36
Figure 4.2: Vectored Block Layout with CARS Survey Planes Highlighted ............................. 37
Figure 4.3: Block Layout and H₂ Injector Detail for Normal Injection .................................... 38
Figure 5.1: Pitot Pressure Profile at Vitiated Air Nozzle Exit ..................................................... 44
Figure 5.2: Temperature Slice with Adiabatic Wall Temperature ............................................. 45
Figure 5.3: Wall Temperature vs. Run Time at Three Locations (Ref [11]) .............................. 46
Figure 5.4: Temperature Slice of Plane 6 at y = 18.2 mm (Connaire) ........................................ 48
Figure 5.5: Mole Fraction Slices of Plane 6 at y = 18.2 mm (Connaire) ................................. 49
Figure 5.6: 5th Degree Polynomial Fits of Exp. and Computed Temperature (Run 1) .......... 50
Figure 5.7: 5th Degree Polynomial Fits of Exp. and Computed Mole Fractions (Run 1) .... 50
Figure 5.8: Experimental Surface Fits of Temperature for Vectored Case ............................. 51
Figure 5.9: Temperature Contours for Run 1 ............................................................................ 52
Figure 5.10: Nitrogen and Oxygen Mole Fractions for Run 1 .................................................. 52
Figure 5.11: Temperature from Runs 1 and 2 (Left: Jach., Right: Connaire) ......................... 53
Figure 5.12: Wall Pressures for Runs 1 and 2 ......................................................................... 54
Figure 5.13: OH Mole Fractions for Runs 1 and 2 (Left: Connaire, Right: Jach.) ............... 55
Figure 5.14: Turbulent Prandtl Number (left) and Turbulent Schmidt Number (right) ....... 56
Figure 5.15: Temperature Contours for Run 3 ........................................................................ 57
Figure 5.16: Nitrogen and Oxygen Mole Fractions for Run 3 ................................................ 58
Figure 5.17: Temperature from Runs 3 and 4 (Left: Jach., Right: Connaire) ....................... 59
Figure 5.18: Wall Pressures for Runs 3 and 4 ....................................................................... 60
Figure 5.19: Temperature Contours for Run 5 ..................................................................... 61
Figure 5.20: Mole Fraction Contours for Run 5 (left: N₂, right: O₂) ........................................ 62
Figure 5.21: Bottom Wall Pressure for Run 5 ........................................................................ 63
Figure 5.22: Temperature Contours for Run 6 ..................................................................... 64
Figure 5.23: Mach Contours on Symmetry Plane for Run 6 .................................................. 65
Figure 5.24: Mach Contours on Symmetry Plane for Run 5 .................................................. 66
Figure 5.25: Mole Fraction Contours for Run 6 (left: N₂, right: O₂) ................................... 67
Figure 5.26: Bottom Wall Pressure for Runs 5 and 6 .............................................................. 67
Figure 5.27: 3D Hydrogen Mole Fraction Contours for Run 6 ................................................ 68
Figure 5.28: Stream Traces Originating in Hydrogen Injector ................................................. 69
Figure 5.29: Mach Number Contours on Symmetry Plane for Unstart Conditions .......... 70
List of Tables

Table 2.1: Troe Parameters for Connaire et al. Mechanism .................................................. 15
Table 2.2: $k$-$\zeta$ Model Closure Coefficients ........................................................................ 19
Table 2.3: Variable Prandtl Number Model Constants .......................................................... 22
Table 2.4: Variable Schmidt Number Model Constants ....................................................... 25
Table 3.1: Inflow Conditions for Vectored Injection ............................................................... 30
Table 3.2: Inflow Conditions for Normal Injection ................................................................. 32
Table 5.1: Runs Presented ..................................................................................................... 47
Table C.1: Abridged Jachimowski Mechanism Reactions ..................................................... 84
Table C.2: Abridged Jachimowski Mechanism Parameters .................................................. 84
Table C.3: Connaire et al. Mechanism Reactions ................................................................. 85
Table C.4: Connaire et al. Mechanism Parameters ............................................................... 86
Table C.5: Connaire et al. Mechanism Third Body Efficiencies ............................................ 87
List of Symbols

Roman Symbols:

- \( A \) Pre-exponential factor / face area
- \( A - G \) Euler Implicit matrix coefficients
- \( a \) Speed of sound
- \( a, T^*, T^{**}, T^{***} \) Fall-off reaction rate constants
- \( a_{1,m} - b_{1,m} \) Thermodynamic curve fit coefficients
- \( C_h - \beta_h \) Variable Prandtl number model constants
- \( C_m \) Species concentration
- \( C_{mix} \) Mixture concentration
- \( C_p \) Specific heat ratio at constant pressure
- \( C_{p,mix} \) Mixture specific heat ratio at constant pressure
- \( C_Y - \beta_Y \) Variable Schmidt number model constants
- \( C_{\mu} - C_{\zeta} \) \( k - \zeta \) model closure coefficients
- \( D \) Binary diffusion coefficient
- \( D_i \) Turbulent diffusion coefficient
- \( E \) Total energy
- \( E_a \) Activation energy
- \( \vec{E}, \vec{F}, \vec{G} \) \( x, y, \) and \( z \) direction inviscid fluxes
- \( \hat{E}, \hat{F}, \hat{G} \) \( \zeta, \eta, \) and \( \zeta \) direction inviscid fluxes
- \( \bar{E}, \bar{F}, \bar{G} \) Average interface fluxes
- \( \vec{E}_v, \vec{F}_v, \vec{G}_v \) \( x, y, \) and \( z \) direction viscous fluxes
- \( \hat{E}_v, \hat{F}_v, \hat{G}_v \) \( \zeta, \eta, \) and \( \zeta \) direction viscous fluxes
- \( e_m \) Species internal energy
- \( e_{mix} \) Mixture internal energy
- \( F \) Fall-off reaction rate function
- \( \vec{F} \) Flux vector
- \( \hat{g} \) Gibbs free energy per mole
- \( H \) Total enthalpy
- \( h^2 \) Enthalpy variance
- \( \Delta h_{f,m} \) Species heat of formation
- \( h_m \) Species enthalpy
- \( \hat{h}_m \) Species enthalpy per mole
- \( h_{mix} \) Mixture enthalpy
- \( J \) Transformation Jacobian
- \( k \) Thermal conductivity / turbulent kinetic energy
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$k_0$</td>
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</tr>
<tr>
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<td>Backward reaction rate coefficient</td>
</tr>
<tr>
<td>$k_{eq</td>
<td>C}$</td>
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<tr>
<td>$k_{eq</td>
<td>P}$</td>
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<td>$k_m$</td>
<td>Species thermal conductivity</td>
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<td>$k_{sc}$</td>
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<td>$M$</td>
<td>Mach number</td>
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<td>$M_i$</td>
<td>Turbulent Mach number</td>
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<td>$m,m$</td>
<td>Forward and backward reaction order</td>
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<td>$\hat{n}_{x_i}$</td>
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<td>Species partial pressure</td>
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<td>$p_r$</td>
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<td>$q_j$</td>
<td>Heat flux vector</td>
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<td>$\mathbf{R}$</td>
<td>Residual vector</td>
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<td>$\hat{\mathbf{R}}$</td>
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<td>$R_{mix}$</td>
<td>Mixture gas constant</td>
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<tr>
<td>$RR_i$</td>
<td>Reaction rate</td>
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<td>$r^{±}$</td>
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<td>Source vector</td>
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<td>Schmidt number</td>
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<td>$\text{Sc}_t$</td>
<td>Turbulent Schmidt number</td>
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<tr>
<td>$s_{ij}$</td>
<td>Instantaneous strain rate tensor</td>
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<tr>
<td>$T$</td>
<td>Temperature</td>
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<tr>
<td>$T_{ij}$</td>
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<tr>
<td>$TB_{m,j}$</td>
<td>Species third body efficiency</td>
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<tr>
<td>$Tu$</td>
<td>Turbulence intensity</td>
</tr>
<tr>
<td>$t$</td>
<td>Time</td>
</tr>
<tr>
<td>$\mathbf{U},\dot{\mathbf{U}}$</td>
<td>Conservative variable vector</td>
</tr>
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<td>$\mathbf{U}_c,\mathbf{\bar{V}}_c,\mathbf{\bar{W}}_c$</td>
<td>Contravariant velocities</td>
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<tr>
<td>$\mathbf{U}_m,\mathbf{\bar{V}}_m,\mathbf{\bar{W}}_m$</td>
<td>Species contravariant velocities</td>
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<tr>
<td>$u_i$</td>
<td>Cartesian velocity in index notation</td>
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<tr>
<td>$u,v,w$</td>
<td>Cartesian velocity components</td>
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<td>$\mathbf{\nu}$</td>
<td>Cell volume</td>
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<td>$V_{m,j}$</td>
<td>Species diffusion velocity in index notation</td>
</tr>
<tr>
<td>$\hat{\mathbf{W}}_m$</td>
<td>Species molecular weight</td>
</tr>
<tr>
<td>$x,y,z$</td>
<td>Cartesian coordinates</td>
</tr>
<tr>
<td>$x_i$</td>
<td>Cartesian coordinates in index notation</td>
</tr>
</tbody>
</table>
\[ \sim \]
\[ Y^{**2} \quad \text{Mass fraction variance} \]
\[ Y_m \quad \text{Species mass fraction} \]
\[ Y_{m,j} \quad \text{Turbulent species diffusion vector} \]

Greek Symbols:

- \( \alpha \): Thermal diffusivity
- \( \alpha_t \): Turbulent thermal diffusivity
- \( \Delta \): Different operator
- \( \delta_{ij} \): Kronecker delta
- \( \varepsilon_h \): Dissipation rate of enthalpy variance
- \( \varepsilon_{ijk} \): Permutation tensor
- \( \varepsilon_Y \): Dissipation rate of \( \sigma_Y \)
- \( \gamma_{mix} \): Mixture specific heat ratio
- \( \eta \): Temperature exponent
- \( \kappa \): Parameter used in kappa scheme
- \( \mu \): Molecular viscosity
- \( \mu_m \): Species molecular viscosity
- \( \mu_t \): Turbulent viscosity
- \( \nu \): Kinematic viscosity
- \( \nu_t \): Turbulent kinematic (eddy) viscosity
- \( \nu_{m,i}, \nu_{m,i}'' \): Species reactant and product stoichiometric coefficients
- \( \theta_d \): Activation temperature
- \( \rho \): Density
- \( \rho_m \): Species density
- \( \sigma \): System spectral radius
- \( \sigma_Y \): Sum of mass fraction variances
- \( \tau_{ij} \): Laminar stress tensor
- \( \omega_i \): Vorticity vector
- \( \omega_m \): Species production rate
- \( \xi, \eta, \zeta \): Generalized Coordinate Directions
- \( \xi_{x_i}, \eta_{x_i}, \zeta_{x_i} \): Metric derivatives in index notation
- \( \psi \): Limiter function
- \( \zeta \): Vorticity variance (enstrophy)

Subscripts:

- \( b \): Backward
- \( C \): Contravariant
- \( CV \): Control volume
- \( E \): Edwards (LDFSS)
- \( eq \): Equilibrium
- \( f \): Forward
$i,j,k$ Grid indices / index notation
$i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}$ Cell faces
$L$ Left
$m$ Species
$mix$ Mixture property
$NS$ Number of species
$R$ Right
$t$ Turbulent
$V$ Viscous
$VL$ van Leer
$w$ Wall
$\infty$ Freestream

Superscripts:

$C$ Convective
$I$ Inviscid
$n$ Time step
$P$ Pressure

Accents:

$-$ Reynolds averaged
$\sim$ Favre averaged / average interface flux
$\wedge$ Per mole
$.$ Time rate of change
$'$ Reynolds fluctuation / reactants
$''$ Favre fluctuation / products

Abbreviations:

CARS Coherent anti-Stokes spectroscopy
CFD Computational Fluid Dynamics
CFL Courant Freidrichs and Lewy
DNS Direct numerical simulation
ENO Essentially non-oscillatory
ILU Incomplete Lower Upper
LDFSS Low diffusion flux splitting scheme
LES Large eddy simulation
MPI Message Passing Interface
PDF Probability density function
RANS Reynolds averaged Navier-Stokes
TVD Total variation diminishing
mmd Minmod
Other symbols:

\[ \partial \] Partial derivative
\[ \nabla \] Gradient operator
1 Introduction

There has always been a need for air-breathing aerospace vehicles to travel higher and faster. Whether it is for more affordable access to orbit, or for defense applications, the need for engines that are capable of propelling an aircraft to hypersonic speeds is clear. Traditional turbojets, in the extreme case, can operate from zero velocity up to around Mach 3. At this point the compressor starts to do more harm than good. By removing the compressor, and thus the need for a turbine, a ramjet engine is created. Ramjets can operate in the range from Mach 3 or 4 to about Mach 5 [19]. At Mach 5, decelerating the flow to subsonic speeds for combustion becomes unreasonable due to the excessive temperatures and thus dissociation of fuel rather than combustion. This illustrates the need for a supersonic combustion ramjet, also known as a scramjet. Rather than mixing and combusting fuel at subsonic speeds, the incoming air is allowed to remain supersonic. The task of mixing and combusting supersonically is a daunting one and the simulation of this process can be equally as difficult. Important factors in the simulation of these types of flows include, but are not limited to, the specification of the turbulent Prandtl and Schmidt numbers and the consideration of turbulence/chemistry interactions. The turbulent Prandtl and Schmidt numbers are inherently variable in the complex three-dimensional flows that are characteristic of current proposed scramjet designs. Since classic turbulence models assume these numbers to be constant and specified ahead of time, a new turbulence model that allows these numbers to vary and also accounts for turbulence/chemistry interactions is required [16][43]. One such model is utilized herein. Another factor that has received little attention in the literature is the role of compressibility on high speed mixing and combustion. It is well known that mixing-layer growth rate decreases with increasing Mach number [40]. This phenomenon becomes especially important in supersonic combustion devices due to the fact that compressibility effects reduce the ability of the fuel to mix with air at supersonic speeds, resulting in less overall combustion.
Some efforts have been made to move toward the calculation, rather than specification, of the turbulent Prandtl and Schmidt numbers as part of the solution. Methods based on the mixing length have been employed as early as 1975, by Reynolds, to calculate both the turbulent Prandtl and Schmidt numbers [30]. In 1988, Nagano developed a two equation model for calculating the turbulent diffusivity, which was used in conjunction with the $k$-$\varepsilon$ turbulence model [28]. However, the model was not developed for high speed flow and thus does not include the effects of compressibility. This model provided the framework for most of the work to follow. In 1993, Sommer et al. developed a variable turbulent Prandtl number model using methods very similar to those used by Nagano [35]. This model was also derived from the incompressible energy equation rather than the compressible energy equation, so compressibility effects, which have been determined to be quite important, are not accounted for. Two additional equations were added to the base incompressible $k$-$\varepsilon$ turbulence model, temperature variance, and its dissipation rate. Solving these four equations allowed for the calculation of the turbulent diffusivity. In general the results for high Mach number, low wall temperature cases were improved over those utilizing the $k$-$\varepsilon$ model alone. In 1999, another approach was taken by Guo et al. to create a variable turbulent Schmidt number model [18]. In addition to the $k$-$\varepsilon$ turbulence model, Guo modeled the turbulent species diffusion vector with a single transport equation. A genetic algorithm technique was applied to efficiently obtain the model constants. Again, the results were improved over the baseline $k$-$\varepsilon$ model for a jet-in-crossflow application.

A company known as Combustion Research and Flow Technology, Inc. (CRAFT Tech) have been investigating the use of variable turbulent Prandtl number methodology for propulsive type flows since 2000 [25]. The formulation is based largely on the work of Sommer and Nagano, but they did also investigate algebraic stress models in addition to the $k$-$\varepsilon$ model. Again the model equations for temperature variation and its dissipation rate are based on the low speed energy equation. The pressure gradient term and the term responsible for energy dissipation are ignored. The current work does not make these simplifications since such assumptions are not valid for scramjet type flows. The model
was later applied by CRAFT Tech to a Large Eddy Simulation (LES) of reacting and non-reacting shear layers at high speeds [6][7]. The purpose of this work was to generate data to be used in improving RANS models. Compressibility corrections were applied in this work, but the model constants were modified in an ad hoc manner, without significant validation. The model was extended to include variable $Pr_t$ and variable $Sc_t$ in 2005 [4].

In 2005, Xiao et al. presented two similar approaches, one for calculating the turbulent Prandtl number ($Pr_t$) as part of the solution [42] and one for calculating the turbulent Schmidt number ($Sc_t$) as part of the solution [41]. Each of these new models used the $k-\zeta$ turbulence model of Robinson and Hassan as a base [31]. With the addition of two equations each, enthalpy variance and its dissipation rate for the variable $Pr_t$ model and concentrations variance and its dissipation rate for the variable $Sc_t$ model, the turbulent diffusivity and the turbulent diffusion coefficient were able to be determined. Improvements were observed for a coaxial jet flow [9] with the variable $Sc_t$ model, and improvements in heat flux predictions were seen with the variable $Pr_t$ model. The variable $Sc_t$ model was later applied to the supersonic combustion experiment of Burrows and Kurkov [5], while using a probability density function (PDF) to address the turbulence/chemistry interactions. In general the variable $Sc_t$ formulation worked well for both mixing and reacting supersonic flows; however, the PDF method for addressing turbulence/chemistry interactions did not necessarily improve the results [22]. A complete turbulence model, where both the $Pr_t$ and $Sc_t$ are calculated as part of the solution was presented by Xiao et al. in 2006 [43]. This work, which employed a new modeling approach for the turbulence/chemistry interactions, showed improvement in predictions for both the coaxial jet and the Burrows and Kurkov combustor. The work also reinforced the fact that the turbulence/chemistry interactions must be accounted for. The latest work, which most of the content herein is based on, applied the complete model to the SCHOLAR supersonic combustion experiments [24][23]. These results are discussed in Chapter 5.
The SCHOLAR combustor has been simulated extensively by Rodriguez and Cutler in conjunction with the actual experiments. Initially, only mixing was considered [13], then the reacting case [10]. Rodriguez and Cutler later continued the work in a more comprehensive study [33]. The simulation utilized the VULCAN CFD code, developed at NASA Langley Research Center. The $k-\omega$ turbulence model was used with various constant values of Pr$_t$ and Sc$_t$. The computed results were seen to vary greatly with the specification of these parameters. The best results were obtained with Pr$_t$ = 0.9 and Sc$_t$ = 1.0, therefore, the constant Pr$_t$/Sc$_t$ runs in the current work use these values. The computational grid used in the current work was also developed from a grid originally generated by Rodriguez.
2 Governing Equations

This section will describe the set of partial differential equations that governs the physics of supersonic multi-component reacting gasses.

2.1 Reacting Gas Equation Set

2.1.1 Navier-Stokes Equations

The governing equations for multi-component compressible chemically reacting flows at high speeds are the Navier-Stokes equations, which consist of conservation of mass, momentum, and energy, along with a set of species mass conservation equations. The number of species equations required is $NS - 1$, where $NS$ is the number of species. By including all of the species equations, the continuity equation may be removed, since the sum of the species mass conservation equations results in the continuity equation. If external forces such as gravity, and body forces are neglected, and thermal equilibrium is assumed, the equations are as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0$$  \hspace{1cm} (2.1)

$$\frac{\partial}{\partial t}(\rho u_j) + \frac{\partial}{\partial x_j}(\rho u_j u_i + \delta_{ij} p - \tau_{ij}) = 0$$  \hspace{1cm} (2.2)

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_j}(\rho H u_j + q_j - \tau_{ij} u_i) = 0$$  \hspace{1cm} (2.3)

$$\frac{\partial}{\partial t}(\rho Y_m) + \frac{\partial}{\partial x_j}(\rho Y_m u_j + \rho Y_m V_{j,m}) = \dot{\omega}_m$$  \hspace{1cm} (2.4)
In these equations, \( \rho \) is the density, \( u_i \) is the velocity, \( p \) is the pressure, \( \tau_{ij} \) is the stress tensor, and \( q_j \) is the heat flux vector. For the species mass conservation equations, \( Y_m \) is the species mass fraction, \( V_{j,m} \) is the diffusion velocity, and \( \dot{w}_m \) is the production rate.

The viscous stress tensor, under the assumption of a Newtonian fluid, can be written as

\[
\tau_{ij} = 2 \mu s_{ij} - \frac{2}{3} \delta_{ij} \mu \frac{\partial u_k}{\partial x_k}
\]  
(2.5)

\[
s_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]  
(2.6)

where \( \mu \) is the molecular viscosity and \( s_{ij} \) is the instantaneous strain rate tensor. The heat flux vector is evaluated using the sum of Fourier’s Law and the heat flux due to diffusion.

\[
q_i = -k \frac{\partial T}{\partial x_i} + \rho \sum_{m=1}^{NS} h_m Y_m V_{m,i}
\]  
(2.7)

Similar to the viscous stress and heat flux, a linear relationship can be developed for the species diffusion mass flux. This is called Fick’s Law [26], and it states that the diffusion mass flux is proportional to the species concentration gradients.

\[
\rho V_{m,i} = \rho D \frac{\partial Y_m}{\partial x_i}
\]  
(2.8)

The binary diffusion coefficient, \( D \), is defined by the Schmidt number (Sc).

\[
Sc = \frac{\mu}{\rho D}
\]  
(2.9)

The total energy and total enthalpy are defined by the following equations.

\[
E = H - \frac{P}{\rho}
\]  
(2.10)

\[
H = h_{\text{mix}} + \frac{u_i u_j}{2}
\]  
(2.11)

The mixture specific enthalpy is defined by a mass fraction weighted sum.

\[
h_{\text{mix}} = \sum_{m=1}^{NS} Y_m h_m
\]  
(2.12)
The species enthalpies, $h_m$, will be defined in Section 2.1.2. The equation of state is used to relate the pressure, bulk density, and temperature. It is known as Dalton’s Law of Partial Pressures.

\[ p = \sum_{m=1}^{N_X} p_m = \rho R_{mix} T \] (2.13)

This law states simply that the pressure is the sum of the partial pressures of each species.

\[ R_{mix} = \hat{R} \sum_{m=1}^{N_S} \frac{Y_m}{\hat{W}_m} \] (2.14)

$\hat{W}_m$ is the molecular weight of species $m$, and $\hat{R}$ is the universal gas constant. The total energy can also be written in the form of Equation (2.11).

\[ E = e_{mix} + \frac{u_1 h_i}{2} \] (2.15)

The mixture internal energy, $e_{mix}$, is also defined in terms of the species enthalpies.

\[ e_{mix} = \sum_{m=1}^{N_X} Y_m e_m = \sum_{m=1}^{N_X} Y_m \left( h_m - \frac{\hat{R} T}{\hat{W}_m} \right) \] (2.16)

### 2.1.2 Thermodynamic Relations

For a high temperature, chemically reacting flow, the flow is assumed to be thermally perfect. Unlike the assumptions of a calorically perfect gas, the specific heats at constant pressure and volume are no longer assumed constant. They are instead functions of temperature. A thermally perfect gas is based on the assumption that the internal energy modes of a molecule are always in a state of equilibrium. Curve fits given in [27] are used to calculate the specific heats along with other related properties. The species enthalpy can easily be obtained from these curve fits using the following equation.

\[ \frac{\hat{h}_m}{\hat{R} T} = a_{1,m} + a_{2,m} \frac{T}{2} + a_{3,m} \frac{T^2}{3} + a_{4,m} \frac{T^3}{4} + a_{5,m} \frac{T^4}{5} + \frac{b_{1,m}}{T} \] (2.17)
The species enthalpy in this equation is defined on a per mole basis. To obtain the enthalpy per unit mass, simply multiply by the species molecular weight. Specific heat, entropy, and Gibbs free energy can be calculated in a similar manner.

The ratio of specific heats for the mixture, \( \gamma_{\text{mix}} \), can be calculated using:

\[
\gamma_{\text{mix}} = \frac{C_{p_{\text{mix}}}}{R_{\text{mix}}} - 1
\]

\[
C_{p_{\text{mix}}} = \sum_{m=1}^{NS} Y_m C_{p_m}
\]

Finally, the laminar viscosity and thermal conductivity must be determined. First the laminar viscosity for each species is calculated using Sutherland’s Law [38]. The laminar thermal conductivity is then calculated from the following relation to the laminar Prandtl number.

\[
k_m = \frac{\nu_m C_{p_m}}{Pr}
\]

Then, using Wilke’s formula [26], the species viscosities and thermal conductivities are combined into a bulk or mixture viscosity and thermal conductivity.

### 2.2 Governing Equations in Vector Form

A convenient way to rewrite the Navier-Stokes equations is in compact vector form. This makes further formulations much simpler. The general form is as follows.

\[
\frac{\partial U}{\partial t} + \frac{\partial (E - E_v)}{\partial x} + \frac{\partial (F - F_v)}{\partial y} + \frac{\partial (G - G_v)}{\partial z} = S
\]

The definitions of these vectors can be found in Appendix A.
2.3 Reynolds and Favre Averaging

While the Navier-Stokes equations describe continuum fluid flow down to the smallest scales of turbulent motion, the discrete computational grids on which the equations are solved are unable to resolve such small scales of motion. The small turbulence scales are very important however, in dissipating energy from larger scale motion and the mean flow. The traditional approach to this problem is not to resolve the smallest features of the flow, but rather to model them using the local characteristics and time history of the flow. This provides a macroscopic view of the affects of turbulence on the mean flow.

There are certainly alternatives to modeling the turbulence. One such alternative is direct numerical simulation (DNS), in which the exact Navier-Stokes equations are resolved down to the smallest turbulence scales. This requires many times more grid points than a solution where the turbulence is completely modeled, and the requirement is ever steeper with increasing Reynolds numbers. Another alternative is to resolve some of the large scale turbulent features and model the scales that occur on the sub-grid level. This is known as large eddy simulation (LES). This is a compromise, but it still requires a significantly higher resolution than simulations that model all turbulence scales. Due to the size of modern engineering problems and the limited computing power that is available, a completely modeled approach is adopted in the current work.

A method called Reynolds averaging is used to convert the governing equations to solve for the mean flow properties rather than the instantaneous properties. There are a number of ways to average the flow properties, but for stationary turbulence, such as that in steady flows, time averaging is the most appropriate [40]. The following equation represents this time averaging process.

\[
F_{\tau}(x_i) = \lim_{T \to \infty} \frac{1}{T} \int_{-T}^{T} f(x_i, t) dt
\]  

\[ (2.22) \]
The instantaneous flow property is represented by \( f(x_i, t) \) while \( F_T(x_i) \) is the time averaged flow property. The instantaneous flow properties can then be expressed by the time averaged mean property plus a fluctuation.

\[
q = \bar{q} + q'
\]  

(2.23)

Here, \( q \) represents any flow property; \( \bar{q} \) is the time averaged quantity and \( q' \) is the fluctuation. This averaging is applied to the velocity and pressure fluctuations.

Applying this time averaging technique to the Navier-Stokes equations results in what is known as the Reynolds Averaged Navier-Stokes (RANS) equations. While this method works well for incompressible flows, more variables must be taken into account if the flow is compressible, namely density and temperature. However, if the same Reynolds averaging technique is used, terms arise that have no analogue to those in the incompressible equations. To alleviate this problem, a different type of averaging is introduced, Favre, or mass-weighted averaging. This average is obtained from the following equation.

\[
\bar{q} = \frac{1}{\bar{\rho}} \lim_{\tau \to \infty} \int_{t}^{t+\tau} \rho(x_i, t) q(x_i, t) dt
\]

(2.24)

Here, \( \bar{\rho} \) represents the Favre averaged quantity, and, just as before, the instantaneous quantity can be written as:

\[
q = \bar{q} + q''
\]

(2.25)

When averaging the equations, correlation terms appear that are not necessarily zero. Consider the averaging of the product of any two variables.

\[
\bar{\phi \psi} = \left( \bar{\phi} + \phi' \right) \left( \bar{\psi} + \psi' \right) = \bar{\phi} \bar{\psi} + \bar{\phi} \psi' + \phi' \bar{\psi} + \phi' \psi'
\]

(2.26)

The terms with only one fluctuating term become zero when averaged, but the product of two fluctuating properties is not necessarily zero if there is a correlation between them.

The density, pressure, stress tensor, heat flux, and species production rate are represented using the Reynolds average, while the other variables use the Favre average.

\[
\begin{align*}
\rho &= \bar{\rho} + \rho', & p &= \bar{p} + p', & \tau_{ij} &= \bar{\tau}_{ij} + \tau'_{ij}, \\
q_i &= \bar{q}_i + q'_i, & \omega_m &= \bar{\omega}_m + \omega'_m
\end{align*}
\]

(2.27)
\[ u_i = \overline{u}_i + u_i^*, \quad V_{i,m} = \overline{V}_{i,m} + V_{i,m}^*, \quad Y_m = \overline{Y}_m + Y_m^*, \]
\[ E = \overline{E} + E^*, \quad H = \overline{H} + H^*, \quad T = \overline{T} + T^* \]

(2.28)

Substituting these quantities into the Navier-Stokes equations and performing the prescribed averaging results in the Favre averaged Navier-Stokes equations, still known as the RANS equations [43].

\[ \frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_i} (\overline{\rho} \overline{u}_i) = 0 \]

(2.29)

\[ \frac{\partial}{\partial t} (\overline{\rho} \overline{Y}_m) + \frac{\partial}{\partial x_j} (\overline{\rho} \overline{u}_j \overline{Y}_m) = \frac{\partial}{\partial x_j} \left( \overline{\rho} \frac{\partial \overline{Y}_m}{\partial x_j} - \overline{\rho} \overline{Y}_m^* \overline{u}_j^* \right) + \overline{\omega}_m \]

(2.30)

\[ \frac{\partial}{\partial t} (\overline{\rho} \overline{u}_i) + \frac{\partial}{\partial x_j} (\overline{\rho} \overline{u}_j \overline{u}_i) = - \frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \overline{v}_j - \overline{\rho} \overline{u}_j^* \overline{u}_i^* \right] \]

(2.31)

\[ \frac{\partial}{\partial t} (\overline{\rho} \overline{H} \overline{u}_i) + \frac{\partial}{\partial x_j} (\overline{\rho} \overline{H} \overline{u}_j \overline{u}_i) = \frac{\partial}{\partial x_i} \left[ \overline{u}_j \left( \overline{v}_j - \overline{\rho} \overline{u}_j^* \overline{u}_i^* \right) \right] - \frac{\partial}{\partial x_i} \left( \overline{q}_i + \overline{\rho} \overline{u}_i^* \overline{h}_i^* \right) \]

(2.32)

Three new terms are introduced in this form of the equations, the turbulent stress tensor, \(- \overline{\rho} \overline{u}_i^* \overline{u}_j^*\), the turbulent heat flux vector, \(\overline{\rho} \overline{u}_j^* \overline{h}_i^*\), and the turbulent species diffusion vector, \(- \overline{\rho} \overline{Y}_m^* \overline{u}_j^*\). These terms are approximated by the turbulence model to be defined in Section 2.5. The turbulent stress tensor is also known as the Reynolds stress tensor.

\[ \text{2.4 Chemical Kinetics} \]

Finite rate chemical kinetics is used to track chemical reactions in the present work. This method is based on the Law of Mass Action (LMA) [26]. This law determines the rate of change of the concentration of a single species in a multi-component flow. This rate is then incorporated into the source term for the species conservation equations.
A chemical mechanism consists of a collection of exchange/recombination reactions and third body reactions, which when combined, result in the global reaction such as that for hydrogen oxidation. The Law of Mass Action for exchange/recombination reactions is:

$$RR_i = k_{f,i} \prod_{m=1}^{NS} C_m^{r_{m,i}} - k_{b,i} \prod_{m=1}^{NS} C_m^{r_{m,i}}$$  \hspace{1cm} (2.33)$$

For third body reactions, which require any third molecule to initiate, the equation becomes:

$$RR_i = \left( k_{f,i} \prod_{m=1}^{NS} C_m^{r_{m,i}} - k_{b,i} \prod_{m=1}^{NS} C_m^{r_{m,i}} \right) \left( \sum_{m=1}^{NS} C_m TB_{m,i} \right)$$  \hspace{1cm} (2.34)$$

$C_m$ is the species concentration, or molar density, which is the species density divided by the molecular weight. The stoichiometric coefficients for the reactants are designated by $v'$ and for the products, $v''$. The effects of the third body are combined into a single term called the third body efficiency, $TB_{m,i}$. Each species has a third body efficiency for each third body reaction. The forward reaction rate coefficient, $k_{f,i}$, is determined by the Arrhenius Law. It takes the following form.

$$k_f = AT^\eta \exp(-\theta_d / T)$$  \hspace{1cm} (2.35)$$

The parameters $A$, $\eta$, and $\theta_d$ are specific to the chemical kinetic mechanism and will be discussed in Sections 2.4.1 and 2.4.2. Rather than require a separate set of parameters for the backward rate coefficient, $k_b$ is calculated using the equilibrium coefficient with the following relation.

$$\frac{k_f}{k_b} = \left. k_{eq} \right|_C = \left. k_{eq} \right|_P \left( \frac{101325}{RT} \right)^{(m''-m')} \hspace{1cm} (2.36)$$

The above equation also demonstrates the conversion of the equilibrium constant from a partial pressure basis to a concentration basis, as indicated by the subscripts. The equilibrium constant for a particular reaction can be calculated from the change in Gibbs free energy.

$$\left. k_{eq} \right|_P = \exp \left[ \frac{-\Delta \tilde{g}}{RT} \right]$$  \hspace{1cm} (2.37)$$
\[
\Delta \hat{g} = \sum_{m}^{NS} (\nu_{m}'' - \nu_{m}') \hat{g}_{m}
\]  
(2.38)

The production rate of each species can be determined using the preceding information.

\[
\dot{\omega}_{m} = \left( \sum_{i=1}^{NR} (\nu_{m,i}'' - \nu_{m,i}') RR \right) \hat{W}_{m}
\]  
(2.39)

2.4.1 Jachimowski Chemical Mechanism

The abridged chemical kinetic mechanism of Jachimowski is one of two models used in this work [21]. The mechanism consists of seven species and seven reactions. The species are N$_2$, O$_2$, H$_2$, H$_2$O, OH, H, and O. The reactions are listed in Table C.1 of Appendix C. Note that the first two reactions are third body reactions, where $M$ represents the third body. Thus, each equation requires a third body (TB) efficiency for each species. The species H$_2$ has $TB = 2.5$ for both reactions and H$_2$O has $TB = 16.0$ for both reactions. All other species have a third body efficiency of 1.0 for both reactions. The mechanism parameters, such as the pre-exponential factor and activation energies are listed in Table C.2.

2.4.2 Connaire et al. Chemical Mechanism

The second chemical model is that of Connaire et al. [8]. This model employs nine species and nineteen reactions. It is slightly more complicated than the Jachimowski mechanism, not just in the magnitude of species and reactions, but in the complexity of the rate expressions. The reactions are listed in Table C.3 of Appendix C. The mechanism parameters and third body efficiencies that are not equal to one are also listed in Appendix C. Note that some of the reactions have two listings. Reactions 14 and 19 are expressed as the sum of two rate expressions. Reactions 9 and 15 employ a different
method for computing the forward rate constant. While the classic definition of the rate constant is a function of the temperature, many chemical reactions are also a function of the pressure. Reactions 9 and 15 are examples of this. At very high pressures the rate constant may be defined by one set of parameters and at very low pressures by another set of parameters, and some blend of the two in between. This is known as a “fall-off” rate constant [26]. The ‘A’ and ‘B’ portions of reactions 9 and 15 represent the lower and upper pressure bounds respectively. A method presented by Troe et al. is used to blend these two limiting cases for intermediate pressures [17]. Using the two sets of parameters specified for the equation, a high-pressure limit rate constant, \( k_\infty \), and a low-pressure limit rate constant, \( k_0 \), are determined. The final forward rate constant is determined from the following equation.

\[
k = k_0 \left( \frac{p_r}{1 + p_r} \right)^F
\]  
(2.40)

The reduced pressure, \( p_r \), is related to the concentration of the mixture.

\[
p_r = \frac{k_0 C_{\text{mix}}}{k_\infty}
\]  
(2.41)

The mixture concentration can be determined by dividing the bulk density by the molecular weight of the mixture. The function \( F \) in the fall-off rate constant is determined from the following relations.

\[
\log F = \left\{ 1 + \left[ \frac{\log p_r + c}{n - d(\log p_r + c)} \right]^2 \right\}^{-1} \log F_{\text{cent}}
\]  
(2.42)

where

\[
c = -0.4 - 0.67 \log F_{\text{cent}}, \quad n = 0.75 - 1.27 \log F_{\text{cent}}, \quad d = 0.14,
\]  
(2.43)

\[
F_{\text{cent}} = (1 - a) \exp(-T / T^{***}) + a \exp(-T / T^*) + \exp(-T^{**} / T)
\]

Required inputs are \( a, T^*, T^{**}, \) and \( T^{***} \). These values are listed in Table 2.1 for reactions 9 and 15.
Table 2.1: Troe Parameters for Connaire et al. Mechanism

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$a$</th>
<th>$T^{***}$</th>
<th>$T^*$</th>
<th>$T^{**}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>0.5</td>
<td>$1.0E-30$</td>
<td>$1.0E+30$</td>
<td>$1.0E+100$</td>
</tr>
<tr>
<td>15</td>
<td>0.5</td>
<td>$1.0E-30$</td>
<td>$1.0E+30$</td>
<td>$1.0E+100$</td>
</tr>
</tbody>
</table>

2.5 Turbulence Closure

As discussed in Section 2.3, the Reynolds and/or Favre averaging of the governing equations results in the addition of three terms. These terms contain more than one fluctuating variable and thus do not go to zero when averaged. To achieve closure, these terms, the Reynolds stress tensor, the turbulent heat flux vector, and the turbulent species diffusion vector, must be modeled. A common assumption for computing the Reynolds stress is called the Boussinesq eddy-viscosity approximation [40]. A new property is defined called the “eddy-viscosity.” Similar to the Newtonian approximation, the Reynolds stress tensor is assumed to be a linear function of the rate of strain tensor with the viscosity $\mu$, replaced by the turbulent viscosity, $\mu_t$. This reduces the number of unknowns from nine to one. There are a number of ways of specifying the eddy-viscosity, such as algebraic models or one/two equation models. The present work utilizes a two equation model, which requires one equation to determine a characteristic velocity of turbulent fluctuations and a second equation to determine a turbulence length scale or equivalent. The $k$-$\zeta$ turbulence model is the two equation model used in the current work and is described in Section 2.5.1.

An argument similar to Fourier’s Law is used to determine the turbulent heat flux using the turbulent diffusivity, $\alpha_t$, and an argument similar Fick’s Law is used to determine the turbulent species diffusion vector using the turbulent diffusion coefficient, $D_t$. Typically, these two extra variables are defined by a constant turbulent Prandtl
number and turbulent Schmidt number, essentially the same way as their laminar counterparts. However, in the current work, these two parameters are modeled using two equations for each that characterize the turbulent heat conduction and turbulent species diffusion. The formulation of these equations can be found in Sections 2.5.2 and 2.5.3.

2.5.1 $k$-$\zeta$ Model

The turbulence model used in the current work is based on the $k$-$\zeta$ model of Robinson and Hassan [31][32][1]. This model has a number of desirable qualities including the absence of damping and wall functions, coordinate system independence, tensorial consistency, and Galilean invariance. The definition of the turbulent kinetic energy is:

$$k = \frac{u_i u_i^*}{2}$$  \hspace{1cm} (2.44)

The enstrophy, $\zeta$, is the variance of vorticity, and is defined by:

$$\zeta = \omega_i \omega_i^*$$  \hspace{1cm} (2.45)

The eddy-viscosity is determined from these two quantities through the following relation.

$$\nu_t = C_\mu k^2 / \zeta$$  \hspace{1cm} (2.46)

All model constants are listed in Table 2.2. The exact Favre averaged turbulent kinetic energy equation is presented below.

$$\frac{\partial}{\partial t}(\bar{p} k) + \frac{\partial}{\partial x_j}(\bar{p} \bar{u}_j k) = T_{ij} \frac{\partial \bar{u}_i}{\partial x_j} - \bar{p} \varepsilon - \bar{u}_i^* \frac{\partial \bar{p}}{\partial x_i} + p' \frac{\partial \bar{u}_i^*}{\partial x_i}$$

$$+ \frac{\partial}{\partial x_j} \left( \frac{\tau_{ij} u_j^*}{2} - p' u_j^* \right)$$  \hspace{1cm} (2.47)

The exact vorticity variance (enstrophy) equation is:
\[
\frac{\partial}{\partial t} \left( \rho \tilde{\omega}_i^2 \right) + \frac{\partial}{\partial x_k} \left( \rho \tilde{u}_k \tilde{\omega}_i^2 + 2\Omega_i \rho \tilde{u}_j^* \tilde{\omega}_i^* + \rho \tilde{u}_i^* \tilde{\omega}_i^* \right) \\
- 2\Omega_i \frac{\partial}{\partial x_k} \left( \rho \tilde{u}_k \tilde{\omega}_i^* \right) = 2 \left( \Omega_m \rho \omega_j^* s_{im} + \overline{s_{im}} \rho \omega_i^* \omega_j^* \right) \\
+ \rho \omega_j^* \omega_j^* s_{im} - \rho \overline{s_{kk}} \omega_i^* \omega_j^* - \Omega_i \rho \omega_j^* s_{kk} - \rho s_{kk} \omega_i^* \omega_j^* \\
+ 2 \epsilon_{ijk} \left[ \frac{\partial \rho}{\partial x_j} \omega_i^* \left( \frac{\partial \rho}{\partial x_k} - \frac{\partial \tau_{km}}{\partial x_m} \right) + \omega_i^* \frac{\partial \rho}{\partial x_j} \left( \frac{\partial \rho}{\partial x_k} - \frac{\partial \tau_{km}}{\partial x_m} \right) \right] + \rho \omega_i^* \frac{\partial^2 \tau_{km}}{\partial x_j \partial x_m} \\
\]

(2.48)

where

\[
\left[ \begin{array}{c} s_j^* = \frac{1}{2} \left( \frac{\partial \tilde{u}_j^*}{\partial x_j} + \frac{\partial \tilde{u}_j^*}{\partial x_i} \right) \\
\overline{s_j} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \end{array} \right] \\
\Omega_i = \epsilon_{ijk} \frac{\partial \tilde{u}_k}{\partial x_j}, \quad \omega_j^* = \epsilon_{ijk} \frac{\partial \tilde{u}_k}{\partial x_j}, \quad \nu = \frac{\mu}{\rho} \\
\]

These two equations are modeled term by term to retain as much of the real physics as possible. The dissipation rate in the \( k \) equation is defined as follows, with the assumption of negligible correlations between velocity gradient and kinematic viscosity fluctuations.

\[
\overline{\rho\epsilon} = \nu \left[ \rho (\omega_i^*)^2 + \frac{4}{3} \rho (u_i^*)^2 \right] + 2\nu \frac{\partial}{\partial x_i} \left[ (\rho u_i^* u_j^*)_{ij} - 2\rho u_i^* u_j^* \right] \\
\]

(2.50)

The second term in Equation (2.50) is simply added to the diffusion term. The term \( \frac{4}{3} \nu \rho (u_i^*)^2 \) is modeled as follows.

\[
\frac{4}{3} \nu \rho (u_i^*)^2 = C_l \overline{\rho k} / \tau, \\
\]

(2.51)

where

\[
\frac{1}{\tau} = \frac{1}{\rho} \left[ k \left( \frac{\partial \rho}{\partial x_i} \right)^2 \right]^{\frac{1}{2}} \\
\]

(2.52)
Typically, this compressibility term is modeled as proportional to the turbulent Mach number, $M_t^2 = 2k/a^2$. For incompressible flows, the sound speed is infinite and the turbulent Mach number goes to zero, but for air, the sound speed is finite, and thus the modeled term never goes to zero, even at low Mach numbers. For constant density flows, such as those at low Mach numbers, the $k$-\(\zeta\) modeled term clearly approaches zero.

The final version of the modeled $k$ and $\zeta$ equations are shown below.

\[
\frac{\partial}{\partial t} (\bar{p}k) + \frac{\partial}{\partial x_j} (\bar{p} \bar{u}_j k) = \frac{\partial}{\partial x_j} \left[ \left( \frac{\mu + \mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + T_{ij} \frac{\partial \bar{u}_i}{\partial x_j} - \frac{1}{C_k} \frac{\bar{p}k}{\tau_p} - \mu \frac{\partial \zeta}{\partial x_j} - \frac{\partial}{\partial x_j} \left( \frac{\partial \Omega}{\partial x_j} \right)
\]

\[= \frac{\partial}{\partial x_j} \left[ \frac{\mu + \mu_t}{\sigma_\zeta} \frac{\partial \zeta}{\partial x_j} \right] + \frac{\mu_t}{\sigma_r} \frac{\partial \Omega_i}{\partial x_j} \left[ \frac{\partial \Omega}{\partial x_i} \right] - \epsilon_{mij} \bar{p} \frac{\partial \Omega_i}{\partial x_j} \left[ \frac{\partial}{\partial x_n} (u^m u^*_n) - \frac{\partial k}{\partial x_m} \right]
\]

\[+ \frac{1}{3} \delta_j \left( \Gamma \frac{\partial \zeta}{\partial x_j} - \frac{\beta_2 T_{ij} \Omega_i \Omega_j}{k \Omega} \right) - \frac{\beta_3}{R_t + \delta} \frac{\bar{p}k}{\zeta} + \frac{2 \beta_3 T_{ij}}{k \nu} \Omega_i \Omega_j \frac{\partial \zeta}{\partial x_j}
\]

\[= \frac{\partial}{\partial x_j} \left( \frac{\partial \Omega}{\partial x_j} \right) + \max[P_\zeta, 0] - 2\bar{p}k \frac{\partial \zeta}{\partial x_j} - C_\zeta \frac{\mu_k \Omega}{\tau_\zeta k}
\]

where

\[
P_\zeta = \frac{(\bar{p}k \Omega / \nu \sigma_p)}{1 + (\sigma_p / \tau_p)(R_t / \zeta)^{1/2}} \frac{D\bar{p}}{Dt},
\]

\[R_t = R_t^2, \quad R_t = \frac{k^2}{\nu^2 \zeta}
\]
The turbulent Prandtl number is an important parameter in supersonic flows. It has a significant influence on heat flux at high speeds and the typical assumption that this number is constant is often inaccurate. A model that calculates the turbulent Prandtl number as part of the solution is used in the present work [42]. To achieve this goal two new equations are derived and modeled, one for the enthalpy variance and one for the dissipation rate of the enthalpy variance. Using these newly calculated parameters, the turbulent diffusivity is defined by the following relation.

\[ \alpha = 0.5(C_h k \tau_h + \nu / \beta_h) \]  

(2.56)

where

\[ \tau_h = \frac{\tilde{h}^2}{\varepsilon_h}, \quad \varepsilon_h = \alpha \left( \frac{\partial \tilde{h}^*}{\partial \chi_i} \right)^2 \]  

(2.57)

\( C_h \) and \( \beta_h \) are model constants. All the model constants for the variable Prandtl number model can be found in Table 2.3. The first step in deriving the enthalpy variance
equation and its dissipation rate equation is to express Favre averaged energy equation as follows.

\[
\frac{\partial}{\partial t} \left( \bar{\rho} \bar{h} \right) + \frac{\partial}{\partial x_j} \left( \bar{\rho} \bar{u}_j \bar{h} \right) = \frac{D \bar{p}}{Dt} - \frac{\partial \bar{q}_i}{\partial x_i} + \bar{\phi} - \frac{\partial}{\partial x_j} \left( \rho h^* u_j^* \right) \tag{2.58}
\]

where

\[
\bar{\phi} = \tau_{ij} \frac{\partial \bar{u}_i}{\partial x_j} + \bar{p} \varepsilon, \quad \varepsilon = \nu \zeta,
\]

\[
- \rho h^* u_j^* \equiv Q_j = \bar{p} \left( \alpha_i \frac{\partial \bar{h}}{\partial x_j} + D_i \sum_{m=1}^{NS} \bar{Y}_m \frac{\partial \bar{Y}_m}{\partial x_j} \right)
\]

When multiple reacting species are present, Equation (2.58) must be rewritten in a way so as to split the entropy into the sensible entropy and that due to reactions.

\[
h_m = \int C_{p_m} dT + \Delta h_{f,m} \tag{2.60}
\]

\[
h = \sum_{m=1}^{NS} Y_m h_m = \sum_{m=1}^{NS} Y_m \int C_{p_m} dT + \sum_{m=1}^{NS} Y_m \Delta h_{f,m} \tag{2.61}
\]

From this, one can derive the exact equations for the enthalpy variance, \( h^* \), and its dissipation rate, \( \varepsilon_h \). They are listed below.

\[
\frac{\partial}{\partial t} \left( \frac{1}{2} \bar{p} \bar{h}^* \right) + \frac{\partial}{\partial x_j} \left( \frac{1}{2} \bar{p} \bar{u}_j \bar{h}^* \right) = -\rho h^* u_j^* \frac{\partial \bar{h}}{\partial x_j} - \frac{\partial}{\partial x_j} \left( \frac{1}{2} \bar{p} u_j^* h^* \right) + h^* S_h \tag{2.62}
\]

\[
\rho \frac{D}{Dt} \varepsilon_h + 2 \rho \alpha \frac{\partial h^*}{\partial x_j} \frac{\partial \bar{h}}{\partial x_j} \bar{u}_j^* + 2 \rho \alpha \frac{\partial u_j^*}{\partial x_k} \frac{\partial \bar{h}}{\partial x_k} \bar{u}_j \bar{h}^* \tag{2.63}
\]

\[
+ 2 \rho \alpha u_j^* \frac{\partial h^*}{\partial x_k} \frac{\partial \bar{h}}{\partial x_k} + u_j^* \rho \alpha \left[ \frac{\partial (h^*)^2}{\partial x_j} \right] + 2 \rho \alpha \frac{\partial u_j^*}{\partial x_k} \frac{\partial h^*}{\partial x_k} \frac{\partial \bar{h}}{\partial x_j}
\]

\[
= 2 \rho \alpha \frac{\partial h^*}{\partial x_k} \frac{\partial}{\partial x_k} \left[ S_h' - \frac{1}{\rho} \frac{\partial}{\partial x_j} (\rho u_j^* h^*) \right]
\]

where

\[
S_h' = -\frac{\partial q_i}{\partial x_i} + \phi'
\]
These equations are then modeled as:

\[
\frac{\partial}{\partial t} (\overline{\rho} h'^{2}/2) + \frac{\partial}{\partial x_j} (\overline{\rho} \overline{u_j} h'^{2}/2) = \frac{\partial}{\partial x_j} \left[ \overline{p}(\gamma \alpha + \alpha_i C_{h,2}) \frac{\partial h'^{2}/2}{\partial x_j} \right] \\
+ 2 \mu \rho S_{ij} \left[ \frac{\partial}{\partial x_j} \left( \frac{Q_i}{\overline{\rho}} \right) + \frac{\partial}{\partial x_i} \left( \frac{Q_j}{\overline{\rho}} \right) \right] - \frac{4}{3} \mu \rho S_{kj} \frac{\partial}{\partial x_j} \left( \frac{Q_j}{\overline{\rho}} \right) \\
- (\gamma - 1) \overline{\rho} h'^{2} \frac{\partial u_i}{\partial x_i} - Q_i \frac{\partial h'}{\partial x_i} + 2 C_{h,4} \mu \sqrt{\overline{h'^{2}}} \zeta - \gamma \overline{\rho} \varepsilon_h \\
- \sum_{m} h'^{2} \overline{\omega_m} \Delta h_{j,m}
\]

and

\[
\frac{\partial}{\partial t} (\overline{\rho} \varepsilon_h) + \frac{\partial}{\partial x_j} (\overline{\rho} \overline{u_j} \varepsilon_h) = -\overline{\rho} \varepsilon_h \left( C_{h,3} b_{jk} - \frac{\delta_{jk}}{3} \right) \overline{\varepsilon_h} \\
+ C_{h,6} \overline{\rho} \frac{\partial \overline{h'}}{\partial x_j} + \frac{\partial}{\partial x_j} \left[ (\gamma \alpha + C_{h,7} \alpha_i) \frac{\partial \varepsilon_h}{\partial x_j} \right] \\
+ C_{h,8} \frac{Q_j}{\tau_h} \overline{\varepsilon_h} \left( \frac{C_{h,9}}{\tau_h} + \frac{C_{h,10}}{\tau_k} \right) \\
+ C_{h,11} \varepsilon_h \left[ \frac{D\overline{\rho}}{Dt} + \overline{\rho} \max \left( \frac{D\overline{\rho}}{Dt}, 0 \right) \right] \\
+ C_{h,13} \left( \overline{\rho} / \overline{\rho} \right) \Delta h^{'2} \sum_{m=1}^{NS} \overline{\alpha_m} \Delta h_{f,m} \\
+ \frac{C_{h,13} \left( \overline{\rho} / \overline{\rho} \right) \Delta h^{'2} \sum_{m=1}^{NS} \overline{\alpha_m} \Delta h_{f,m}}{\tau_Y + \tau_h}
\]

where

\[
b_{jk} = \frac{T_{jk}}{\overline{\rho} k} + \frac{2}{3} \delta_{jk}, \quad \tau_k = \frac{k}{\nu_s} \quad \tau_Y = \frac{k}{\nu_s}
\]

\( \Delta h_{f,m} \) is the heat of formation of species \( m \). \( \tau_Y \) is a parameter used in the variable turbulent Schmidt number formulation to be defined in Section 2.5.3. Note the final term in the modeled enthalpy variance equation, \( \sum_{m} h'^{2} \overline{\omega_m} \Delta h_{f,m} \). This term is a mechanism for
turbulence/chemistry interactions and the modeling of this term is described in Section 2.5.4.

<table>
<thead>
<tr>
<th>Constant</th>
<th>Value</th>
<th>Constant</th>
<th>Value</th>
</tr>
</thead>
<tbody>
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</tr>
<tr>
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<td>0.25</td>
</tr>
<tr>
<td>$C_{h,4}$</td>
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<td>$C_{h,11}$</td>
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</tr>
<tr>
<td>$C_{h,5}$</td>
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<td>$C_{h,12}$</td>
<td>−0.86</td>
</tr>
<tr>
<td>$C_{h,6}$</td>
<td>−0.12</td>
<td>$C_{h,13}$</td>
<td>−5.0</td>
</tr>
<tr>
<td>$C_{h,7}$</td>
<td>1.45</td>
<td>$\beta_h$</td>
<td>0.5</td>
</tr>
<tr>
<td>$C_{h,8}$</td>
<td>0.7597</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

2.5.3 Variable Turbulent Schmidt Number Model

Just as with the turbulent Prandtl number, the specification of the turbulent Schmidt number can have a profound influence on the simulation of a supersonic chemically reacting flow. Again, this value is traditionally specified as a constant depending on the type of problem, but for complex three-dimensional flows, this assumption is typically invalid. The specification of a turbulent Schmidt number that is too high can result in a flame blowout, while on the other end of the spectrum, if the number is too low, the simulation may unstart. A method similar to that of the variable turbulent Prandtl number is adopted for the variable turbulent Schmidt number in the present work [41]. Two equations are derived and modeled, one for the concentrations variance, and one for its dissipation rate. Using these new parameters, the turbulent binary diffusion coefficient is defined as follows.
\[ D_r = 0.5(C_\gamma k \tau_r + \nu_r / \beta_r) \]  

(2.68)

where

\[ \tau_r = \sigma_r / \varepsilon_r, \quad \sigma_r = \sum_{m=1}^{NS} \tilde{Y}_m^*, \quad \varepsilon_r = \sum_{m=1}^{NS} D \left( \frac{\partial Y_m^*}{\partial x_i} \right)^2 \]  

(2.69)

\( \sigma_r \) is the sum of the mass fraction variances, and \( \varepsilon_r \) is its dissipation rate.

The derivation of model equations for each of these quantities begins with the exact Favre averaged species conservation equation.

\[ \frac{\partial}{\partial t} (\bar{\rho} \bar{Y}_m^*) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_j \bar{Y}_m^*) = \frac{\partial}{\partial x_j} \left( \bar{\rho}D \frac{\partial \bar{Y}_m^*}{\partial x_j} - \bar{\rho} \bar{Y}_m^* \bar{u}_j' \right) + \bar{\omega}_m \]  

(2.70)

From this, one can derive the exact equations governing the sum of the mass fraction variances and its dissipation rate. They are as follows.

\[ \frac{\partial}{\partial t} (\bar{\rho} \bar{\sigma}_r) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_j \bar{\sigma}_r) = \frac{\partial}{\partial x_j} \left( \bar{\rho}D \frac{\partial \bar{\sigma}_r}{\partial x_j} - \sum_{m=1}^{NS} \bar{\rho} \bar{u}_j \bar{Y}_m^* \right) \]  

(2.71)

\[ + 2 \sum_{m=1}^{NS} \left[ - \bar{\rho} \bar{u}_j \bar{Y}_m^* \frac{\partial \bar{Y}_m^*}{\partial x_j} - \bar{\rho}D \left( \frac{\partial \bar{Y}_m^*}{\partial x_j} \right)^2 + \bar{\omega}_m \bar{Y}_m^* \right] \]

\[ \bar{\rho} D \frac{\partial \varepsilon_r}{\partial t} + \sum_{m=1}^{NS} \left[ 2 \rho D \frac{\partial \bar{Y}_m^*}{\partial x_k} \frac{\partial \bar{Y}_m^*}{\partial x_j} \frac{\partial \bar{u}_j}{\partial x_k} + 2 \rho D \frac{\partial \bar{u}_j}{\partial x_k} \frac{\partial \bar{Y}_m^*}{\partial x_j} \right] \]

\[ + \rho D \frac{\partial \bar{u}_j}{\partial x_j} \left( \frac{\partial \bar{Y}_m^*}{\partial x_k} \right)^2 + 2 \rho D \frac{\partial \bar{u}_j}{\partial x_k} \frac{\partial \bar{Y}_m^*}{\partial x_j} \frac{\partial \bar{Y}_m^*}{\partial x_k} + 2 \rho D \frac{\partial \bar{u}_j}{\partial x_k} \frac{\partial \bar{Y}_m^*}{\partial x_j} \frac{\partial \bar{Y}_m^*}{\partial x_k} \]  

(2.72)

\[ = \sum_{m=1}^{NS} \left[ 2 \rho D \frac{\partial \bar{Y}_m^*}{\partial x_k} \frac{\partial \bar{Y}_m^*}{\partial x_j} \left( \frac{\partial \bar{u}_j}{\partial x_k} \right) \right. \]

\[ \left. - \frac{1}{\rho} \frac{\partial}{\partial x_j} \left( \bar{\rho} \bar{u}_j \bar{Y}_m^* \right) \right] \]

(2.73)

where

\[ S'_i = \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial \bar{Y}_m^*}{\partial x_j} \right) + \hat{\omega}_m' \]

These equations are modeled using the same techniques used for the equations in the \( k-\zeta \) model and the variable Prandtl number model. These modeled equations are shown below.
\[
\frac{\partial}{\partial t} (\overline{\rho} \sigma_y) + \frac{\partial}{\partial x_j} (\overline{\rho} \overline{u}_j \sigma_y) = \frac{\partial}{\partial x_j} \left[ \overline{\rho} (D + C_{Y,1} D_t) \frac{\partial \sigma_y}{\partial x_j} \right] \\
+ 2 \sum_{m=1}^{NS} \overline{\rho} D_t \left( \frac{\partial \overline{\mu}_m}{\partial x_j} \right)^2 - 2 \overline{\rho} \varepsilon_y + 2 \sum_{m=1}^{NS} \omega_m Y_m^n
\]

\[
\frac{\partial}{\partial t} (\overline{\rho} \varepsilon_y) + \frac{\partial}{\partial x_j} (\overline{\rho} \overline{u}_j \varepsilon_y) = \frac{\partial}{\partial x_j} \left[ \overline{\rho} (D + C_{Y,3} D_t) \frac{\partial \varepsilon_y}{\partial x_j} \right] \\
+ 2 \overline{\rho} \varepsilon_y \left( \frac{1}{3} \frac{\partial \overline{u}_i}{\partial x_i} + C_{Y,2} b_k \frac{\partial \overline{u}_j}{\partial x_k} \right) + C_{Y,3} \overline{\rho} k \sum_{m=1}^{NS} \frac{\partial}{\partial x_j} \sqrt{\overline{Y}_m} \frac{\partial \overline{Y}_m}{\partial x_j} \\
+ \overline{\rho} D_{Y,41} D_t \sum_{m=1}^{NS} \left( \frac{\partial^2 \overline{Y}_m}{\partial x_j \partial x_j} \right)^2 + \overline{\rho} D_{Y,42} \sum_{m=1}^{NS} \overline{Y}_m \frac{\partial^2 \overline{Y}_m}{\partial x_j \partial x_k} \\
+ \overline{\rho} D_{Y,6} \frac{C_{Y,6}}{\tau_\varepsilon} \sum_{m=1}^{NS} \left( \frac{\partial \overline{Y}_m}{\partial x_j} \right)^2 - C_{Y,7} \overline{\rho} \frac{\varepsilon_y}{\tau_\varepsilon} + C_{Y,9} \overline{\rho} k \sum_{m=1}^{NS} \sqrt{\overline{Y}_m} \overline{Y}_m \omega_m \\
+ C_{Y,p} \frac{\overline{\rho}}{\overline{\rho} \tau_\varepsilon} \max \left( \frac{D\overline{\rho}}{D t}, 0.0 \right)
\]

(2.74)

(2.75)

All of the model constants can be found in Table 2.4. Note the last term in the \( \sigma_y \) equation, \( 2 \sum_{m=1}^{NS} \omega_m Y_m^n \). Similar to the variable Prandtl number model, a term is present here as well that is a mechanism for turbulence/chemistry interactions. The modeling of this term is discussed in Section 2.5.4.
Table 2.4: Variable Schmidt Number Model Constants

<table>
<thead>
<tr>
<th>Constant</th>
<th>Value</th>
<th>Constant</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_Y$</td>
<td>0.065</td>
<td>$C_{Y,6}$</td>
<td>0.5</td>
</tr>
<tr>
<td>$C_{Y,1}$</td>
<td>1.0</td>
<td>$C_{Y,7}$</td>
<td>0.78125</td>
</tr>
<tr>
<td>$C_{Y,2}$</td>
<td>0.095</td>
<td>$C_{Y,8}$</td>
<td>0.4</td>
</tr>
<tr>
<td>$C_{Y,3}$</td>
<td>−0.025</td>
<td>$C_{Y,9}$</td>
<td>4.4</td>
</tr>
<tr>
<td>$C_{Y,41}$</td>
<td>0.45</td>
<td>$C_{T,p}$</td>
<td>−0.1</td>
</tr>
<tr>
<td>$C_{Y,42}$</td>
<td>−1.0</td>
<td>$\beta_Y$</td>
<td>0.5</td>
</tr>
<tr>
<td>$C_{Y,5}$</td>
<td>1.0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

2.5.4 Turbulence / Chemistry Interactions

As mentioned in Sections 2.5.2 and 2.5.3, terms arise in the enthalpy variance and concentrations variance equations that act as mechanisms for the interactions between turbulence and chemistry. There are a multitude of methods available for the estimation of these two terms. A common method makes use of either an assumed or an evolution Probability Density Function (PDF). It has been found that assumed PDF’s are unable to reasonably calculate higher order terms such as those containing chemical production source terms [3]. Evolution PDF’s on the other hand may be able to accurately calculate these terms, but the cost in computation time increases dramatically, potentially by a factor of ten. Considering these limitations, a modeling approach is adopted in the interest of saving computational time and retaining the effects of the terms [43]. The method in general provides good agreement with validation experiments. The turbulence/chemistry interaction terms, along with their corresponding models, are listed below. The term that appears in the enthalpy variance equation is:

$$\sum \bar{h}^n \bar{\omega}_m \Delta h_{f,m} = C_{h,12} \sqrt{\bar{h}^n} \sum \bar{\omega}_m \Delta h_{f,m}$$  \(2.76\)

The term that appears in the concentrations variance equation is:
\[ 2 \sum \overline{Y_m^* \omega_m} = C_{Y,s} \sum \sqrt{\overline{Y_m^{**2} \omega_m}} \]  
(2.77)

For both of these models, \( \overline{\omega_m} \) is calculated using the mean temperature and mass fractions. Refer to Table 2.3 and Table 2.4 for the model constants.

### 2.6 Complete Equation Set

Once the six turbulence equations are incorporated into the reacting gas equation set, the result is a system of 19 coupled nonlinear partial differential equations. For an explanation of the solution methods employed, refer to Appendix E. Just as before, the system of equations can be written in compact vector form for a generalized coordinate system. See Equation (B.2). Refer to Appendix D for these vectors.

#### 2.6.1 Solution Methods

A finite volume method is used to solve this set of equations. An Essentially Non-Oscillatory (ENO) and/or Total Variation Diminishing (TVD) scheme is used in conjunction with the Low Diffusion Flux Splitting Scheme (LDFSS) of Edwards, and the system is advanced in time using a planar implicit scheme. The viscous and diffusion terms are evaluated using central differences.

An alternate version of the code was developed, which solved the turbulence equations separately. The species and conservation equations were solved using the planar implicit scheme, then the six turbulence equations were solved sequentially using a three-dimensional scheme. This modification resulted in a significant speed improvement without changing the computed results.

Appendix E contains a more detailed explanation of the numerical formulation.
3 Experimental Overview

This chapter describes the experiments that are used for model validation in the present study. The experiment is one that has been adopted by a working group of the NATO Research and Technology Organization for use in CFD validation. The experiment is known as SCHOLAR. The sections below describe the two experimental configurations as well as the measurement techniques used.

3.1 The SCHOLAR Experiments

The SCHOLAR experiments were performed at NASA Langley Research Center’s Direct Connect Supersonic Combustion Test Facility (DCSCTF) [11][29][36]. The experiments were conducted with the intention of being used for CFD validation of supersonic combustion. The model consists of hydrogen being injected normally or at a 30° angle to a vitiated air stream at Mach 2.0. The initial experiment, with vectored injection was designed using the VULCAN CFD code [39] with emphasis on avoiding large regions of subsonic flow. This resulted in a situation where chemical reactions lagged mixing and combustion did not initiate until far downstream of the injector. This proved to be difficult for CFD simulations, therefore another experiment, with normal hydrogen injection was conducted to complement the vectored injection case. Along with pressure and temperature measurements along the four walls of the combustor, two-dimensional slices of temperature and species mole fractions were extracted using a method called coherent anti-Stokes Raman spectroscopy (CARS). These measurements were taken at a number of planes upstream and downstream of the hydrogen injector. This technique is described in section 3.2 along with samples of the data obtained.
3.1.1 Vectored Injection Case

The first SCHOLAR model employs vectored hydrogen injection [29]. The hydrogen is injected at Mach 2.5 and a 30° angle to the vitiated air stream. Vitiated air is the result of hydrogen burning in oxygen enriched air. This technique is used to raise the enthalpy of the incoming gas to that of hypersonic flight conditions. A schematic of the experiment is shown in Figure 3.1.

![Figure 3.1: Schematic of Vectored Injection SCHOLAR Experiment](image)

The planes at which CARS measurements are taken are labeled in this figure as well. The planes are numbered 1, 3, 5, 6, and 7. The combustor consists of a straight isolator section following the vitiated air nozzle. There is then a small outward step on the upper wall followed by another short straight section. The remainder of the duct has a 3° divergence on the top wall. The hydrogen injector is located at the beginning of the divergent section. Note the different material utilized in the construction of the combustor. The section around the hydrogen injector, reaching to just downstream of plane 5, is made of copper. The remaining downstream section is made of steel. The duct was not cooled and thus runs were limited to about 20 seconds, with the duct being
allowed to cool between runs. As a result of this, the wall temperatures are constantly increasing with a rate depending on the location and local wall material. Measurements are available for the wall temperatures as a function of time [11], but the simulation is not time accurate, and thus these measurements cannot be used to provide a temperature boundary condition. The specification of wall temperatures is discussed further in Section 4.3.1. For clarification, a detail view of the hydrogen injector region is shown in Figure 3.2.

![Figure 3.2: Detail of Vectored Hydrogen Injector](image)

The enthalpy of the vitiated air stream is set to be that of Mach 7 flight and an equivalence ratio of 1.0. Listed in Table C.1 are the stagnation conditions and flow rates for both the heater and the hydrogen injector.
Table 3.1: Inflow Conditions for Vectored Injection

<table>
<thead>
<tr>
<th>Location</th>
<th>Flow Rates</th>
<th>Stagnation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heater :</td>
<td>0.915 ± 0.008 kg/s Air</td>
<td>Pressure 0.765 ± 0.008 MPa</td>
</tr>
<tr>
<td></td>
<td>0.0284 ± 0.0006 kg/s H₂</td>
<td>Temperature 1827 ± 75 K</td>
</tr>
<tr>
<td></td>
<td>0.300 ± 0.005 kg/s O₂</td>
<td></td>
</tr>
<tr>
<td>H₂ Injector :</td>
<td>Corresponds to equivalence ratio of 1.0</td>
<td>Pressure 3.44 ± 0.065 MPa</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Temperature 302 ± 4 K</td>
</tr>
</tbody>
</table>

3.1.2 Normal Injection Case

The second SCHOLAR model employs normal hydrogen injection [36]. There are some minor differences in the geometry of the combustor, but the major difference is the fuel being injected normal to the vitiated air stream at Mach 1.0. A schematic of this configuration can be seen in Figure 3.3, and a detailed view of the injector region is shown in Figure 3.4.

Figure 3.3: Schematic of Normal Injection SCHOLAR Experiment
This configuration presents a different challenge. While the vectored injection case had delayed ignition, this model has a small recirculation region ahead of the hydrogen injector that acts like a flame holder. Only planes 1, 3, 6, and 7 are used for CARS measurements in this experiment. The same pressure and temperature data are obtained for the centerline of each wall, but the wall temperature data was not available. This turns out to be an issue, which will be discussed in Chapter 5. The inflow conditions for the normal injection case are listed in Table 3.2. It was initially planned to use the same conditions as those for the vectored injection case, but the higher temperatures and pressures deformed the combustor and thus the enthalpy had to be reduced. The enthalpy was reduced to that of Mach 6 flight and the equivalence ratio was reduced to 0.7.
Table 3.2: Inflow Conditions for Normal Injection

<table>
<thead>
<tr>
<th>Location</th>
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<th>Stagnation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heater</td>
<td>1.196 ± 0.006 kg/s Air</td>
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<tr>
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<td>0.0231 ± 0.0006 kg/s H₂</td>
<td>Temperature 1490 ± 75 K</td>
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<tr>
<td></td>
<td>0.281 ± 0.003 kg/s O₂</td>
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<tr>
<td>H₂ Injector</td>
<td>Corresponds to equivalence</td>
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</tr>
<tr>
<td></td>
<td>ratio of 0.7</td>
<td>Temperature 290 ± 5 K</td>
</tr>
</tbody>
</table>

3.2 CARS Measurement Techniques

A method known as coherent anti-Stokes Raman spectroscopy (CARS) was used to obtain temperature profiles at the planes mentioned above. In the later experiments of references [29] and [36], a dual-pump CARS method was used, which allowed not only temperature measurements, but also the measurement of absolute mole fractions of nitrogen, oxygen, and hydrogen. Using a number of lasers passing through the same location in the combustor, the temperature and species mole fractions can be determined from the output intensity at different Raman shifts. The slots through which these lasers travel are located on either side of the duct at the distances indicated in the figures above. Each slot is 4.8 mm wide and has a window mounted at the Brewster angle to minimize reflections. To avoid condensation on the windows, warm dry air is blown over the inside of the window between it and the duct wall. Some of this may be entrained in the flow within the combustor, but has been decided to have negligible effects. This air (~400 K) may skew the temperature measurements slightly near the left and right walls however. Also, it turns out that the original measurements for hydrogen mole fractions may contain errors and are thus excluded from analysis in the current work.
3.3 Experimental Data Fitting

Experimental data fitting is an important issue when comparing with CFD simulations. The CARS data has a large amount of scatter, thus many measurements are required to obtain spatially resolved averages. Because it is not practical to accumulate a large sample, numerical techniques were used to smooth and present the data. A program called Table Curve 3D® was used to generate the surface fits for the 2D array of data at each plane. A large number of methods are available to generate these averages, many of which are examined in reference [12] to determine the best option for the data that was obtained. A preliminary CFD analysis was conducted in reference [13], and the methods for comparison with computation and experiment were investigated in an attempt to determine the best way to analyze the two sets of data. Figure 3.5 shows an example of the CARS scatter data for temperature and the curve fit that has been applied to it. This data represents a horizontal slice of plane 6 about half way between the top and bottom walls (at y = 18.2 mm). This particular location is used throughout the current work for comparison between experiment and computation. Similar plots are available for species mole fractions.
Figure 3.5: Example of CARS Measurements and Curve Fit (Plane 6, y = 18.2 mm)
4 Implementation

The code used in the present work is called REACTMB [15], which has been under development at NC State University for the past several years. It is a parallel general purpose Navier-Stokes solver for multi-phase multi-component reactive flows at all speeds. It employs a second order essentially non-oscillatory and/or total variation diminishing scheme based on the Low Diffusion Flux Splitting Scheme of Edwards, which is described in Appendix E.

4.1 Multiblock Parallel Approach

Parallelization is achieved through domain decomposition. The grid is divided into many smaller blocks, which are distributed among a number of processing nodes in a computing cluster. The Message Passing Interface (MPI) is then used for communication among processors [34]. The data from the edges of each block is passed to the processor containing the adjacent block. The computations were carried out on the IBM Blade Center at NC State University’s High Performance Computing Center.

4.2 Computational Geometry

The computational geometries for the two cases were generated using the GRIDGEN® program. The block layout for the vectored injection case is shown in Figure 4.1. The figure also shows a detail of the hydrogen injector with all grid points activated. A “butterfly” type grid topology is used in this region to avoid singularities.
and oddly shaped cells. Note that symmetry is used on the vertical centerplane so that only half of the combustor needs to be modeled.

![Figure 4.1: Block Layout and H₂ Injector Detail for Vectored Injection](image)

The grid for the vectored injection case employs 378 blocks and approximately 7.5 million grid points. It runs on 50 processors. For clarification, a view from the side of the symmetry plane is shown in Figure 4.2, including the survey planes for the CARS system.
The grid for the normal injection case is similar and was created by the same means. The block layout for the normal injection case is shown in Figure 4.3.
This grid contains 600 blocks and approximately 6.9 million grid points. It also runs on 50 processors. The number of blocks is increased for this case so as to obtain a reasonable load balance among the 50 processors. The fact that the vectored injection grid only consists of 378 blocks has nothing to do with the complexity. Note that the injector is contoured rather than stepped, as it is in the schematic. This is simply an approximation to make it easier on the solver and does not have much of an effect on the flow at the tip of the injector.
4.3 Wall and Inlet Boundary Conditions

For the representation of boundary conditions, the ghost cell method is employed. Rather than imposing boundary conditions directly on the fluxes at a wall or inlet, an imaginary cell on the opposite side of the boundary is created. The data in these cells is defined in a way such that the flux at the interface between them corresponds to the physical boundary conditions, such as the no-slip velocity condition and constant or adiabatic wall temperature. When higher order flux reconstruction schemes are used, multiple layers of cells may be required. The code can accommodate up to three layers of ghost cells. Since symmetry is utilized, a symmetry boundary condition is necessary. This is achieved by merely mirroring all scalar properties into the ghost cells from the interior cells. Care must be taken with the velocity vector however. Since the plane is of constant $z$, the $w$ velocity component must be made negative. The other components are simply copied.

4.3.1 Wall Boundaries

A number of different wall boundary conditions are required for the present simulation. The first condition corresponds to the no-slip condition.

\[ u_w = v_w = w_w = 0 \]  \hspace{1cm} (4.1)

\[ \frac{\partial p}{\partial n} |_w = 0 \]  \hspace{1cm} (4.2)

The direction normal to the wall is represented by $n$. The velocities become zero at the wall by applying the negative of all three velocity components to the ghost cells. The zero pressure gradient is enforced by simply setting the ghost cell pressure to the nearest internal cell pressure. Higher order approximations of this are also possible.
For the species equations, the normal concentration gradient must be zero at the wall.

\[ \frac{\partial Y_m}{\partial n} \bigg|_{w} = 0 \]  

(4.3)

This is enforced in a manner similar to the pressure.

There are various options for the wall temperature. The first and simplest condition is an adiabatic wall. Since the heat flux is proportional to the temperature gradient, the normal temperature gradient at the wall must be zero for it to be adiabatic. Conditions similar to the pressure and mass fractions can be used for this. The second possibility is to have an isothermal wall, meaning that the temperature is constant. To accomplish this, the temperature is extrapolated from the first internal layer of cells through the wall into the ghost cell. Many times this can result in a negative temperature in the ghost cell. This of course must be limited to a small positive value, or the calculation of the viscosity or other thermal properties in that cell will cause the program to crash. A third option is the isothermal ghost cell wall. This is somewhere between an adiabatic wall and an isothermal wall. The wall temperature is allowed to change but still remains close to the specified ghost cell value.

For the turbulence model, \( k = 0 \) at the walls. For \( \zeta \), the wall condition reduces to the following.

\[ \nu \zeta_w = \frac{\partial}{\partial n} \left( \nu \frac{\partial k}{\partial n} \right) \bigg|_{w} \]  

(4.4)

The boundary conditions for the variable turbulent Prandtl/Schmidt number models are similar to those of the \( k-\zeta \) model. \( \sigma_y \) and \( \tilde{h}^* \) must be zero at the walls, and a condition similar to Equation (4.4) holds for the dissipation rates.
4.3.2 Inflow and Outflow Boundaries

Both of the inflow boundaries, the vitiated air nozzle and the hydrogen nozzle, are subsonic. With grid aligned subsonic flow, there is one characteristic that propagates backward, out of the domain. For this reason, some information must be extrapolated from the flow inside the boundary. The velocity components are best suited for this. For the $k$-$
abla$ turbulence model, the incoming turbulence intensity $Tu$ and the initial length scale $(v_t / v)$ must be specified.

The outflow boundary is supersonic for this combustor; therefore all characteristics are propagating out of the domain. This means that the entire solution must be extrapolated into the ghost cells.
5 Results and Discussion

This chapter presents the results that have been obtained using the procedures and models described in the previous sections for both the vectored injection experiment and the normal injection experiment. Below is a list of the important factors investigated in this work.

- Wall temperatures and thermal boundary conditions. Since the walls were not cooled, a variety of methods were investigated.
- Specification of various inflow conditions such as turbulence intensity, length scale \( (\nu_l / \nu) \), and OH concentration.
- Grid resolution and refinement for the vectored injection case.
- Role of software in comparing computed data with experimental data.
- Variable vs. constant turbulent Prandtl/Schmidt numbers.
- Role of chemical kinetic mechanisms.
- Role of the compressibility term.

5.1 General Results

As mentioned above, one of the factors investigated was the effect of the inflow conditions on the solution. The sensitivities of several parameters were examined. First is the initial turbulence intensity, which is defined as:

\[
Tu = 100 \sqrt{\frac{2 k}{3 u^2}}
\]  
(5.1)
This term is basically used to specify the initial turbulent kinetic energy. Some turbulence models are sensitive to this value, but the $k-\zeta$ model is not. Values from 5% to 25% were inspected. Little to no influence on the solution was observed. The second factor, the initial turbulent length scale $(v_l / v)_{\infty}$, also had only a minor impact on the solution. The pressure along the bottom wall in the combustor section seemed to be loosely related to the specification of this value. Values from 5 to 2000 were used. In the lower range, from 5 to 500, the pressure increased very slightly with an increase in $(v_l / v)_{\infty}$. However, any increase above 500 did not seem to change the solution. Finally, the effects of freestream OH concentration were observed. Other than the baseline case, where the freestream OH mass fraction was zero, values from $1.0 \times 10^{-6}$ to $1.0 \times 10^{-3}$ were considered. It was observed that the degree of combustion was increased with the addition of OH in the freestream composition. This, in turn, produced higher pressures in the combustor.

The freestream turbulence intensity was set to 25% for all of the runs presented here, and the turbulent length scale was 2000. The freestream OH mass fraction was $1.0 \times 10^{-5}$ for the vectored injection case and $1.0 \times 10^{-6}$ for the normal injection case.

The experimental data set included a pitot pressure profile for the vitiated air nozzle exit. The quality of the flow in the combustor clearly depends on how well the nozzle output can be matched. Figure 5.1 shows the computed and experimental profiles, and there is good agreement between the two. Note that this data is for the vectored injection case and thus an enthalpy equivalent to Mach 7 flight. Pitot pressure data was not available for the normal injection case.
A final general consideration is how the wall temperatures were specified. The first attempt employed the adiabatic wall temperature for all surfaces. This was simple to implement, but resulted in wall temperatures and temperatures in the near wall region to be much higher than the experimental values. Figure 5.2 shows a horizontal slice of the temperature on plane 6 at $y = 18.2$ mm, with the computed solution overlaid on the experimental scatter. Note the large over prediction near the walls due to the adiabatic wall temperature. This is undesirable, since colder walls would remove energy from the flow. This could have a substantial effect on the flow downstream in the combustor.
The second option explored for the wall temperature was the use of a constant wall temperature. This is a difficult assumption to make since the wall temperature is varying throughout the geometry of the combustor due to material differences and the fact that the walls are uncooled and constantly increasing in temperature. The final solution was to use a constant ghost cell temperature method. This holds the actual wall temperature close to the specified value, but lets it increase slightly if the internal flow is hot enough. Rather than specify a single temperature for the entire system, the code was modified to allow different temperatures for different portions of the duct. In Figure 5.3, taken from reference [11], the wall temperatures in different sections of the combustor are listed against the run time. Using this data, approximate average temperatures were chosen for each section of the combustor. In the hydrogen injector, a ghost cell temperature of 300 K was used due to the low stagnation temperature. A temperature of 500 K was used for the copper section and 700 K was used for the steel section. The results presented in the subsequent sections utilize this varied constant ghost cell temperature method.
The results from the latest set of runs, at the above conditions, are presented below in Sections 5.2 and 5.3. There are six runs that are of interest, four for the vectored injection case, and two for the normal injection case. Table 5.1 lists the runs and the conditions for each.
Table 5.1: Runs Presented

<table>
<thead>
<tr>
<th>Case</th>
<th>Run #</th>
<th>Pr$_t$/Sc$_t$</th>
<th>Chem. Mech.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vectored:</td>
<td>1</td>
<td>variable</td>
<td>Connaire</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>variable</td>
<td>Jachimowski</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>constant</td>
<td>Connaire</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>constant</td>
<td>Jachimowski</td>
</tr>
<tr>
<td>Normal:</td>
<td>5</td>
<td>constant</td>
<td>Jachimowski</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>variable</td>
<td>Jachimowski</td>
</tr>
</tbody>
</table>

The turbulent Prandtl and Schmidt numbers were set to 0.9 and 1.0 respectively for the constant Pr$_t$/Sc$_t$ cases. These choices were based on the results from reference [33].

5.2 Vectored Injection Model

Mentioned above is the fact that grid resolution was investigated. A fine grid was created for the vectored injection case that contained approximately 9 million points and was run on 60 processors. It was found that this grid did not provide any improvement in the solution.

Refer to Section 3.1.1 for information on the original experiment and refer to Section 4.2 for information on the computational geometry used for the vectored injection case.

5.2.1 Variable Pr$_t$/Sc$_t$ Runs

Runs 1 and 2 use the variable turbulent Prandtl/Schmidt number model described in Sections 2.5.2 and 2.5.3. As explained in previous sections, there are two types of
experimental data, wall pressures along the length of the duct and CARS surveys at 5 planes along the length of the duct. For the CARS data, both the raw data and the software generated surface fits are available. The majority of comparisons will be made to the surface fits. However, the results for a single slice of plane 6 are shown first to demonstrate the role of smoothing in the comparison of experimental and computed data. Figure 5.4 presents a horizontal temperature slice of plane 6, similar to reference [29]. The slice is at \( y = 18.2 \) mm, which is about half way between the top and bottom walls. The computed data is for the Connaire mechanism (Run 1). There are large variations in temperature across the duct. This indicates that the fuel and air are not well mixed. While the computed curve does not match the experimental curve fit, it does lie within the experimental scatter.

![Figure 5.4: Temperature Slice of Plane 6 at \( y = 18.2 \) mm (Connaire)](image-url)
Figure 5.5 shows nitrogen and oxygen mole fraction slices at the same location. The profiles follow the same trends as the experimental data, but again, do not follow the curve fit applied to the experimental data.

In an effort to obtain a more reasonable comparison between computed and experimental data, the same curve fit was applied to both sets of data. Figure 5.6 shows the same slice as Figure 5.4, but with a 5th degree polynomial fit applied to both the raw experimental data and the computed solution. A 5th degree polynomial was chosen since, when applied to the experimental scatter, it most closely resembled the original curve fit, which is also shown in the figure for reference. Clearly, when subjected to the same smoothing, the computed solution displays very good agreement with the experimental data. Similar results are seen for the nitrogen and oxygen mole fractions, shown in Figure 5.7. The Jachimowski mechanism provides similar results.
Figure 5.6: 5\textsuperscript{th} Degree Polynomial Fits of Exp. and Computed Temperature (Run 1)

Figure 5.7: 5\textsuperscript{th} Degree Polynomial Fits of Exp. and Computed Mole Fractions (Run 1)
Figure 5.8 shows the CARS surface fits of temperature for the vectored injection model. Regardless of the fact that the data is slightly asymmetric, the computed results are shown on the left side of each slice and the experimental data on the right side. The temperature contours for the Connaire mechanism (Run 1) plotted against the smoothed experimental data are shown in Figure 5.9. Note the thin combustion region as opposed to the smoothed experimental data. Also, there is indication of ignition on plane 5 for the computed solution that is not reflected in the experimental data.

![Figure 5.8: Experimental Surface Fits of Temperature for Vectored Case](image)
In Figure 5.10, results for nitrogen and oxygen mole fractions are presented in a similar manner. The computed results again show similar patterns, but with more distinct interfaces.
Figure 5.11 only shows computed temperatures; the left side of each plane contains the results for the Jachimowski mechanism while the right half contains the result from the Connaire mechanism. This is to show the differences between the two chemical mechanisms. It can be seen that there is very little difference between the two. The species are nearly identical for each mechanism as well. While the patterns and extent of combustion are similar, there is a slightly smaller amount of combustion on plane 5 for the Jachimowski model. The purpose of this figure is to show the similarity of the results from each chemical mechanism.

![Figure 5.11: Temperature from Runs 1 and 2 (Left: Jach., Right: Connaire)](image)

The pressure distributions along the center of the bottom wall for the experiment and runs 1 and 2 are shown in Figure 5.12. The lack of smoothness in the pressure most likely comes from the fact that the flow is not well mixed. Since regions of cold fluid are near regions of hot fluid, the pressure is directly affected through the equation of state.
Note that the pressure distribution for both models is very similar. This reinforces the observations made above that were based on temperature and mole fraction contours. While the agreement is reasonable up to around 0.4 meters, the pressure further downstream is significantly underpredicted. The computed solution does not seem to have the same pressure rise due to ignition and combustion as the experiment.

As mentioned earlier, combustion depends on higher concentrations of OH. Figure 5.13 reflects this statement. Notice that both chemical mechanisms show equal amounts of OH in the combustion zone.

Figure 5.12: Wall Pressures for Runs 1 and 2
Contour plots of turbulent Prandtl number and turbulent Schmidt number are shown in Figure 5.14. The CARS survey planes are shown along with the symmetry plane. The purpose of this figure is to show that these numbers are indeed variable, and most of the change takes place in the combustion regions.
As listed at the beginning of the chapter, the effects of the compressibility term in the \( k \) equation were investigated. By setting the model constant \( C_1 \) to zero, the term is effectively turned off. With absence of this compressibility term, unstart conditions resulted. This was true for both the vectored injection and normal injection case. Refer to section 5.3.2 for details on the normal injection case. This result stresses the importance of including the effects of compressibility in the turbulence model for supersonic reactive flows.

### 5.2.2 Constant \( \text{Pr}_t / \text{Sc}_t \) Runs

Runs 3 and 4 were for the vectored injection model with constant turbulent Prandtl and Schmidt numbers. Figure 5.15 shows the temperature data from run 3, which used the Connaire chemical mechanism. Keep in mind that the experimental data is smoothed and the computed data is not. The pattern of combustion does not appear to be much different than for the variable \( \text{Pr}_t/\text{Sc}_t \) model, but the flame is thinner and less
intense. Also, plane 5 shows a smaller amount of combustion than is observed with the variable model. This is likely due to the Schmidt number being higher than that for the variable case. Recall that the turbulent Schmidt number is specified as 1.0 for the constant Pr/Sc case.

Figure 5.15: Temperature Contours for Run 3

Figure 5.16 shows the species mole fractions for run 3. The results are slightly degraded over those for the variable Pr/Sc case.
As with the variable case, a direct comparison between the temperature predictions for the Connaire mechanism and the Jachimowski mechanism is shown in Figure 5.17. This reinforces the fact that there are very little differences between the two chemical mechanisms.
Figure 5.17: Temperature from Runs 3 and 4 (Left: Jach., Right: Connaire)

The computed pressure distribution for both chemical mechanisms is shown with the experimental data in Figure 5.18. The pressure from run 1 is shown as well for a variable Pr/Sc comparison. Note that there is almost no change from the variable too the constant model implying that the pressure distribution does not seem to depend on the choice of Pr/Sc model.
5.3 Normal Injection Model

For information on the original normal injection experiment, refer to section 3.1.2, and for information on the computational model used, refer to section 4.2. Only the Jachimowski chemical mechanism was considered for the normal injection case. This should be adequate given the similarity of the two mechanisms for the vectored injection case.
5.3.1 Constant Pr$_t$ / Sc$_t$ Run

As with the vectored injection case, the constant Pr$_t$/Sc$_t$ run for the normal injection case used Pr$_t = 0.9$ and Sc$_t = 1.0$. Note that only planes 1, 3, 6 and 7 were used in this experiment. Figure 5.19 shows the computed and experimental temperature contours from these four planes, and Figure 5.20 shows the nitrogen and oxygen mole fraction contours. In general, the extent of the reaction in the downstream portion of the duct is minimal, much lower than the experimental data. The species profiles reflect this despite the fact that they appear to have slightly better agreement. The air appears to have penetrated to the center of the duct, according to the distribution of nitrogen there.

Figure 5.19: Temperature Contours for Run 5
Figure 5.20: Mole Fraction Contours for Run 5 (left: $N_2$, right: $O_2$)
Figure 5.21 shows the bottom wall pressure for Run 5 and the experimental pressure data. Notice that the location of the initial pressure spike is not captured very well. The pressure “plateau” that is exhibited by the experimental data is not reproduced in the computed result. This is at least part of the reason that the downstream pressure is well underpredicted. The experimental pressure trend suggests that there is an area of large scale separation or intense combustion downstream of the isolator, a phenomenon which has yet to be reproduced in the computation.
5.3.2 Variable Pr \(_t\) / Sc \(_t\) Run

The variable Pr \(_t\) / Sc \(_t\) run, in general, produced better results than the constant case. Figure 5.22 shows the computed temperature profiles for run 6. Notice the significant increase in combustion on plane 3. Also, unlike the vectored injection case, the variable model for this run actually predicted a different flame structure in the downstream portion of the duct. Rather than a vertical “sheet,” the flame takes a “tube” like shape. Although the temperature distribution is still much lower than the experimental data, the shape more closely matches, especially on plane 6. There is also a small region of high temperature upstream of the step, indicating that there is an area of recirculation and/or very low-speed flow allowing hydrogen to diffuse upstream.

![Figure 5.22: Temperature Contours for Run 6](image)
This is confirmed in Figure 5.23, which shows Mach number contours on the symmetry plane in the vicinity of the hydrogen injector. The recirculation upstream of the hydrogen injector and behind the step is quite large. The result is a complex shock-boundary layer interaction on the top and bottom wall at the step. This allows some hydrogen to get entrained along the top wall and diffuse upstream. Since the flow is near stagnation at this point, the temperature is very high and reactions occur quickly.

**Figure 5.23: Mach Contours on Symmetry Plane for Run 6**

Contrast this situation with that of Run 5, which is shown in Figure 5.24. The recirculation ahead of the hydrogen injector is thin here, thus the incoming flow is not obstructed. This is likely the source of the major differences in the flow structure downstream.
Figure 5.24: Mach Contours on Symmetry Plane for Run 5

Figure 5.25 shows the species mole fraction profiles for nitrogen and oxygen. This figure shows that the fuel plume did not penetrate as far as it did for the constant Pr_t/Sc_t case. This is more consistent with the experimental data as well.

Figure 5.26 shows the bottom wall pressure for both runs 5 and 6. The different flow structures that are noted above are reflected in the pressure data. The variable model shows the initial pressure rise at precisely the same location as the experimental data. However, the pressure “plateau” is still not reproduced. While the variable model shows slightly higher pressure downstream, the experiment is still greatly underpredicted. Recall that the experimental wall temperatures were unavailable. The wall temperatures from the vectored injection case were used as a substitute, but upon further examination of the temperature data, it appears that this was a poor substitute. The wall temperatures are higher for the normal injection case and likely more uniform throughout. This could be a major factor in the underprediction of the downstream pressure in the duct.
Figure 5.25: Mole Fraction Contours for Run 6 (left: N₂, right: O₂)

Figure 5.26: Bottom Wall Pressure for Runs 5 and 6
Figure 5.27 and Figure 5.28 are presented to highlight the flow structure in the region upstream of the hydrogen injector. Figure 5.27 is a view from the side of the symmetry plane. The hydrogen spreads to the area behind the step and across the duct to the outer wall. Figure 5.28 shows stream traces that originate in and near the hydrogen injector. While the majority of the fuel plume travels directly downstream, a small portion is entrained in the helical flow that moves from the symmetry plane toward the outer wall. More hydrogen is allowed to travel upstream behind the step once it has reached the outer wall of the duct.

Figure 5.27: 3D Hydrogen Mole Fraction Contours for Run 6
One final consideration is the role of the compressibility term in the solution. It was mentioned in the vectored injection section that when this term is neglected, or set to zero, an unstart results. Figure 5.29 shows the Mach number contours on the symmetry plane in the region upstream of the step. A normal shock has moved upstream of the isolator and thus the flow downstream of it and the majority of the flow in the combustor is largely subsonic. Clearly the compressibility term plays an important role and must be carefully accounted for.
Figure 5.29: Mach Number Contours on Symmetry Plane for Unstart Conditions
6 Conclusions

The turbulence model employed in the current work removes uncertainties in specifying the turbulent Prandtl and Schmidt numbers. Classic turbulence models assume these numbers to be constant and they must be specified before hand. In reality, these numbers are not constant for complex three dimensional flows, and the chosen values can have profound effects on the solution. The model also accounts for turbulence/chemistry interactions, which are certainly necessary for scramjet type flows. Also, an item which has received little attention in the literature is the role of the compressibility correction in the turbulence model. The current results show that neglecting this term results in an unstart condition for this specific experiment. Despite these efforts to improve the modeling, the prediction of ignition location is still difficult. Other factors such as grid resolution and chemical kinetic models can also have a profound effect on ignition location.

In general, the current model shows early ignition and a lack of significant combustion downstream. Even so, the computed temperature profiles do fall within experimental scatter, and when subjected to the same curve fits, the two show very good agreement. This stresses the fact that care must be taken when comparing computed results with smoothed CARS data.

For the normal injection case, the recirculation ahead of the injector acts as a flame holder as predicted, but past the initial shock system, the pressure and amount of combustion are lower than the experiment. Again, there are a number of factors other than the turbulence model that can affect these predictions, but in general, the variable Prt/Scτ model provides better results than the constant model.

It is not practical to generate a large sample when CARS measurements are employed. Thus, the accuracy of the experimental data depends on the size of the sample collected, and statistical methods have to be employed to determine mean properties. Because of this, a more meaningful method of comparing theory and experiments
employing CARS is the use of an LES/RANS approach. Such calculations provide “samples” that require smoothing to determine the mean flow. Thus, using the same smoothing technique for theory and experiment would result in better evaluation of existing turbulence models.
References


Appendix
Appendix A: Governing Equations Vectors

The first term, $\vec{U}$, is the vector of conservative variables, which is as follows.

$$
\vec{U} = \begin{bmatrix}
\rho_a \\
\vdots \\
\rho_{NS} \\
\rho u \\
\rho v \\
\rho w \\
\rho E
\end{bmatrix}
$$

(A.1)

The inviscid flux vectors are represented by $\vec{E}$, $\vec{F}$, and $\vec{G}$.

$$
\vec{E} = \begin{bmatrix}
\rho u \\
\vdots \\
\rho_{NS} u \\
\rho u^2 + p \\
\rho u v \\
\rho u w \\
\rho H u
\end{bmatrix}, \quad
\vec{F} = \begin{bmatrix}
\rho v \\
\vdots \\
\rho_{NS} v \\
\rho v^2 + p \\
\rho v u \\
\rho v w \\
\rho H v
\end{bmatrix}, \quad
\vec{G} = \begin{bmatrix}
\rho w \\
\vdots \\
\rho_{NS} w \\
\rho w u \\
\rho w v \\
\rho w^2 + p \\
\rho H w
\end{bmatrix}
$$

(A.2)

The viscous flux vectors are $\vec{E}_v$, $\vec{F}_v$, and $\vec{G}_v$. 
Finally, $\vec{S}$ is the vector of source terms, which are only non-zero for the species equations.

\[
\vec{S} = \begin{bmatrix}
\dot{\omega}_1 \\
\vdots \\
\dot{\omega}_N \end{bmatrix}
\]

Note that the species densities can be written as either $\rho_m$, as it is here, or as the bulk density times the species mass fraction, $\rho Y_m$. 

\[
(A.4)
\]
Appendix B: Transformation to Generalized Coordinates

As written, the equations are only easily applicable on Cartesian grids. However, the Navier-Stokes equations can be rewritten for a generalized coordinate system, which can then be applied to any curvilinear grid without modification. This generalized coordinate system is defined by three new coordinates: \( \xi = \xi(x, y, z) \), \( \eta = \eta(x, y, z) \), and \( \zeta = \zeta(x, y, z) \). This transforms the physical space of the problem to a Cartesian computational space that has equal unit spacing in all three coordinate directions. The partial derivatives can be represented by the following.

\[
\begin{align*}
\frac{\partial}{\partial x} &= \frac{\partial \xi}{\partial x} \frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial x} \frac{\partial}{\partial \eta} + \frac{\partial \zeta}{\partial x} \frac{\partial}{\partial \zeta} \\
\frac{\partial}{\partial y} &= \frac{\partial \xi}{\partial y} \frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial y} \frac{\partial}{\partial \eta} + \frac{\partial \zeta}{\partial y} \frac{\partial}{\partial \zeta} \\
\frac{\partial}{\partial z} &= \frac{\partial \xi}{\partial z} \frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial z} \frac{\partial}{\partial \eta} + \frac{\partial \zeta}{\partial z} \frac{\partial}{\partial \zeta}
\end{align*}
\]

(B.1)

The metric derivatives, such as \( \partial \xi/\partial x \) are represented using the shorthand \( \bar{\xi} \). The transformed RANS equations are written here in the vector conservation form [20].

\[
\frac{\partial \hat{U}}{\partial t} + \frac{\partial (\hat{E} - \hat{E}_r)}{\partial \xi} + \frac{\partial (\hat{F} - \hat{F}_r)}{\partial \eta} + \frac{\partial (\hat{G} - \hat{G}_r)}{\partial \zeta} = \hat{S}
\]

(B.2)

The vector of conserved variables is defined by the following.

\[
\hat{U} = \begin{bmatrix}
\bar{\rho}_i \\
\vdots \\
\bar{\rho}_{NS} \\
\bar{\rho}u \\
\bar{\rho}v \\
\bar{\rho}w \\
\bar{\rho}E
\end{bmatrix}
\]

(B.3)

The generalized inviscid flux vectors are defined as:
Finally, the generalized viscous flux vectors are as follows.

\[
\hat{E} = \frac{\xi_x}{J} \hat{E} + \frac{\xi_y}{J} \hat{F} + \frac{\xi_z}{J} \hat{G} = \frac{1}{J} \begin{bmatrix}
\vec{\rho}_1 \vec{\tilde{U}}_c \\
\vdots \\
\vec{\rho}_{\text{NS}} \vec{\tilde{U}}_c \\
\vec{\rho}_1 \vec{\tilde{V}}_c \\
\vdots \\
\vec{\rho}_{\text{NS}} \vec{\tilde{V}}_c \\
\vec{\rho}_1 \vec{\tilde{W}}_c \\
\vdots \\
\vec{\rho}_{\text{NS}} \vec{\tilde{W}}_c
\end{bmatrix}
\]  

(B.4)

\[
\hat{F} = \frac{\eta_x}{J} \hat{E} + \frac{\eta_y}{J} \hat{F} + \frac{\eta_z}{J} \hat{G} = \frac{1}{J} \begin{bmatrix}
\vec{\rho}_1 \vec{\tilde{V}}_c \\
\vdots \\
\vec{\rho}_{\text{NS}} \vec{\tilde{V}}_c \\
\vec{\rho}_1 \vec{\tilde{W}}_c \\
\vdots \\
\vec{\rho}_{\text{NS}} \vec{\tilde{W}}_c
\end{bmatrix}
\]  

(B.5)

\[
\hat{G} = \frac{\xi_x}{J} \hat{E} + \frac{\xi_y}{J} \hat{F} + \frac{\xi_z}{J} \hat{G} = \frac{1}{J} \begin{bmatrix}
\vec{\rho}_1 \vec{\tilde{W}}_c \\
\vdots \\
\vec{\rho}_{\text{NS}} \vec{\tilde{W}}_c \\
\vec{\rho}_1 \vec{\tilde{U}}_c \\
\vdots \\
\vec{\rho}_{\text{NS}} \vec{\tilde{U}}_c
\end{bmatrix}
\]  

(B.6)

\[
\hat{E}_v = \frac{1}{J} \begin{bmatrix}
-\vec{\rho}_1 \vec{\tilde{U}}_1 + \left( \xi_x Y_{1,x} + \xi_y Y_{1,y} + \xi_z Y_{1,z} \right) \\
\vdots \\
-\vec{\rho}_{\text{NS}} \vec{\tilde{U}}_{\text{NS}} + \left( \xi_x Y_{\text{NS},x} + \xi_y Y_{\text{NS},y} + \xi_z Y_{\text{NS},z} \right) \\
\xi_x \left( \tau_{xx} + T_{xx} \right) + \xi_y \left( \tau_{xy} + T_{xy} \right) + \xi_z \left( \tau_{xz} + T_{xz} \right) \\
\xi_x \left( \tau_{yx} + T_{yx} \right) + \xi_y \left( \tau_{yy} + T_{yy} \right) + \xi_z \left( \tau_{yz} + T_{yz} \right) \\
\xi_x \left( \tau_{zx} + T_{zx} \right) + \xi_y \left( \tau_{zy} + T_{zy} \right) + \xi_z \left( \tau_{zz} + T_{zz} \right) \\
\xi_x \left( \tilde{u}(\tau_{xx} + T_{xx}) + \tilde{v}(\tau_{xy} + T_{xy}) + \tilde{w}(\tau_{xz} + T_{xz}) + q_x + Q_x \right) + \xi_y \left( \tilde{u}(\tau_{yx} + T_{yx}) + \tilde{v}(\tau_{yy} + T_{yy}) + \tilde{w}(\tau_{yz} + T_{yz}) + q_y + Q_y \right) + \xi_z \left( \tilde{u}(\tau_{zx} + T_{zx}) + \tilde{v}(\tau_{zy} + T_{zy}) + \tilde{w}(\tau_{zz} + T_{zz}) + q_z + Q_z \right)
\end{bmatrix}
\]  

(B.7)
\[
\hat{F}_v = \frac{1}{J} \begin{bmatrix}
-\overline{\rho} \tilde{V}_1 + (\eta_x Y_{1,x} + \eta_y Y_{1,y} + \eta_z Y_{1,z}) \\
\vdots \\
-\overline{\rho}_{NS} \tilde{V}_{NS} + (\eta_x Y_{NS,x} + \eta_y Y_{NS,y} + \eta_z Y_{NS,z}) \\
\eta_x (\tilde{r}_{xx} + T_{xx}) + \eta_y (\tilde{r}_{xy} + T_{xy}) + \eta_z (\tilde{r}_{xz} + T_{xz}) \\
\eta_x (\tilde{r}_{yx} + T_{yx}) + \eta_y (\tilde{r}_{yy} + T_{yy}) + \eta_z (\tilde{r}_{yz} + T_{yz}) \\
\eta_x (\tilde{r}_{zx} + T_{zx}) + \eta_y (\tilde{r}_{zy} + T_{zy}) + \eta_z (\tilde{r}_{zz} + T_{zz}) \\
\eta_x (\tilde{w}_x + \tilde{r}_{xx} + \tilde{m}_x + \tilde{q}_x + Q_x) \\
+ \eta_y (\tilde{w}_y + \tilde{r}_{xy} + \tilde{m}_y + \tilde{q}_y + Q_y) \\
+ \eta_z (\tilde{w}_z + \tilde{r}_{xz} + \tilde{m}_z + \tilde{q}_z + Q_z)
\end{bmatrix}
\]

\[
\hat{G}_v = \frac{1}{J} \begin{bmatrix}
-\overline{\rho} \tilde{W}_1 + (\zeta_x Y_{1,x} + \zeta_y Y_{1,y} + \zeta_z Y_{1,z}) \\
\vdots \\
-\overline{\rho}_{NS} \tilde{W}_{NS} + (\zeta_x Y_{NS,x} + \zeta_y Y_{NS,y} + \zeta_z Y_{NS,z}) \\
\zeta_x (\tilde{r}_{xx} + T_{xx}) + \zeta_y (\tilde{r}_{xy} + T_{xy}) + \zeta_z (\tilde{r}_{xz} + T_{xz}) \\
\zeta_x (\tilde{r}_{yx} + T_{yx}) + \zeta_y (\tilde{r}_{yy} + T_{yy}) + \zeta_z (\tilde{r}_{yz} + T_{yz}) \\
\zeta_x (\tilde{r}_{zx} + T_{zx}) + \zeta_y (\tilde{r}_{zy} + T_{zy}) + \zeta_z (\tilde{r}_{zz} + T_{zz}) \\
\zeta_x (\tilde{w}_x + \tilde{r}_{xx} + \tilde{m}_x + \tilde{q}_x + Q_x) \\
+ \zeta_y (\tilde{w}_y + \tilde{r}_{xy} + \tilde{m}_y + \tilde{q}_y + Q_y) \\
+ \zeta_z (\tilde{w}_z + \tilde{r}_{xz} + \tilde{m}_z + \tilde{q}_z + Q_z)
\end{bmatrix}
\]

The turbulent Reynolds stress tensor, the turbulent species diffusion vector, and the turbulent heat flux vector are represented here by \(T_{i,j}, Y_{m,i}\), and \(Q_i\) respectively. The source vector is as follows.

\[
\hat{S} = \frac{1}{J} \begin{bmatrix}
\overline{\omega}_1 \\
\vdots \\
\overline{\omega}_{NS} \\
0 \\
0 \\
0 \\
0
\end{bmatrix}
\]

The contravariant velocity components are those that are defined in the grid aligned coordinate system. These are defined below along with the contravariant species diffusion velocities.
\[ \tilde{U}_c = \xi_x \tilde{u} + \xi_y \tilde{v} + \xi_z \tilde{w} \]
\[ \tilde{V}_c = \eta_x \tilde{u} + \eta_y \tilde{v} + \eta_z \tilde{w} \]
\[ \tilde{W}_c = \zeta_x \tilde{u} + \zeta_y \tilde{v} + \zeta_z \tilde{w} \]

\[ \tilde{U}_m = \xi_x \tilde{V}_{x,m} + \xi_y \tilde{V}_{y,m} + \xi_z \tilde{V}_{z,m} \]
\[ \tilde{V}_m = \eta_x \tilde{V}_{x,m} + \eta_y \tilde{V}_{y,m} + \eta_z \tilde{V}_{z,m} \quad m = 1, 2, \ldots, \text{NS} \]
\[ \tilde{W}_m = \zeta_x \tilde{V}_{x,m} + \zeta_y \tilde{V}_{y,m} + \zeta_z \tilde{V}_{z,m} \]

Finally, the transformation Jacobian, \( J \), is defined by:
\[ J = \frac{\partial (\xi, \eta, \zeta)}{\partial (x, y, z)} \]

The inverse of the Jacobian, \( 1/J \), can be interpreted as the cell volume and is evaluated as such.
Appendix C: Chemical Kinetic Mechanism Parameters

Table C.1: Abridged Jachimowski Mechanism Reactions

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_1$</td>
<td>$H + OH + M \leftrightarrow H_2O + M$</td>
</tr>
<tr>
<td>$R_2$</td>
<td>$H + H + M \leftrightarrow H_2 + M$</td>
</tr>
<tr>
<td>$R_3$</td>
<td>$H_2 + O_2 \leftrightarrow OH + OH$</td>
</tr>
<tr>
<td>$R_4$</td>
<td>$H + O_2 \leftrightarrow OH + O$</td>
</tr>
<tr>
<td>$R_5$</td>
<td>$OH + H_2 \leftrightarrow H_2O + H$</td>
</tr>
<tr>
<td>$R_6$</td>
<td>$O + H_2 \leftrightarrow OH + H$</td>
</tr>
<tr>
<td>$R_7$</td>
<td>$OH + OH \leftrightarrow H_2O + O$</td>
</tr>
</tbody>
</table>

Table C.2: Abridged Jachimowski Mechanism Parameters

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$A$ (cal/mol)</th>
<th>$\eta$</th>
<th>$E_a$ (mol cm sec K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$2.21E+22$</td>
<td>$-2.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>2</td>
<td>$7.30E+17$</td>
<td>$-1.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>3</td>
<td>$1.70E+13$</td>
<td>$0.0$</td>
<td>$48000.0$</td>
</tr>
<tr>
<td>4</td>
<td>$1.20E+17$</td>
<td>$-0.9$</td>
<td>$16800.0$</td>
</tr>
<tr>
<td>5</td>
<td>$2.20E+13$</td>
<td>$0.0$</td>
<td>$5150.0$</td>
</tr>
<tr>
<td>6</td>
<td>$5.06E+04$</td>
<td>$2.7$</td>
<td>$6268.0$</td>
</tr>
<tr>
<td>7</td>
<td>$6.30E+12$</td>
<td>$0.0$</td>
<td>$1090.0$</td>
</tr>
</tbody>
</table>
Table C.3: Connaire et al. Mechanism Reactions

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_1$</td>
<td>$H + O_2 \leftrightarrow O + OH$</td>
</tr>
<tr>
<td>$R_2$</td>
<td>$O + H_2 \leftrightarrow H + OH$</td>
</tr>
<tr>
<td>$R_3$</td>
<td>$OH + H_2 \leftrightarrow H + H_2O$</td>
</tr>
<tr>
<td>$R_4$</td>
<td>$O + H_2O \leftrightarrow OH + OH$</td>
</tr>
<tr>
<td>$R_5$</td>
<td>$H_2 + M \leftrightarrow H + H + M$</td>
</tr>
<tr>
<td>$R_6$</td>
<td>$O + O + M \leftrightarrow O_2 + M$</td>
</tr>
<tr>
<td>$R_7$</td>
<td>$O + H + M \leftrightarrow OH + M$</td>
</tr>
<tr>
<td>$R_8$</td>
<td>$H + OH + M \leftrightarrow H_2O + M$</td>
</tr>
<tr>
<td>$R_{9A}$</td>
<td>$H + O_2 + M \leftrightarrow HO_2 + M$</td>
</tr>
<tr>
<td>$R_{9B}$</td>
<td>$H + O_2 \leftrightarrow HO_2$</td>
</tr>
<tr>
<td>$R_{10}$</td>
<td>$HO_2 + H \leftrightarrow H_2 + O_2$</td>
</tr>
<tr>
<td>$R_{11}$</td>
<td>$HO_2 + H \leftrightarrow OH + OH$</td>
</tr>
<tr>
<td>$R_{12}$</td>
<td>$HO_2 + O \leftrightarrow OH + O_2$</td>
</tr>
<tr>
<td>$R_{13}$</td>
<td>$HO_2 + OH \leftrightarrow H_2O + O_2$</td>
</tr>
<tr>
<td>$R_{14A}$</td>
<td>$HO_2 + HO_2 \leftrightarrow H_2O_2 + O_2$</td>
</tr>
<tr>
<td>$R_{14B}$</td>
<td>$HO_2 + HO_2 \leftrightarrow H_2O_2 + O_2$</td>
</tr>
<tr>
<td>$R_{15A}$</td>
<td>$H_2O_2 + M \leftrightarrow OH + OH + M$</td>
</tr>
<tr>
<td>$R_{15B}$</td>
<td>$H_2O_2 \leftrightarrow OH + OH$</td>
</tr>
<tr>
<td>$R_{16}$</td>
<td>$H_2O_2 + H \leftrightarrow H_2O + OH$</td>
</tr>
<tr>
<td>$R_{17}$</td>
<td>$H_2O_2 + H \leftrightarrow H_2 + HO_2$</td>
</tr>
<tr>
<td>$R_{18}$</td>
<td>$H_2O_2 + O \leftrightarrow OH + HO_2$</td>
</tr>
<tr>
<td>$R_{19A}$</td>
<td>$H_2O_2 + OH \leftrightarrow H_2O + HO_2$</td>
</tr>
<tr>
<td>$R_{19B}$</td>
<td>$H_2O_2 + OH \leftrightarrow H_2O + HO_2$</td>
</tr>
<tr>
<td>Reaction</td>
<td>$A , (\text{cal/mol})$</td>
</tr>
<tr>
<td>----------</td>
<td>------------------------</td>
</tr>
<tr>
<td>1</td>
<td>$1.91E+14$</td>
</tr>
<tr>
<td>2</td>
<td>$5.08E+4$</td>
</tr>
<tr>
<td>3</td>
<td>$2.16E+8$</td>
</tr>
<tr>
<td>4</td>
<td>$2.97E+6$</td>
</tr>
<tr>
<td>5</td>
<td>$4.57E+19$</td>
</tr>
<tr>
<td>6</td>
<td>$6.17E+15$</td>
</tr>
<tr>
<td>7</td>
<td>$4.72E+18$</td>
</tr>
<tr>
<td>8</td>
<td>$4.50E+22$</td>
</tr>
<tr>
<td>$9A$</td>
<td>$3.48E+16$</td>
</tr>
<tr>
<td>$9B$</td>
<td>$1.48E+12$</td>
</tr>
<tr>
<td>10</td>
<td>$1.66E+13$</td>
</tr>
<tr>
<td>11</td>
<td>$7.08E+13$</td>
</tr>
<tr>
<td>12</td>
<td>$3.25E+13$</td>
</tr>
<tr>
<td>13</td>
<td>$2.89E+13$</td>
</tr>
<tr>
<td>$14A$</td>
<td>$4.20E+14$</td>
</tr>
<tr>
<td>$14B$</td>
<td>$1.30E+11$</td>
</tr>
<tr>
<td>$15A$</td>
<td>$1.27E+17$</td>
</tr>
<tr>
<td>$15B$</td>
<td>$2.95E+14$</td>
</tr>
<tr>
<td>16</td>
<td>$2.41E+13$</td>
</tr>
<tr>
<td>17</td>
<td>$6.03E+13$</td>
</tr>
<tr>
<td>18</td>
<td>$9.55E+6$</td>
</tr>
<tr>
<td>$19A$</td>
<td>$1.00E+12$</td>
</tr>
<tr>
<td>$19B$</td>
<td>$5.80E+14$</td>
</tr>
</tbody>
</table>
Table C.5: Connaire et al. Mechanism Third Body Efficiencies

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$H_2O$</th>
<th>$H_2$</th>
<th>$Ar/He$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>12.0</td>
<td>2.5</td>
<td>1.0</td>
</tr>
<tr>
<td>6</td>
<td>12.0</td>
<td>2.5</td>
<td>0.83</td>
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<tr>
<td>7</td>
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<td>0.75</td>
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<td>8</td>
<td>12.0</td>
<td>0.73</td>
<td>0.38</td>
</tr>
<tr>
<td>9</td>
<td>14.0</td>
<td>1.3</td>
<td>0.67</td>
</tr>
<tr>
<td>15</td>
<td>12.0</td>
<td>2.5</td>
<td>0.45</td>
</tr>
</tbody>
</table>
Appendix D: Complete Equation Set in Vector Form

\[ \hat{U} = \begin{bmatrix} \bar{p}_1 \\ \vdots \\ \bar{p}_{NS} \\ \bar{p} u \\ \bar{p} v \\ \bar{p} w \\ \bar{p} \bar{E} \\ \bar{p} k \\ \bar{p} \zeta \\ \bar{p} \sigma_y \\ \bar{p} \varepsilon_y \\ \bar{p} h'^{2} \\ \bar{p} \varepsilon_h \end{bmatrix} \] \quad (D.1)

The inviscid flux vectors are:

\[ \hat{E} = \frac{1}{J} \begin{bmatrix} \bar{p}_i \bar{U}_c \\ \vdots \\ \bar{p}_{NS} \bar{U}_c \\ \bar{p} \bar{U}_c + \xi, \bar{p} \\ \bar{p} \bar{v} \bar{U}_c + \xi, \bar{p} \\ \bar{p} \bar{w} \bar{U}_c + \xi, \bar{p} \\ \bar{p} \bar{H} \bar{U}_c \\ \bar{p} k \bar{U}_c \\ \bar{p} \zeta \bar{U}_c \\ \bar{p} \sigma_y \bar{U}_c \\ \bar{p} \varepsilon_y \bar{U}_c \\ \bar{p} h'^{2} \bar{U}_c \\ \bar{p} \varepsilon_h \bar{U}_c \end{bmatrix}, \quad \hat{F} = \frac{1}{J} \begin{bmatrix} \bar{p}_i \bar{V}_c \\ \vdots \\ \bar{p}_{NS} \bar{V}_c \\ \bar{p} \bar{V}_c + \eta, \bar{p} \\ \bar{p} \bar{v} \bar{V}_c + \eta, \bar{p} \\ \bar{p} \bar{w} \bar{V}_c + \eta, \bar{p} \\ \bar{p} \bar{H} \bar{V}_c \\ \bar{p} k \bar{V}_c \\ \bar{p} \zeta \bar{V}_c \\ \bar{p} \sigma_y \bar{V}_c \\ \bar{p} \varepsilon_y \bar{V}_c \\ \bar{p} h'^{2} \bar{V}_c \end{bmatrix}, \quad \hat{G} = \frac{1}{J} \begin{bmatrix} \bar{p}_i \bar{W}_c \\ \vdots \\ \bar{p}_{NS} \bar{W}_c \\ \bar{p} \bar{W}_c + \zeta, \bar{p} \\ \bar{p} \bar{v} \bar{W}_c + \zeta, \bar{p} \\ \bar{p} \bar{w} \bar{W}_c + \zeta, \bar{p} \\ \bar{p} \bar{H} \bar{W}_c \\ \bar{p} k \bar{W}_c \\ \bar{p} \zeta \bar{W}_c \\ \bar{p} \sigma_y \bar{W}_c \\ \bar{p} \varepsilon_y \bar{W}_c \\ \bar{p} h'^{2} \bar{W}_c \end{bmatrix} \] \quad (D.2)
The viscous flux vectors are as follows. Note the use of index notation to simplify the expressions.

\[
\hat{E}_v = \frac{1}{J} \begin{bmatrix}
- \bar{\rho} \bar{U}_1 + \xi_{x_1} Y_{1,j} \\
\vdots \\
- \bar{\rho}_{NS} \bar{U}_{NS} + \xi_{x_{NS}} Y_{NS,j} \\
\xi_{x_1} (\bar{r}_{x_1} + T_{x_1}) \\
\xi_{x_2} (\bar{r}_{x_2} + T_{x_2}) \\
\xi_{x_3} (\bar{r}_{x_3} + T_{x_3}) \\
\xi_{x_4} (\bar{u}_j (\bar{r}_j + T_{x_5}) + \bar{q}_i + Q_i) \\
\xi_{x_5} \left( \frac{\mu + \mu_i}{3} \right) \frac{\partial k}{\partial x_i} \\
\xi_{x_6} \left( \mu + \frac{\mu_i}{\sigma_k} \right) \frac{\partial \zeta}{\partial x_i} \\
\xi_{x_7} \bar{\rho} (D + C_{Y,1} D_1) \frac{\partial \sigma_y}{\partial x_i} \\
\xi_{x_8} \bar{\rho} (D + C_{Y,5} D_1) \frac{\partial \varepsilon_y}{\partial x_i} \\
\xi_{x_9} \bar{\rho} (\gamma \alpha + C_{h,2} \alpha_i) \frac{\partial h^{n^2}/2}{\partial x_i} \\
\xi_{x_10} \bar{\rho} (\gamma \alpha + C_{h,5} \alpha_i) \frac{\partial \varepsilon_h}{\partial x_i}
\end{bmatrix}
\]

\[
\hat{F}_v = \frac{1}{J} \begin{bmatrix}
- \bar{\rho} \bar{V}_1 + \eta_{x_1} Y_{1,j} \\
\vdots \\
- \bar{\rho}_{NS} \bar{V}_{NS} + \eta_{x_{NS}} Y_{NS,j} \\
\eta_{x_1} (\bar{r}_{x_1} + T_{x_1}) \\
\eta_{x_2} (\bar{r}_{x_2} + T_{x_2}) \\
\eta_{x_3} (\bar{r}_{x_3} + T_{x_3}) \\
\eta_{x_4} (\bar{u}_j (\bar{r}_j + T_{x_5}) + \bar{q}_i + Q_i) \\
\eta_{x_5} \left( \frac{\mu + \mu_i}{3} \right) \frac{\partial k}{\partial x_i} \\
\eta_{x_6} \left( \mu + \frac{\mu_i}{\sigma_k} \right) \frac{\partial \zeta}{\partial x_i} \\
\eta_{x_7} \bar{\rho} (D + C_{Y,1} D_1) \frac{\partial \sigma_y}{\partial x_i} \\
\eta_{x_8} \bar{\rho} (D + C_{Y,5} D_1) \frac{\partial \varepsilon_y}{\partial x_i} \\
\eta_{x_9} \bar{\rho} (\gamma \alpha + C_{h,2} \alpha_i) \frac{\partial h^{n^2}/2}{\partial x_i} \\
\eta_{x_10} \bar{\rho} (\gamma \alpha + C_{h,5} \alpha_i) \frac{\partial \varepsilon_h}{\partial x_i}
\end{bmatrix}
\]

(D.3)
\[
\hat{G}_v = \frac{1}{J} \begin{bmatrix}
- \bar{p}_1 \hat{W}_1 + \zeta_{x_i} Y_{ij} \\
\vdots \\
- \bar{p}_{NS} \hat{W}_{NS} + \zeta_{x_i} Y_{NS,j} \\
\zeta_{x_i} (\bar{r}_{ix} + T_{ix}) \\
\zeta_{x_i} (\bar{r}_{iy} + T_{iy}) \\
\zeta_{x_i} (\bar{r}_{iz} + T_{iz}) \\
\zeta_{x_i} (\bar{u}_j (\bar{r}_{ij} + T_{ij}) + \bar{q}_j + Q_1) \\
\zeta_{x_i} \left( \frac{\mu}{3} + \frac{\mu_k}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \\
\zeta_{x_i} \left( \mu + \frac{\mu_k}{\sigma_k} \right) \frac{\partial \zeta}{\partial x_i} \\
\zeta_{x_i} (D + C_{x,y_i} D_j) \frac{\partial \sigma_y}{\partial x_i} \\
\zeta_{x_i} (D + C_{x,y} D_j) \frac{\partial e_y}{\partial x_i} \\
\zeta_{x_i} \bar{p} (\gamma \alpha + C_{h,2} \alpha_i) \frac{\partial h^{n^2}/2}{\partial x_i} \\
\zeta_{x_i} \bar{p} (\gamma \alpha + C_{h,7} \alpha_i) \frac{\partial \varepsilon_h}{\partial x_i}
\end{bmatrix}
\]
Finally, the source vector is:

\[
\hat{S} = \frac{1}{J} \begin{bmatrix}
\bar{\omega}_1 \\
\vdots \\
\bar{\omega}_{NS} \\
0 \\
0 \\
0 \\
0 \\
0 \\
S_k \\
S_\zeta \\
S_{\sigma_y} \\
S_{er} \\
S_k' \\
S_{sa}
\end{bmatrix}
\]  

Refer to Section 2.5 for the turbulence source terms.
Appendix E: Numerical Formulation

The purpose of this appendix is to describe the procedures and approximations used to solve the set of equations presented in Section 2.6. A finite volume discretization is employed. This method is chosen for a number of reasons. Unlike finite difference, finite volume does not result in geometric conservation errors on highly deformed grids. Using a finite volume discretization is also easily applied to the strong conservation form of the equations. This allows for the formation of discontinuous, or weak, solutions to the differential equations [20]. A second order Essentially Non-Oscillatory (ENO) or Total Variation Diminishing (TVD) limiting scheme is used along with the Low Diffusion Flux Splitting Scheme (LDFSS) of Edwards [14]. Planar relaxation is used to advance the steady state solution.

E.1 Finite Volume Discretization

In a finite volume discretization, information is stored at cell centers rather than at the nodes of the mesh. The cell properties are considered constant across the entire cell, so the representation could be viewed as a piecewise constant model. This technique requires the integral form of the governing equations rather than the differential form. To obtain the integral form, the equations are integrated over a finite control volume.

\[
\int_{V} \left( \frac{\partial \tilde{U}}{\partial t} + \nabla \cdot \tilde{F} \right) dV_{CV} = \tilde{S} \tag{E.1}
\]

Gauss’ theorem is used to convert the volume integral of the flux to a surface integral. This equation set is then applied to each cell of the computational mesh.

\[
\int_{V} \frac{\partial \tilde{U}}{\partial t} dV_{CV} + \int_{A_{CV}} (\tilde{F} \cdot \hat{n}) dA_{CV} = \tilde{S} \tag{E.2}
\]
Assuming the volume of a cell does not change over time, the volume integral simply becomes the cell volume times the partial derivative of the conservative variable vector with respect to time. The surface integral is decomposed into a discrete sum of the flux over each face of the cell. For a structured mesh, there are six faces, two associated with each coordinate direction. For notational purposes, the indices \( i, j, \) and \( k \), are associated with the \( \xi, \eta, \) and \( \zeta \) directions respectively. Assuming the flux to be constant across each cell face, the integral equation can be rewritten in the following form.

\[
\nu \frac{\partial \vec{U}}{\partial t} + \tilde{E}_{i+\frac{1}{2},j,k} - \tilde{E}_{i-\frac{1}{2},j,k} + \tilde{F}_{i,j+\frac{1}{2},k} - \tilde{F}_{i,j-\frac{1}{2},k} + \tilde{G}_{i,j,k+\frac{1}{2}} - \tilde{G}_{i,j,k-\frac{1}{2}} = \vec{S} \tag{E.3}
\]

The tilde over the flux vectors denotes an average over the face. The \( \pm \frac{1}{2} \) on the indices denotes the cell face to the right or left of the cell center. This equation can now be integrated in time using a number of schemes. A planar implicit scheme is used in the current work and it is described in Section E.4.

### E.2 Flux Reconstruction Scheme

As mentioned above, the flux scheme is based on the Low Diffusion Flux Splitting Scheme (LDFSS) of Edwards. Due to the mixed character of the Navier-Stokes equations and the inviscid subset, the Euler equations, care must be taken in the reconstruction of the flux at the cell interfaces. In supersonic flow, the mathematical character of the equations is hyperbolic, meaning that information can only propagate in one direction. In subsonic flow, the mathematical character is elliptic, which means that information propagates in all directions. Both of these flow conditions can easily arise in typical engineering problems, and thus care must be taken to ensure that the directions of information propagation are accurately represented in the flux reconstruction. A method known as “upwinding” is used here.
E.2.1 Inviscid Flux Splitting

The LDFSS upwind differencing technique is similar to the flux vector splitting scheme of van Leer. LDFSS incorporates some ideas of flux difference splitting in order to increase the ability to sharply capture stationary and moving contact waves as well as maintain the monotonicity of strong discontinuities. The inviscid flux at a cell interface is separated into the convective portion and the pressure portion.

\[ \vec{E}_{i+\frac{1}{2}} = \vec{E}_{i+\frac{1}{2}}^C + \vec{E}_{i+\frac{1}{2}}^p \]  

(E.4)

The \( j \) and \( k \) indices are constant throughout and are therefore not shown. The convective portion of the inviscid flux is defined as:

\[ \vec{E}_{i+\frac{1}{2}}^C = A_{i+\frac{1}{2}} \bar{a}_{i+\frac{1}{2}} \left( \bar{\rho}_L C_E^+ \phi_L^C + \bar{\rho}_R C_E^- \phi_R^C \right) \]  

(E.5)

The ‘\( L \)’ and ‘\( R \)’ represent the state to the left and to the right of the interface. For a first order spatial scheme, this can simply be the data at ‘\( i \)’ and ‘\( i + 1 \)’ respectively. The current work employs a more accurate representation of this data that is extrapolated to the interface from each direction. This method is described in Section E.3. The pressure portion of the flux is:

\[ \vec{E}_{i+\frac{1}{2}}^p = A_{i+\frac{1}{2}} \left[ \left( D^+ P_L^* + D^- P_R^* \right) \phi^p \right] \]  

(E.6)

The \( \phi \) vectors are listed below.
\[
\phi_{L/R}^C = \begin{bmatrix}
\tilde{Y}_t \\
\vdots \\
\tilde{Y}_{NS} \\
\tilde{u} \\
\tilde{v} \\
\tilde{w} \\
\tilde{H} \\
k \\
\zeta \\
\sigma_Y \\
\hat{v}_y \\
\hat{h}^{*2} \\
\epsilon_h
\end{bmatrix}_{L/R}, \quad \phi^p = \begin{bmatrix}
0 \\
\vdots \\
0 \\
\hat{n}_{x,i+\frac{1}{2}} \\
\hat{n}_{y,i+\frac{1}{2}} \\
\hat{n}_{z,i+\frac{1}{2}} \\
0 \\
0 \\
0 \\
0 \\
0 \\
0 \\
0
\end{bmatrix}
\] (E.7)

\(A_{i+\frac{1}{2}}\) is the area of the interface and is defined by the following, given the metric derivatives at that face.

\[
A_{i+\frac{1}{2}} = \sqrt{\left(\frac{\xi_x}{J}\right)^2 + \left(\frac{\xi_y}{J}\right)^2 + \left(\frac{\xi_z}{J}\right)^2} \quad (E.8)
\]

This can of course be applied in the other coordinate directions as well. The normal vectors that show up in the pressure flux are defined as follows.

\[
\hat{n}_{x,i+\frac{1}{2}} = \frac{\xi_x}{A_{i+\frac{1}{2}}}, \quad \hat{n}_{y,i+\frac{1}{2}} = \frac{\xi_y}{A_{i+\frac{1}{2}}}, \quad \hat{n}_{z,i+\frac{1}{2}} = \frac{\xi_z}{A_{i+\frac{1}{2}}} \quad (E.9)
\]

Since a common sound speed is used at the interface, the Mach numbers at the left and right state must be redefined as:

\[M_L = \tilde{U}_L / a_{i+\frac{1}{2}}, \quad M_R = \tilde{U}_R / a_{i+\frac{1}{2}} \quad (E.10)\]

Recall that the tilde over the \(U\) denotes the interface aligned velocity. The pressure splitting terms are defined below.

\[
D^+ = \alpha_L^+(1 + \beta_L) - \beta_L P_L^+, \quad D^- = \alpha_R^-(1 + \beta_R) - \beta_R P_R^- \quad (E.11)
\]

\[
P_L^+ = \frac{\alpha_L^+}{4} (M_L + 1)^3 (2 - M_L), \quad P_R^- = \frac{\alpha_R^-}{4} (M_R - 1)^3 (2 + M_R) \quad (E.12)
\]
The $\alpha$’s and $\beta$’s account for switches in Eigen values at sonic and stagnation points. They are:

$$\alpha_L^+ = \frac{1}{2} \left[ 1.0 + \mathrm{sign}(M_L) \right], \quad \alpha_R^- = \frac{1}{2} \left[ 1.0 - \mathrm{sign}(M_R) \right]$$  \hspace{1cm} (E.13)

$$\beta_L = -\max\left[ 0.0, 1.0 - \mathrm{int}\left[ |M_L| \right] \right], \quad \beta_R = -\max\left[ 0.0, 1.0 - \mathrm{int}\left[ |M_R| \right] \right]$$  \hspace{1cm} (E.14)

The van Leer scheme defines the split Mach numbers as:

$$C_{IL}^+ = \alpha_L^+(1 + \beta_L)M_L - \beta_L M_L^+, \quad C_{VL}^- = \alpha_R^-(1 + \beta_R)M_R - \beta_R M_R^-$$  \hspace{1cm} (E.15)

$$M_L^+ = \frac{1}{4}(M_L + 1)^2, \quad M_R^- = -\frac{1}{4}(M_R - 1)^2$$  \hspace{1cm} (E.16)

Using this computed data, the LDFSS redefines the split Mach numbers.

$$C_E^+ = C_{VL}^+ - M_{\frac{E}{2}}^+, \quad C_E^- = C_{VL}^- + M_{\frac{E}{2}}^-$$  \hspace{1cm} (E.17)

where

$$M_{\frac{E}{2}}^+ = M_{\frac{E}{2}} \left( 1 - \frac{(\overline{p}_L - \overline{p}_R)}{2 \overline{p}_L a_{\frac{E}{2}}} \right), \quad M_{\frac{E}{2}}^- = M_{\frac{E}{2}} \left( 1 + \frac{(\overline{p}_L - \overline{p}_R)}{2 \overline{p}_R a_{\frac{E}{2}}} \right),$$ \hspace{1cm} (E.18)

$$M_{\frac{E}{2}} = \frac{1}{2} \left[ C_{VL}^+ - \alpha_L^+ M_L - C_{VL}^- + \alpha_R^- M_R \right]$$

This method can be applied to the interface on the opposite side of the cell by a simple index shift. The $\eta$ and $\zeta$ coordinate direction fluxes are computed similarly.

E.2.2 Viscous Flux Calculation

The viscous and diffusion terms in the flux are calculated using simple central differences about the cell interface. This provides a second order discretization for these terms. The total flux is the sum of the inviscid and viscous fluxes.

$$\vec{E}_{i+\frac{1}{2}} = \vec{E}_{i+\frac{1}{2}}^i + \vec{E}_{i+\frac{1}{2}}^v$$  \hspace{1cm} (E.19)

The fluxes at the other five faces of each cell are determined in the same manner.
E.3 Higher Order Extension

A higher order spatial discretization can be achieved if the conservative or primitive variables are extrapolated to the cell interfaces rather than assuming that the properties are constant across the entire cell. A method known as the Monotone Upwind Scheme for Conservation Laws (MUSCL extrapolation) is used in the current work [20]. Rather than assuming a piecewise constant distribution of properties, the data is assumed to be piecewise linear or quadratic. The Kappa scheme is based on this idea.

\[ \tilde{u}_L = \tilde{u}_i + \frac{1}{4} \left( (1 - \kappa) \Delta \tilde{u}_{i-1} + (1 + \kappa) \Delta \tilde{u}_i \right) \]  
(E.20)

\[ \tilde{u}_R = \tilde{u}_{i+1} - \frac{1}{4} \left( (1 - \kappa) \Delta \tilde{u}_{i+1} + (1 + \kappa) \Delta \tilde{u}_i \right) \]  
(E.21)

\[ \Delta \tilde{u}_i = \tilde{u}_{i+1} - \tilde{u}_i \]  
(E.22)

Again, the \( j \) and \( k \) indices are assumed to be constant, and this method can be applied in those directions as well. The resulting extrapolation depends on the value chosen for \( \kappa \). A full upwind, full downwind, or a weighted average can result.

As with most high order schemes, some numerical dispersion is induced in regions with steep gradients or near discontinuities. A method called “slope limiting” is used to reduce or eliminate these oscillations. By limiting the slopes on either side of the interface, it can be ensured that no new local maxima or minima develop in the solution. One class of limiting schemes is called Total Variation Diminishing (TVD) schemes. This method ensures that the so called total variation of the solution will either decrease or remain the same. The total variation is:

\[ TV = \sum_{\text{All Interfaces}} |\tilde{u}_{i+1} - \tilde{u}_i| \]  
(E.23)

The slopes are scaled by a function of the ratio of the adjacent slopes. One such limiting function is called the Van Albada limiter. The functional form of this limiter is as follows, where \( r \) is the ratio of two adjacent slopes.

\[ \Psi(r) = \frac{r^2 + r}{1 + r^2} \]  
(E.24)
This is a smooth limiter that lies in the middle of the second order TVD range and is generally not too compressive or too dissipative. However, it does tend toward the dissipative extreme as the value of $r$ increases. This limiter also has the property of being symmetric, which means that the following relation holds.

$$\Psi\left(\frac{1}{r}\right) = \frac{1}{r} \Psi\left(r\right)$$  \hspace{1cm} (E.25)

When this is the case, the dependence on kappa vanishes and the final extrapolated variables are obtained with the following equations.

$$\tilde{u}_L = \bar{u}_i + \frac{1}{2} \Psi\left(\frac{r_{i+1/2}^-}{r_{i+1/2}^+}\right) \left(\bar{u}_{i+1} - \bar{u}_{i-1}\right)$$  \hspace{1cm} (E.26)

$$\tilde{u}_R = \bar{u}_{i+1} - \frac{1}{2} \Psi\left(\frac{r_{i+3/2}^-}{r_{i+3/2}^+}\right) \left(\bar{u}_{i+2} - \bar{u}_{i+1}\right)$$  \hspace{1cm} (E.27)

$$r_{i+1/2}^+ = \frac{\Delta \bar{u}_i}{\Delta \bar{u}_{i+1}}, \quad r_{i+3/2}^- = \frac{\Delta \bar{u}_i}{\Delta \bar{u}_{i-1}}$$  \hspace{1cm} (E.28)

Another class of extrapolation methods is called Essentially Non-Oscillatory (ENO) schemes. When symmetric limiters are applied to the kappa scheme, the data model is essentially reduced to linear model, losing any ability to produce piecewise quadratic data. ENO schemes attempt to recover this loss by extending the stencil of the extrapolation. The main goal of these schemes is to maintain smooth extremes in a solution. The SONIC-A scheme, which is an ENO extension of the van Leer TVD limiter is defined by the following set of equations.

$$\tilde{u}_L = \bar{u}_i + a_i \frac{\Delta x}{2}, \quad \tilde{u}_R = \bar{u}_{i+1} - a_{i+1} \frac{\Delta x}{2}$$  \hspace{1cm} (E.29)

$$a_i = \text{sign}(t_i) \min \left[ \frac{\bar{s}_{i+1/2} + \bar{s}_{i-1/2}}{2}, \max\left[2|s_i|, \frac{\bar{t}_i}{2}\right] \right]$$  \hspace{1cm} (E.30)

$$\bar{s}_{i+1/2} = s_{i+1/2} - \frac{\Delta x}{2} \text{mmd} \left[ \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}, \frac{u_{i+2} - 2u_{i+1} + u_i}{\Delta x^2}, \frac{u_{i+2} - 2u_{i+1} + u_i}{\Delta x^2} \right]$$  \hspace{1cm} (E.31)

$$\bar{s}_{i-1/2} = s_{i-1/2} + \frac{\Delta x}{2} \text{mmd} \left[ \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}, \frac{u_{i-2} - 2u_{i-1} + u_{i-2}}{\Delta x^2} \right]$$  \hspace{1cm} (E.32)
Once the variables are extrapolated to the cell interfaces, the fluxes can be calculated using the methods described in Section E.2.

E.4 Time Integration

The goal of the numerical solver is to advance the solution in time until a steady state is reached, such that the solution does not change with further advancement. An implicit method is chosen over an explicit method meaning that the residual is evaluated at the next time step rather than the current time step. The residual is simply the sum of the fluxes minus the source vector for each cell.

\[
\begin{align*}
\nabla \cdot \left( \frac{\partial \tilde{u}_{i,j,k}}{\partial t} \right) &= - \left( \tilde{E}_{i+\frac{1}{2},j,k} - \tilde{E}_{i-\frac{1}{2},j,k} + \tilde{F}_{i,j+\frac{1}{2},k} - \tilde{F}_{i,j-\frac{1}{2},k} + \tilde{G}_{i,j,k+\frac{1}{2}} - \tilde{G}_{i,j,k-\frac{1}{2}} - \tilde{S} \right) \\
&\equiv -\tilde{R}_{i,j,k}
\end{align*}
\]

The time discretization is called the backward Euler scheme, which is as follows.

\[
\begin{align*}
\nu \left( \frac{\tilde{u}^{n+1} - \tilde{u}^n}{\Delta t} \right) + \tilde{R}(\tilde{u}^{n+1}) &= 0
\end{align*}
\]

Consider a system of equations consisting of all equations solved per mesh cell times the number of mesh cells. The system is denoted by the nonlinear operator \( \tilde{R}(\tilde{u}) \). This system is then linearized as follows.

\[
\begin{align*}
\left( \frac{\nu}{\Delta t} + \frac{\partial \tilde{R}}{\partial \tilde{u}} \right) (\tilde{u}^{n+1} - \tilde{u}^n) &= -\tilde{R}(\tilde{u}^n)
\end{align*}
\]

Some simplifications are taken in formulating the system Jacobian \( \partial \tilde{R} / \partial \tilde{u} \). First, consider the residual vector to be spatially first order, regardless of the spatial order of the residual on the right hand side of the equation. Also, the Jacobian is formulated based...
only on the inviscid fluxes. The residual vector for a single mesh cell is a function of the
data in that cell and the six adjacent cells.

\[
\vec{R}_{i,j,k}^{n+1} = \vec{E}_{i,j,k}^{n+1} \left( \vec{u}_{i,j,k}^{n+1} \right) - \vec{E}_{i,j,k}^{n} \left( \vec{u}_{i,j,k}^{n} \right)
\]

\[
+ \vec{F}_{i,j,k}^{n+1} \left( \vec{u}_{i,j,k}^{n+1} \right) - \vec{F}_{i,j,k}^{n} \left( \vec{u}_{i,j,k}^{n} \right)
\]

\[
+ \vec{G}_{i,j,k}^{n+1} \left( \vec{u}_{i,j,k}^{n+1} \right) - \vec{G}_{i,j,k}^{n} \left( \vec{u}_{i,j,k}^{n} \right)
\]

(E.38)

Differentiating this with respect to the conservative variable vector produces the
following equation for the Euler Implicit form.

\[
A_{i,j,k} \Delta u_{i-1,j,k}^{n+1} + B_{i,j,k} \Delta u_{i,j-1,k}^{n+1} + C_{i,j,k} \Delta u_{i,j,k-1}^{n+1} + D_{i,j,k} \Delta u_{i,j,k}^{n+1}
\]

\[
+ E_{i,j,k} \Delta u_{i,j,k+1}^{n+1} + F_{i,j,k} \Delta u_{i,j+1,k}^{n+1} + G_{i,j,k} \Delta u_{i,j,k}^{n+1} = -\vec{R}(\vec{u}_{i,j,k}^{n})
\]

(E.39)

where \( A \) through \( G \) are as follows,

\[
A_{i,j,k} = -\left( \frac{\partial \vec{E}}{\partial \vec{u}_{i-1,j,k}} \right)_{i,j,k}
\]

(E.40)

\[
B_{i,j,k} = -\left( \frac{\partial \vec{F}}{\partial \vec{u}_{i,j-1,k}} \right)_{i,j,k}
\]

(E.41)

\[
C_{i,j,k} = -\left( \frac{\partial \vec{G}}{\partial \vec{u}_{i,j,k-1}} \right)_{i,j,k}
\]

(E.42)

\[
D_{i,j,k} = \left( \frac{\partial \vec{E}}{\partial \vec{u}_{i,j,k}} \right)_{i,j,k} + \left( \frac{\partial \vec{E}}{\partial \vec{u}_{i,j,k}} \right)_{i,j,k}
\]

\[
+ \left( \frac{\partial \vec{F}}{\partial \vec{u}_{i,j,k}} \right)_{i,j,k} + \left( \frac{\partial \vec{G}}{\partial \vec{u}_{i,j,k}} \right)_{i,j,k} + \left( \frac{\partial \vec{G}}{\partial \vec{u}_{i,j,k}} \right)_{i,j,k} + \frac{\nu}{\Delta t}
\]

(E.43)

\[
E_{i,j,k} = -\left( \frac{\partial \vec{G}}{\partial \vec{u}_{i,j,k+1}} \right)_{i,j,k+1}
\]

(E.44)

\[
F_{i,j,k} = -\left( \frac{\partial \vec{G}}{\partial \vec{u}_{i,j,k+1}} \right)_{i,j,k+1}
\]

(E.45)

\[
G_{i,j,k} = -\left( \frac{\partial \vec{G}}{\partial \vec{u}_{i,j,k+1}} \right)_{i,j,k+1}
\]

(E.46)

With nine chemical species, each of these flux Jacobians is a 19 by 19 matrix. Another
simplification used here is to let the interface fluxes be determined by the Lax-Friedrichs
scheme. This allows for the simple calculation of derivatives. The Lax-Friedrichs scheme is:

$$\tilde{E}_{i+1/2,j,k} = \frac{1}{2} \left( \tilde{E}_{i,j,k} + \tilde{E}_{i+1,j,k} + \sigma_{i+1/2,j,k} t \left( \tilde{u}_{i,j,k} - \tilde{u}_{i+1,j,k} \right) \right)$$  \hspace{1cm} (E.47)

Sigma is the maximum Eigen value, or spectral radius of the system. The flux Jacobians for the Navier-Stokes equations can be found in Hirsch [20]. Two final approximations include zeroing many of the more complicated entries in the flux Jacobians and assuming that the flux Jacobians approximately cancel in the $D$ coefficient. This makes the $D$ matrix diagonal.

While this is sufficient for non-reactive systems, systems with chemical source terms require further accommodations. The characteristic times for chemical reactions are significantly smaller than any of those present in the convective or diffusive terms. Therefore, to solve the system implicitly, the source terms must be linearized in addition to the inviscid fluxes. This results in an additional term, $\partial \tilde{S} / \partial \tilde{u}$, in the $A$ matrix, and while the matrix itself may be complicated, the derivation of it is straightforward.

An iterative technique is adopted to approximately solve this linear system. The method is a combination of two techniques, incomplete lower/upper (ILU) decomposition and symmetric Gauss-Seidel. On each plane of constant $i$, ILU is used in the $j$ and $k$ directions while symmetric Gauss-Seidel iteration is used in the $i$ direction.

The linear system can be written as follows.

$$\left( \frac{\nu}{\Delta t} + \frac{\partial \tilde{R}}{\partial \tilde{u}} - \frac{\partial \tilde{S}}{\partial \tilde{u}} \right) \Delta \tilde{u}^{n+1} = -\tilde{R}^n$$  \hspace{1cm} (E.48)

$$A \Delta \tilde{u}^{n+1} = -\tilde{R}^n$$

The ILU method simplifies the $A$ matrix into lower, upper, and diagonal matrices [37].

$$A \Delta \tilde{u}^{n+1} = (L + D + U) \Delta \tilde{u}^{n+1} = -R^n$$  \hspace{1cm} (E.49)

$$L = A + B + C$$  \hspace{1cm} (E.50)

$$U = E + F + G$$  \hspace{1cm} (E.51)

$D$ is defined as follows:

$$D_{i,j,k} = D_{i,j,k} - A_{i,j,k} D_{i+1,j,k} G_{i+1,j,k} - B_{i,j,k} D_{i+1,k} F_{i+1,k} - C_{i,j,k} D_{i+1,k} E_{i,j,k+1}$$  \hspace{1cm} (E.52)
This is performed in both directions. $A$ is approximated by the ILU scheme as follows.

$$A_{ILU} = (L + D)D^{-1}(D + U)$$  \hspace{1cm} (E.53)

Using this approximation, a symmetric Gauss-Seidel technique is used to update the solution in the $i$ direction with a forward and backward sweep defined as follows.

$$\Delta \tilde{u}_{i,j,k}^{n+1/2} = \left( D_{i,j,k}^n \right)^{-1} \left( -\tilde{R}_{i,j,k}^n - L_{i,j,k}^n \Delta \tilde{u}_{i-1,j,k}^{n+1/2} \right)$$  \hspace{1cm} (E.54)

$$\Delta \tilde{u}_{i,j,k}^{n+1} = \Delta \tilde{u}_{i,j,k}^{n+1/2} - U_{i,j,k}^n \Delta \tilde{u}_{i+1,j,k}^{n+1}$$  \hspace{1cm} (E.55)

Once the two sweeps have been performed, the solution is updated.

The time step is determined using the Courant Friedrichs and Lewy (CFL) condition based on the local maximum Eigen values of the system. Since the only solution of interest is the steady state solution, the temporal accuracy of the preceding iterations is not of concern. This allows local time stepping to be used, which increases convergence rates, but decreases the accuracy of any intermediate solution. The time step is defined by the following.

$$\frac{\nu_{i,j,k}}{\Delta t} = \frac{A_z \left( |\tilde{U}_c| + a \right) + A_n \left( |\tilde{V}_c| + a \right) + A_z \left( |\tilde{W}_c| + a \right)}{CFL}$$  \hspace{1cm} (E.56)

The $A$'s represent average projected areas in the three coordinate directions. The CFL maybe be specified as high as 5 for the current work.

E.4.1 Alternate Solver (Sequential Solution of Turbulence Equations)

Two different methods were used to solve the turbulence equations. One method includes the six turbulence equations in the planar ILU scheme. The alternative method solves the species and conservation equations with the planar ILU scheme and then solves the turbulence equations sequentially using a three-dimensional ILU method similar to the one described above. The latter is the method of choice and the overall result is a much faster computation with solutions that are not noticeably different from the inclusive solver.