DEVELOPMENT OF A NUMERICAL TOOL TO STUDY THE MIXING PHENOMENON OCCURRING DURING MODE ONE OPERATION OF A MULTI-MODE EJECTOR-AUGMENTED PULSED DETONATION ROCKET ENGINE

by

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To my wife Megan, I am well aware of the sacrifices you have made throughout this process. I would not have been successful without your support. I love you.
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A special thanks to every professor I had while in attendance at UTA, I appreciate their patience. There were most certainly occasions when I asked too many questions and yet they were always willing to engage in conversation. I am especially grateful to Dr. Han, his passion for teaching without question facilitated the learning process. Whilst some engineering courses can be a grind, Dr. Han was invariably able to keep it interesting.

To my parents, Lindsey and Annette Dawson, their contributions are immeasurable. Without there support, this endeavor would have been impossible. I take pride in having such a close family and that fundamental familial structure was a vital support system, undeniably the root of my success.

I would like to express my deepest gratitude to my brothers, from whom I have received perpetual encouragement and inspiration. I am extremely fortunate to be so blessed.

And lastly...my best friend, life partner, and kick in the pants when I need one...my lovely wife Megan. You are my universe and are truly one of a kind. Love you.
Don’t be afraid of perfection. In the words of Julius Caesar... *VENI VIDI VICI*!
ABSTRACT

DEVELOPMENT OF A NUMERICAL TOOL TO STUDY THE MIXING PHENOMENON OCCURRING DURING MODE ONE OPERATION OF A MULTI-MODE EJECTOR-AUGMENTED PULSED DETONATION ROCKET ENGINE

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Supervising Professor: Dr. Donald Wilson

A novel multi-mode implementation of a pulsed detonation engine, put forth by Wilson et al. [2], consists of four modes; each specifically designed to capitalize on flow features unique to the various flow regimes. This design enables the propulsion system to generate thrust through the entire flow regime. The multi-mode ejector-augmented pulsed detonation rocket engine operates in mode one during take-off conditions through the acceleration to supersonic speeds. Once the mixing chamber internal flow exceeds supersonic speed, the propulsion system transitions to mode two. While operating in mode two, supersonic air is compressed in the mixing chamber by an upstream propagating detonation wave and then exhausted through the convergent-divergent nozzle. Once the velocity of the air flow within the mixing chamber exceeds the Chapman-Jouguet Mach number, the upstream propagating detonation wave no longer has sufficient energy to propagate upstream and consequently the propulsive system shifts to mode three. As a result of the inability of the
detonation wave to propagate upstream, a steady oblique shock system is established just upstream of the convergent-divergent nozzle to initiate combustion. And finally, the propulsion system progresses on to mode four operation, consisting purely of a pulsed detonation rocket for high Mach number flight and use in the upper atmosphere as is needed for orbital insertion. Modes three and four appear to be a fairly significant challenge to implement, while the challenge of implementing modes one and two may prove to be a more practical goal in the near future. A vast number of potential applications exist for a propulsion system that would utilize modes one and two, namely a high Mach number hypersonic cruise vehicle. There is particular interest in the dynamics of mode one operation, which is the subject of this study. Several advantages can be obtained by use of this technology. Geometrically, the propulsion system is fairly simple and the rapid combustion process results in an engine cycle which is more efficient compared to its combined-cycle counterparts.

The flow path geometry consists of an inlet system, followed just downstream by a mixing chamber where an ejector structure is placed within the flow path. Downstream of the ejector structure is a duct leading to a convergent-divergent nozzle. During mode one operation and within the ejector, products from the detonation of a stoichiometric hydrogen/air mixture are exhausted directly into the surrounding secondary air stream. Mixing then occurs between both the primary and secondary flow streams, at which point the air mass containing the high pressure, high temperature reaction products is convected downstream towards the nozzle.

The engine cycle is engineered to a specific number of detonations per second, creating the pulsating characteristic of the primary flow. The pulsing nature of the primary flow serves as a momentum augmentation, enhancing the thrust and specific impulse at low speeds. Consequently, it is necessary to understand the transient
mixing process between the primary and secondary flow streams occurring during mode one operation.

Using OPENFOAM®, a numerical tool is developed to simulate the dynamics of the turbulent detonation process along with detailed chemistry in order to understand the physics involved with the stream interactions. The computational code has been developed within the framework of OPENFOAM®, an open-source alternative to commercial CFD software. A conservative formulation of the Farve averaged Navier-Stokes equations are used to facilitate programming and numerical stability.

Time discretization is accomplished by using the Crank-Nicolson method, achieving second-order convergence in time. Species mass fraction transport equations are implemented and a Seulex ODE solver was used to resolve the system of ordinary differential equations describing the hydrogen-air reaction mechanism detailed in Appendix A. The Seulex ODE solution algorithm is an extrapolation method based on the linearly implicit Euler method with step size control. A second-order total variation diminishing method with a modified Sweby flux limiter was used for space discretization. And finally the use of operator splitting (PISO algorithm, and chemical kinetics) is essential due to the significant differences in characteristic time scales evolving simultaneously in turbulent reactive flow. Capturing the turbulent nature of the combustion process was done using the k-ω-SST turbulence model, as formulated by, [1]. Mentor’s formulation is well suited to resolve the boundary layer while remaining relatively insensitive to freestream conditions, blending the merits of both the k-ω and k-ε models. Further development of the tool is possible, most notably with the Numerical Propulsion System Simulation application. NPSS allows the user to take advantage of a zooming functionality in which high-fidelity models of engine components can be integrated into NPSS models, allowing for a more robust propulsion system simulation.
A more comprehensive understanding of the multi-mode ejector-augmented pulsed detonation rocket engine can be achieved with a systematic study of the impact pulsed flow has on thrust production. Although a significant increase in computational requirements, adding nozzle geometry to this study would illuminate any problems associated with pulsed flow through a nozzle. Additionally, a study including nozzle geometry would bring more clarity in regards to the efficiency of the propulsion design.
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\( q_0 \)  Dynamic Pressure  \( \text{N/m}^2 \)

\( q_j \)  Component Energy Flux  \( \text{W/m}^2 \)

\( R \)  Source Term Vector

\( R \)  Universal Gas Constant  \( \text{J/K-mol} \)

\( r_R \)  Grid Refinement Ratio

\( S_f \)  Face Area Vector  \( \text{m}^2 \)

\( \tilde{S}_{ij} \)  Mass Averaged Mean Deviatoric Component of Strain Rate Tensor

\( Sc_{t,i} \)  Turbulent Schmidt Number

\( S_\phi \)  Source Term from General Transport Equation

\( S_{ij} \)  Deviatoric Component of the Strain Rate Tensor

\( s_k \)  Molar Entropy  \( \text{J/kmol-K} \)

\( s_{ij} \)  Instantaneous Strain-Rate Tensor

\( \bar{T} \)  Mass Averaged Mean Temperature  \( \text{K} \)

\( T'' \)  Mass Averaged Fluctuating Temperature  \( \text{K} \)

\( T_s \)  Sutherland’s Constant  \( \text{K} \)

\( T_{ref} \)  Sutherland’s Reference Temperature  \( \text{K} \)

\( T \)  Temperature  \( \text{K} \)

\( T_{to} \)  Total temperature  \( \text{K} \)

\( T_0 \)  Freestream Temperature  \( \text{K} \)

\( T_3 \)  Mixing Chamber Inlet Temperature  \( \text{K} \)

\( \mathbf{U}^0 \)  Initial Velocity Condition Vector  \( \text{m/s} \)

\( u^+ \)  Dimensionless Velocity used in the Law of the Wall

\( \bar{u}_i \)  Mass Averaged Mean Component Velocity  \( \text{m/s} \)

\( u''_i \)  Mass Averaged Fluctuating Component Velocity  \( \text{m/s} \)

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<td>( \pi_{max} )</td>
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<td>( \Psi )</td>
<td>JANAF Polynomial Function for Specific Heat at Constant Pressure</td>
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</table>
\( \psi \)  Static Temperature Ratio

\( \Psi_{FL} \)  Flux Limiting Function

\( \rho \)  Mass Density \( \text{kg/m}^3 \)

\( \rho' \)  Time Averaged Fluctuating Mass Density \( \text{kg/m}^3 \)

\( \sigma_k \)  Turbulence Model Blending Function

\( \sigma_\omega \)  Turbulence Model Blending Function

\( \sigma_{k1,k2,\omega1,\omega2} \)  Turbulence Model Calibration Parameters

\( \tau_c \)  Chemical Time Scale \( s \)

\( \tau_{ij} \)  Viscous Stress Tensor

\( \tau'_{ij} \)  Mass Averaged Fluctuating Viscous Stress Tensor

\( \tau_{mix} \)  Turbulent Micro-Mixing Scale \( s \)

\( \tilde{\Omega}_{ij} \)  Rate of Rotation \( 1/s \)

\( \tilde{\tau}_{ij} \)  Mass Averaged Mean Viscous Stress Tensor

\( \zeta \)  Second Coefficient of Viscosity \( \text{kg/m} \cdot \text{s} \)

CEA  Chemical Equilibrium with Applications

CFD  Computational Fluid Dynamics

CFL  Courant-Friedrichs-Lewy Condition

CJ  Chapman-Jouguet

JANAF  Joint Army Navy Air Force

LW  Lax-Wendroff: Second-Order Central Differencing Scheme

NPSS  Numerical Propulsion Simulation System

ODE  Ordinary Differential Equation

PaSR  Partially Stirred Reactor

PISO  Pressure Implicit with Splitting of Operators

PSR  Perfectly Stirred Reactor

RR  Reaction Rate Modifier
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tr>
<td>SST</td>
<td>Shear Stress Transport</td>
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<tr>
<td>SSTO</td>
<td>Single Stage to Orbit</td>
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<td>TVD</td>
<td>Total Variation Diminishing</td>
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<td>WB</td>
<td>Warming-Beam: Second-Order Upwind Scheme</td>
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<td>WF</td>
<td>Wall Function Boundary Condition</td>
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<td>WT</td>
<td>Wave Transmissive Boundary Condition</td>
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<td>ZG</td>
<td>Zero Gradient Boundary Condition</td>
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CHAPTER 1
INTRODUCTION

Hypersonic flight has been an area of focus for researchers since World War II. The German V-2 Rocket was the first manufactured object to achieve hypersonic speed, and in February 1949 its upper-stage reached a velocity of 8,288 kilometers/hour. The applications of hypersonic flight are boundless. From military applications to transporting medical payloads and even commercial transport, hypersonic flight could very well be the future of aviation. Although hypersonic flight has numerous advantages, there remains a litany of challenges to overcome before hypersonic flight can be considered practical. Firstly, the flight vehicle will travel at speeds in which temperatures are sufficient for dissociation to become noticeable within the gases surrounding the vehicle. As a result, we must concern ourselves with high temperature gas dynamics, which can have a substantial impact on the flow field dynamics. Because of increased temperatures, the flight vehicle structure will be exposed to massive heat loads coupled with extreme dynamic loading, necessitating a robust structural design. Many questions also remain regarding the optimized propulsion system design for hypersonic flight. Regardless of these challenges, however, the advantages for hypersonic flight far exceed the required work and cost associated with developing a hypersonic aviation infrastructure. Once hypersonic flight technology is practical, cost efficient and easily reproducible, only then will the business opportunities begin to materialize. The propulsion system should have a design capable of frequent and reliable usage, thus enabling a frequent fly rate. The propulsion system should also be capable of accelerating from static conditions to hypersonic speed,
along a constant dynamic pressure trajectory. This is a challenging endeavor considering the integrated nature typical of hypersonic aircraft, for example, the role the vehicle’s forebody will have in maintaining sufficient density as well as manipulation of the actual inlet capture area. Both factors are extremely important in the ability of the propulsion system to produce adequate thrust.

Keeping these constraints in mind, propulsion system options are limited and a legitimate engineering challenge exists in order to achieve our goals of hypersonic aviation. As a consequence, modifications to existing engine designs, combined-cycle systems, or new technology altogether are inevitable. Combined-cycle systems bridge the thrust gap between turbine based systems and ram/scramjet systems, unfortunately at the cost of added weight attributed to the dual flow paths. The multi-mode ejector-augmented pulsed detonation rocket engine, proposed by Wilson et al. [2], is thought to possess sufficient thrust as well as two additional advantages; firstly, the propulsion system uses a single flow path and, secondly, their is no rotating machinery. These design features could reduce the propulsion system weight, and the lack of rotating machinery greatly simplifies the design. Therefore, the multi-mode ejector-augmented pulsed detonation rocket engine is potentially a viable concept for either hypersonic or SSTO applications. However, this study is concerned specifically with the mixing phenomenon occurring during the stream interaction of mode one operation. Prior to narrowing the focus of this research, subsequent sections offer a brief review of the operational high points for each mode, as well as a basic review of pulsed detonation engine mechanics and detonation wave physics.

1.1 Mechanics of a Pulsed Detonation Engine Cycle

Currently, propulsion systems operate using deflagration, deflagration is the rapid but subsonic burning of fuel. Pulsed detonation engines, however, operate on
the supersonic detonation of fuel. Interestingly, supersonic detonation turns out to be very advantageous. Because combustion occurs so rapidly, the reacting mixture does not have time to expand and the combustion takes place at constant volume essentially. Constant volume combustion is more efficient than open-cycle designs, which leads to superior fuel efficiency [2].

The pulse detonation engine cycle begins by filling the detonation tube with a stoichiometric hydrogen/air mixture through injection valves. Detonation properties exhibit some dependence on the ambient conditions within the detonation tube. More specifically, deflagration-to-detonation occurs more readily at higher pre-detonation pressures. Prior to the mixture reaching the open end of the detonation tube, the detonation is initiated at the closed end by an ignition system. Traveling towards the open end of the detonation tube, an unsteady expansion wave propagates behind the detonation wave while chemical reactions continuously feed the detonation wave with energy. When the detonation wave exits the detonation tube, a purging process due to the pressure gradient which exists between the ends of the detonation tube unfolds. Finally commencement of the blowdown process begins as clean fresh air is injected into the detonation tube, whereby any remaining combustion products are purged. Reaction products are purged to avoid auto ignition of the new fuel/oxidizer mixture, signaling the beginning of the next detonation cycle [2]. A visual representation of this can be seen in Figure 1.1 [3].

1.2 Mode One: Ejector-Augmented Pulsed Detonation Rocket

The ejector-augmented pulsed detonation rocket, as stated previously, provides the means to generate enhanced thrust and specific impulse at low speeds. Operationally, this mode is designed for take-off to moderate supersonic speeds while the
mixing chamber remains subsonic. This concept would be similar to the conventional air-augmented ejector rocket except in this case the primary flow is pulsed.

1.3 Mode Two: Detonation Wave Scramjet

Mode two would operate at Mach numbers from approximately 4 to 8. While in operation, increased pressures are achieved with the use of unsteady upstream propagating detonation waves yielding pressure values higher than those attainable during typical scramjet deflagration burning [2]. Here the mixing chamber is supersonic and fuel may be injected upstream of the nozzle to further increase momentum. In this mode, for mixing chamber Mach numbers less than the CJ Mach number, ignition at a downstream location will cause an upstream propagating detonation wave. Upstream propagation will continue until the energy within the wave is no longer sufficient for upstream propagation, at which point the wave is extinguished.
1.4 Mode Three: Steady Oblique Detonation Wave Engine

During mode three operation, the system may operate at Mach numbers in the approximate range of 8 to 12. Once the mixing chamber Mach number exceeds the CJ Mach number, the upstream propagating detonation waves produced in mode two are convected downstream. Approaching the convergent section of the nozzle, detonation waves tend to stabilize as steady oblique detonation waves. Hydrogen and oxygen may be injected in a pulsating fashion as the flow passes through the convergent section to promote flow transition to oblique detonation waves. A high frequency ignition source is needed to initiate the detonation process.

1.5 Mode Four: Pulsed Detonation Rocket

In mode four, a purely pulsed detonation rocket is employed at very high Mach numbers and altitudes. Mode four would be reserved for orbital insertion among other potential space applications. However, applications involving lower atmospheric hypersonic flight vehicles will utilize modes one and two. As the central focus of this research paper, the process to understand mode one operation begins with understanding the physics present in detonation waves.

1.6 Physics of a Detonation Wave

Several models exist to describe the chemistry involved in detonation waves. However, most of these models make simplifying assumptions which unfortunately limit the models ability to accurately describe the processes that actually occurs during a detonation wave. Presently, the Zel’dovich-von Neumann-Döring, or ZND model, appropriately captures the chemistry by admission of finite-rate chemical reactions, thus allowing for the chemical kinetic non-equilibrium inherent in detonation
wave chemistry. This assumption directly leads to the structure of the detonation wave. First, an infinitely thin shock wave compresses a fuel/oxidizer mixture to a high pressure peak referred to as the von Neumann spike which is accompanied by a discontinuous increase in temperature. At the von Neumann spike point, the reactive mixture remains unreacted. The spike marks the onset of the zone of exothermic chemical reactions, resulting in the detonation products expanding backwards with respect to the moving shock reference frame. Flow immediately following the shock, in the reference frame in which the shock is stationary, is subsonic [4]. Because of this, energy released behind the shock can be transported to the shock front for its support. Essentially, all of the chemical energy is harnessed to propagate the shock wave forward [4]. If you will notice in Figure. 1.2 [4], the wave structure is clearly seen.

The assumption of finite-rate chemical reactions necessitates the use of a reaction model, a detailed description of a hydrogen-air reaction mechanism can be found in Appendix A. Finite-rate chemistry implies a delay in the reactions due to the fi-
nite time required to initiate the reactions, thus an induction zone is formed. When the chemical reactions begin, a reasonable increase in temperature occurs in parallel with a reduction in pressure and density as can be seen in the reaction zone. As the chemical reactions race towards completion, the physical flow variables such as temperature, pressure and density approach the Chapman-Jouguet conditions. Once the reaction products are exhausted into the surrounding air stream, rarefaction waves start the process of ejecting heated reaction products while also further adjusting the temperature and pressure within the detonation tube to match the left wall boundary conditions [2]. Finally, a purging process signals the completion of the cycle and is necessary to remove any remaining heated reaction products, preventing fuel/oxidizer auto-ignition.
CHAPTER 2
NUMERICAL FORMULATION

This chapter will review the formulation of the Favre averaged Navier-Stokes equations in conjunction with the k-ω-SST turbulence model as derived by [5]. Included is an elucidation of the equations governing the transport properties while concluding with an explication of the equations relevant to the chemical kinetics and combustion model.

2.1 Favre Averaged Navier Stokes Equations

Turbulence was initially defined as an irregular motion which in general makes its appearance in fluids, gaseous or liquid, when they flow past solid surfaces or even when neighboring streams of the same fluid pass over one another [6]. However, as our understanding of turbulence has progressed, researchers have deemed ”irregular motion” to be too imprecise. In order to clarify the definition, Hinze defined turbulence as fluid motion with an irregular condition of flow in which the various quantities show a random variation with time and space coordinates, so that statistically distinct average values can be discerned [6]. And finally, Bradshaw (Cebeci and Smith [7]), completed the definition by adding the statement that turbulence has a wide range of scales. Thus, turbulent time and length scales are represented by frequencies and wavelengths which are determined by a Fourier analysis of the turbulent-flow time history.

Turbulence plays a particularly significant role in the mixing process relative to the dual flow streams within the multi-mode ejector-augmented pulsed detona-
tion rocket engine. During mode one operation, the velocity of the secondary flow stream will be lower than that of the ejector exhaust products (primary flow stream). As a result of the velocity differences, flow instabilities are created at the interface and turbulence begins to dominate the flow. In this case, turbulence operates as a mechanism to transfer energy from the primary flow stream to the secondary flow stream. Turbulence is such a unique phenomenon, scientist have largely been unsuccessful in formulating a numerical model to accurately simulate turbulence across all flow regimes and geometries. Statistical formulation of the Navier-Stokes equations is necessary thus facilitating the use of Reynolds and Favre decomposition techniques as well as time and mass averaged variables. These reformulated Navier-Stokes equations are coupled with chemical species mass fraction transport equations, chemical kinetic equations, perfect gas equation of state, and turbulent closure approximations formulated using Mentor’s k-ω-SST model.

For motion in a compressible medium, a solution to the equations governing conservation of mass, momentum, and energy must be found. Below are the instantaneous equations using Einstein’s tensor notation where repeated indices are summed.

**Mass conservation**

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0 \tag{2.1}
\]

**Momentum conservation**

\[
\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_j u_i) = - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} (\tau_{ij}) + \rho g \tag{2.2}
\]
Energy conservation

\[
\frac{\partial}{\partial t} \left[ \rho \left( e + \frac{1}{2} u_i u_i \right) \right] + \frac{\partial}{\partial x_j} \left[ \rho u_j \left( h + \frac{1}{2} u_i u_i \right) \right] = \frac{\partial}{\partial x_j} (u_i \tau_{ij}) - \frac{\partial q_j}{\partial x_j} + \dot{Q}_{\text{source}} \quad (2.3)
\]

In order to remove the internal energy term from the energy conservation equation, the following definition is used,

\[
e = h - \frac{p}{\rho} \quad (2.4)
\]

Substituting Equation 2.4 into Equation 2.3 yields.

\[
\frac{\partial}{\partial t} \left[ \rho \left( h - \frac{p}{\rho} + \frac{1}{2} u_i u_i \right) \right] + \frac{\partial}{\partial x_j} \left[ \rho u_j \left( h + \frac{1}{2} u_i u_i \right) \right] = \frac{\partial}{\partial x_j} (u_i \tau_{ij}) - \frac{\partial q_i}{\partial x_j} + \dot{Q}_{\text{source}} \quad (2.5)
\]

Re-arrange and you have.

\[
\frac{\partial}{\partial t} \left[ \rho h + \frac{1}{2} \rho u_i u_i \right] + \frac{\partial}{\partial x_j} \left[ \rho u_j h + \frac{1}{2} \rho u_j u_i u_i \right] = \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_j} (u_i \tau_{ij}) - \frac{\partial q_i}{\partial x_j} + \dot{Q}_{\text{source}} \quad (2.6)
\]

Starting with Reynolds decomposition, the instantaneous velocity \( u_i(x, t) \) can be expressed as the sum of a mean \( u_i(x) \) and a fluctuating component \( u'_i(x, t) \), yielding

\[
u_i(x, t) = u_i(x) + u'_i(x, t) \quad (2.7)
\]
Time averaging Equation 2.7 can be accomplished with the following integral,

$$ u_i(x) = \lim_{T \to \infty} \frac{1}{T} \int_t^{t+T} u_i(x, t) \, dt \quad (2.8) $$

where \( u_i(x) \) is the time averaged or mean velocity. Taking the time average of the mean velocity is again the same time averaged value,

$$ \overline{u_i}(x) = \lim_{T \to \infty} \frac{1}{T} \int_t^{t+T} u_i(x) \, dt \quad (2.9) $$

in which the overbar is shorthand for the time average. Equation 2.8 can be proven by taking the time average of the fluctuating velocity component, as defined in Equation 2.7, resulting in the following.

$$ \overline{u'_i}(x, t) = \lim_{T \to \infty} \frac{1}{T} \int_t^{t+T} [u_i(x, t) - \overline{u_i}(x)] \, dt = u_i(x) - \overline{u_i}(x) = 0 \quad (2.10) $$

Reynolds decomposition can be applied to other flow variables, such as density, and the results are the same. For example,

$$ \rho = \overline{\rho} + \rho' \quad (2.11) $$

where the mean density \( \overline{\rho} \), and fluctuating density \( \rho' \), comprise the constituent components of a Reynolds decomposition applied to density. Time averaging Equation 2.11 leaves only the mean component.
Substituting Equations 2.11 and 2.7 into the compressible continuity equation yields the following.

\[
\frac{\partial}{\partial t}(\bar{\rho} + \rho') + \frac{\partial}{\partial x_i}(\bar{\rho}u_i + \rho'u_i + \bar{\rho}'u_i' + \rho'u_i') = 0 \quad (2.12)
\]

As demonstrated by Equation 2.10, time averaging a fluctuating component is equal to zero. However, no \textit{a priori} reason exist for the mean of the product of two fluctuating quantities to vanish, as there is no mathematical proof to declare its equivalency to zero. Due to the statistical nature of Reynolds decomposition, these terms are considered to be correlated if the mean product of two fluctuating quantities is not equal to zero [6]. Thus, from time averaging the convection term in Equation 2.12, $\rho'u_i$ and $\bar{\rho}u_i'$ are dropped leaving,

\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}u_i + \rho'u'_i) = 0 . \quad (2.13)
\]

Through Reynolds decomposition and time averaging, these correlation terms are introduced into the Navier-Stokes equations. Herein lies the fundamental problem with turbulence modeling and is coined the "turbulent closure problem".

Simplification is achieved by defining a mass averaged velocity which can be expressed as [6],

\[
\bar{u}_i = \frac{1}{\bar{\rho}} \lim_{T \rightarrow \infty} \frac{1}{T} \int_t^{t+T} \rho(x, t)u_i(x, t)dt \quad (2.14)
\]

where $\bar{\rho}$ is the conventional Reynolds averaged density.
Thus, after re-arranging Equation 2.14 and remembering the conventional time averaging technique in Equations 2.7 through 2.10, the following is true

\[ \bar{\rho} \bar{u}_i = \bar{\rho} \bar{u}_i = \bar{\rho} u_i + \rho' u'_i \] (2.15)

Consequently, Equation 2.13 can be recast in the form

\[ \frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \bar{u}_i) = 0 \] (2.16)

Using a mass averaged approach, it is customary to decompose the instantaneous velocity into the mass averaged component \( \bar{u}_i \), and fluctuating component \( u''_i \) [6], whereby:

\[ u_i = \bar{u}_i + u''_i \] (2.17)

Simply multiply Equation 2.17 through by \( \rho \) while executing the time averaging as described by Equations 2.7 through 2.10 yields

\[ \bar{\rho} \bar{u}_i = \bar{\rho} \bar{u}_i + \bar{\rho} u''_i \] (2.18)

Recalling Equation 2.15, the following is necessarily true,

\[ \bar{\rho} u''_i = 0 \] (2.19)
Thus, time averaging the mass averaged fluctuating velocity component causes the fluctuating term to vanish. These averaging techniques are used entirely as mathematical simplifications and carry no physical significance. Hence, density fluctuations are effectively removed from the averaged equations, however, the impact that density fluctuations have on turbulence still persists [6]. In order to mass average Equations 2.1, 2.2 and 2.6, the following decomposed flow variables will be used.

\[ U_i = \bar{u}_i + u'' \]  \hspace{1cm} (2.20)
\[ \rho = \bar{\rho} + \rho' \]  \hspace{1cm} (2.21)
\[ h = \bar{h} + h'' \]  \hspace{1cm} (2.22)
\[ T = \bar{T} + T'' \]  \hspace{1cm} (2.23)
\[ q_j = \bar{q}_j + q_j'' \]  \hspace{1cm} (2.24)
\[ \tau_{ij} = \bar{\tau}_{ij} + \tau_{ij}'' \]  \hspace{1cm} (2.25)

However, if \(|\bar{\tau}_{ij}| \gg |\tau_{ij}''|\), stress fluctuations can be neglected [8]. Making the substitutions and performing both the time and mass averaging operations results in the Favre (mass) averaged mean conservation equations. To simplify the mass averaged energy conservation equation, the following definition is used. In Equation 2.26, \(k\) represents the turbulent kinetic energy

\[ \bar{H} = \bar{h} + \frac{\bar{u}_i \bar{u}_i}{2} + k \]  \hspace{1cm} (2.26)
Mass conservation

\[ \frac{\partial \bar{p}}{\partial t} + \frac{\partial}{\partial x_i} (\rho \bar{u}_i) = 0 \] (2.27)

Momentum conservation

\[ \frac{\partial}{\partial t} (\rho \bar{u}_i) + \frac{\partial}{\partial x_j} (\rho \bar{u}_j \bar{u}_i) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} (\bar{\tau}_{ji} - \rho \bar{u}_j'' \bar{u}_i'') + \bar{g} \] (2.28)

Energy conservation

\[ \frac{\partial}{\partial t} (\rho \bar{H}) + \frac{\partial}{\partial x_j} (\rho \bar{u}_j \bar{H}) = \frac{\partial}{\partial x_j} \left[ -\bar{q}_j - \rho \bar{u}_j'' \bar{H} + \bar{\tau}_{ij} \bar{u}_i'' - \rho \bar{u}_j'' \bar{u}_i'' \frac{2}{2} \right] + \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_j} [\bar{u}_i (\bar{\tau}_{ij} - \rho \bar{u}_j'' \bar{u}_i'')] + \dot{Q}_{source} \] (2.29)

The constitutive relation between stress and strain rate for a Newtonian fluid is,

\[ \tau_{ij} = 2\mu s_{ij} + \zeta \frac{\partial u_k}{\partial x_i} \delta_{ij} \] (2.30)

where \( s_{ij} \) is the instantaneous strain-rate tensor and \( \delta_{ij} \) is the Kronecker delta. Two commonly used assumptions will be utilized to simplify my analysis. First, the second coefficient of viscosity \( \zeta \) is related to \( \mu \) by,

\[ \zeta = -\frac{2}{3} \mu . \] (2.31)
Compact notation of the viscous stress tensor can be accomplished as follows

\[ \tau_{ij} = 2\mu S_{ij} \quad (2.32) \]

where \( S_{ij} \) is the deviatoric component of the strain rate tensor,

\[ S_{ij} = s_{ij} - \frac{1}{3}s_{kk}\delta_{ij} \quad (2.33) \]

and the Favre averaged viscous stress is given by,

\[ \tilde{\tau}_{ij} = 2\tilde{\mu}\tilde{S}_{ij} \quad . \quad (2.34) \]

The Favre averaged heat flux, \( \overline{q}_j \), is defined as,

\[ \overline{q}_j = -\kappa \frac{\partial \bar{T}}{\partial x_j} - \kappa \frac{\partial T''}{\partial x_j} + \sum_{i=1}^{N_s} h_i j_i \quad (2.35) \]

where \( \kappa \) is thermal conductivity, \( j_i \) is the species mass-diffusion flux [4], and \( h_i \) is the species specific enthalpy.

\[ j_i = \rho D \frac{\partial Y_i}{\partial x_i} \]

\( D \) is the species mass diffusion coefficient. Temperature fluctuations, the second term in Equation 2.35, can be neglected if they are much smaller in comparison to the mean temperature. This is true for virtually all flows [8].
The third term in Equation 2.35 is an enthalpy source term in which the sensible enthalpy contribution by each species is accounted for. The second assumption requires each gas species to be thermally perfect and as a consequence the specific heat at constant pressure and enthalpy are functions of temperature only. This assumption can be expressed as,

\[ c_{p,i} = \Psi_1(T) \tag{2.36} \]

\[ dh_i = c_{p,i}dT. \tag{2.37} \]

Integrating Equation 2.37 yields

\[ h_i(T) = h^f_i(T_{ref}) + \int_{T_{ref}}^{T} c_{p,i}(T)dT \tag{2.38} \]

in which \( h^f_i(T_{ref}) \) is termed the heat of formation for species \( i \) at the reference temperature 298.15 K. For most species, the heat of formation is zero in the natural state and can be found in a thermodynamic database such as JANAF. However, for this research, Equations 2.36 and 2.37 are evaluated using \( \Psi \), a polynomial fitting function used by NASA CEA. Valid within the temperature range of 200 K to 5000 K, the necessary temperature coefficients were pulled from JANAF tables. Seven coefficients are needed for each of the high and low temperature ranges. The molar thermodynamic properties are defined as follows,

\[ \frac{c_{p,i}}{R} = \sum_{i=1}^{5} a_{i,k}T^{(i-1)} = a_{1,i} + a_{2,i}T + a_{3,i}T^2 + a_{4,i}T^3 + a_{5,i}T^4 \tag{2.39} \]
\[
\frac{h_i}{R} = \sum_{i=1}^{6} \frac{a_{i,k}}{i} T^i = a_{1,i} T + \frac{a_{2,i}}{2} T^2 + \frac{a_{3,i}}{3} T^3 + \frac{a_{4,i}}{4} T^4 + \frac{a_{5,i}}{5} T^5 + \frac{a_{6,i}}{6} T^6 \tag{2.40}
\]

\[
\frac{s_i}{R} = a_{1,i} \ln T + a_{2,i} T + \frac{a_{3,i}}{2} T^2 + \frac{a_{4,i}}{3} T^3 + \frac{a_{5,i}}{4} T^4 + a_{7,i} \tag{2.41}
\]

where \( R \) is the universal gas constant. Remaining thermodynamic properties can be determined using the above properties. The specific heat at constant pressure, enthalpy and entropy can be normalized by the species molecular weight to obtain mass-based quantities. This facilitates the use of mass fractions to define fuel-air ratios. Mixture properties, specific heat at constant pressure and enthalpy, are determined from species properties by,

\[
c_p(T) = \sum_{i=1}^{N_s} Y_i c_{pi}(T) \tag{2.42}
\]

\[
h(T) = \sum_{i=1}^{N_s} Y_i h_i(T) . \tag{2.43}
\]

Equations 2.42 and 2.43 depend on both temperature and species mass fraction. Using the definition of enthalpy, the temperature gradient terms of Equation 2.35 can be written as,

\[
-\frac{\kappa}{c_p} \frac{\partial T}{\partial x_j} = -\frac{\kappa}{c_p} \frac{\partial h}{\partial x_j} .
\]
The energy flux can be defined.

\[ q_j = -\frac{\kappa}{c_p} \frac{\partial \tilde{h}}{\partial x_j} + \sum_{i=1}^{N_s} \tilde{h}_i \hat{j}_i \]  \hspace{1cm} (2.44)

Substituting Equations 2.34 and 2.44 into Equations 2.28 and 2.39 respectively, gives the following

\[ \frac{\partial \tilde{p}}{\partial t} + \frac{\partial}{\partial x_i} (\tilde{p} \tilde{u}_i) = 0 \]  \hspace{1cm} (2.45)

\[ \frac{\partial}{\partial t} (\tilde{p} \tilde{u}_i) + \frac{\partial}{\partial x_j} (\tilde{p} \tilde{u}_j \tilde{u}_i) = -\frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial}{\partial x_j} (2\tilde{\mu} \tilde{S}_{ij} - \tilde{\rho}u''_j u''_i) + \tilde{p} \tilde{g} \]  \hspace{1cm} (2.46)

\[ \frac{\partial}{\partial t} (\tilde{p} \tilde{H}) + \frac{\partial}{\partial x_j} (\tilde{p} \tilde{u}_j \tilde{H}) = \frac{\partial}{\partial x_j} \left[ \frac{\kappa}{c_p} \frac{\partial \tilde{h}}{\partial x_j} - \sum_{i=1}^{N_s} \tilde{h}_i \hat{j}_i - \tilde{\rho}u''_j \tilde{h}'' \right] \\
+ \frac{\partial}{\partial x_j} \left[ \tau_{ij} u''_i - \tilde{\rho}u''_j u''_i \right] + \frac{\partial \tilde{p}}{\partial t} + \frac{\partial}{\partial x_j} \left[ \tilde{u}_i (2\tilde{\mu} \tilde{S}_{ij} - \tilde{\rho}u''_j u''_i) \right] + \dot{Q}_{\text{source}} \]  \hspace{1cm} (2.47)

As a consequence of the decomposition techniques, correlation terms have been introduced into the reformulated Navier-Stokes equations. These correlation terms have no laminar counterpart and require a closure approximation to achieve a closed system of equations. The closure process begins with the Reynolds stress tensor \(-\tilde{\rho}u''_j u''_i\), which appears in both the energy and momentum equations. This stress tensor is essentially the stress experienced by the mean flow due to the turbulent fluctuations [9].

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To close the term, Mentor’s shear stress transport (SST) model makes use of the Boussinesq approximation,

\[ -\rho \overline{u'' j u'' i} = 2\mu_t \tilde{S}_{ij} - \frac{2}{3} \rho k \delta_{ij} \]  \hfill (2.48)

where \( \mu_t \) is known as the eddy viscosity.

Next term requiring closure is the Reynolds heat flux vector \( \overline{\rho u'' j h''} \). The heat flux vector represents the heat flux experienced by the mean flow due to the correlation term involving turbulent fluctuations of velocity and enthalpy, and this term can be defined as [9]

\[ \overline{\rho u'' j h''} = -\kappa_t \frac{\partial \tilde{T}}{\partial x_j} = -\frac{\kappa_t}{c_p} \frac{\partial \tilde{h}}{\partial x_j} . \]  \hfill (2.49)

Turbulent transport terms are the remaining two terms requiring a closure approximation. Known as the turbulent work terms, these terms appear in both the conservation of energy and turbulent kinetic energy equations. Using the gradient-diffusion hypothesis, the turbulent transport terms are expressed as [9],

\[ \overline{\tau_{ij} u''_i - \rho u''_j u''_i u''_i} = (\overline{\mu} + \mu_t) \frac{\partial k}{\partial x_j} \]  \hfill (2.50)

where \( \sigma_k \) is a calibration parameter [5]. Substituting Equations 2.48 through 2.50 into Equations 2.45 through 2.47 give the equations in their final form.
Mass Conservation

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho \tilde{u}_i) = 0 \]  \hspace{1cm} (2.51)

Momentum Conservation

\[ \frac{\partial}{\partial t} (\rho \tilde{u}_i) + \frac{\partial}{\partial x_j} (\rho \tilde{u}_j \tilde{u}_i) = - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ 2(\bar{\mu} + \mu_t) \tilde{S}_{ij} - \frac{2}{3} \rho k \delta_{ij} \right] + \rho g \]  \hspace{1cm} (2.52)

Energy Conservation

\[ \frac{\partial}{\partial t} (\rho \tilde{H}) + \frac{\partial}{\partial x_j} (\rho \tilde{u}_j \tilde{H}) = \bar{\rho} \alpha_{eff} \frac{\partial^2}{\partial x_j^2} (\tilde{h}) + \frac{\partial p}{\partial t} + \dot{q}_{source} \]  \hspace{1cm} (2.53)

In the interest of minimizing computational overhead, a few assumptions are applied to Equation 2.53. The turbulent transport terms, Equation 2.50, can be neglected as their impact only becomes noticeable in the hypersonic regime [9]. Additionally, all species Lewis numbers have been assumed equal to unity, in effect implying the mass and thermal diffusivities are equivalent. Finally, the viscous dissipation term as well as radiative heat sources are neglected. These final assumptions reduce the energy equation to the following,

\[ \frac{\partial}{\partial t} (\bar{\rho} \tilde{H}) + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j \tilde{H}) = \bar{\rho} \alpha_{eff} \frac{\partial^2}{\partial x_j^2} (\tilde{h}) + \frac{\partial p}{\partial t} + \dot{q}_{reaction} \]  \hspace{1cm} (2.54)
where \( \alpha_{eff} = (\kappa/\bar{p}c_p + \kappa_t/\bar{p}c_p) \) and \( \dot{q}_{reaction} \) is the heat of formation defined by

\[
\dot{q}_{reaction} = - \sum_{i=1}^{N_s} \Delta h_{f,i}^0
\]

This source term from Equation 2.54 represents the heat increase caused by the chemical reactions.

2.2 Turbulence Model

Selection of the turbulence model is important. The starting point for the development of the SST model was the need for the accurate prediction of flows with strong adverse pressure gradients and separation. Available turbulence models consistently failed to compute such flows. In particular, the otherwise popular k-\( \epsilon \) model was not able to capture the proper behavior of turbulent boundary layers up to separation [10]. The k-\( \omega \) model is substantially more accurate than the k-\( \epsilon \) model in the near wall layers, and has therefore been successful for flows with moderate adverse pressure gradients, but fails for flows with pressure induced separation [10]. In addition, the \( \omega \) equation shows a strong sensitivity to the values of \( \omega \) in the freestream outside the boundary layer [1]. Mentor combined the Wilcox k-\( \omega \) turbulence model with the standard k-\( \epsilon \) model, and the zonal formulation is based on blending functions which ensure a proper selection of the k-\( \omega \) and k-\( \epsilon \) zones without user interaction [10]. Blending of the calibration parameters is used, while a production limiter is implemented, completing the model’s closure approximations [9].
The turbulent kinetic energy equation can be written as [1]

**Turbulent Kinetic Energy**

\[
\frac{\partial}{\partial t}(\bar{\rho}k) + \frac{\partial}{\partial x_i}(\bar{\rho}\bar{u}_i k) = \tilde{P}_k - \beta^*\bar{\rho}\omega k + (\bar{\mu} + \sigma_k \mu_t) \frac{\partial^2}{\partial x_i^2}(k)
\]

Here, \( \tilde{P}_k \), is the production limiter used in the SST model to prevent the build-up of turbulence in stagnation regions [1]. The production limiter can be defined as follows

\[
P_k = \mu_t \frac{\partial \bar{u}_i}{\partial x_j} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \rightarrow \tilde{P}_k = \min(P_k, 10, \beta^*\bar{\rho}\omega k) \tag{2.55}
\]

**Specific Turbulent Dissipation**

\[
\frac{\partial}{\partial t}(\bar{\rho}\omega) + \frac{\partial}{\partial x_i}(\bar{\rho}\bar{u}_i \omega) = \frac{\alpha}{\nu_t} \frac{\partial \bar{u}_i}{\partial x_j} \left( 2\mu_t \bar{S}_{ij} - \frac{2}{3} \bar{\rho} k \delta_{ij} \right) - \beta \bar{\rho} \omega^2 \\
+ (\bar{\mu} + \sigma_\omega \mu_t) \frac{\partial^2}{\partial x_i^2}(\omega) + 2(1 - F_1)\bar{\rho} \sigma_\omega^2 \frac{1}{\omega} \frac{\partial k}{\partial x_i} \frac{\partial \omega}{\partial x_i} \tag{2.56}
\]

Calibration parameters include the following [1], \( \beta^* = 0.09, \beta_1 = 0.075, \beta_2 = 0.0828, \sigma_{k1} = 0.85034, \sigma_{k2} = 1, \sigma_{\omega1} = 0.5, \sigma_{\omega2} = 0.85616, \alpha_1 = 0.5532, \) and \( \alpha_2 = 0.4403 \), where,

\[
\sigma_k = F_1(\sigma_{k1} - \sigma_{k2}) + \sigma_{k2} \tag{2.57}
\]

\[
\sigma_{\omega} = F_1(\sigma_{\omega1} - \sigma_{\omega2}) + \sigma_{\omega2} \tag{2.58}
\]

\[
\beta = F_1(\beta_1 - \beta_2) + \beta_2 \tag{2.59}
\]

\[
\alpha = F_1(\alpha_1 - \alpha_2) + \alpha_2 \tag{2.60}
\]
while the turbulent kinematic viscosity is $\nu_t = \mu_t/\bar{\rho}$. $F_1$ is a blending function defined by,

$$F_1 = \tanh(\text{arg}_1^4)$$  \hspace{1cm} (2.61)

$$\text{arg}_1 = \min \left[ \max \left( \frac{\sqrt{k}}{0.09 \omega d}, \frac{500 \nu}{d^2 \omega} \right), \frac{4 \bar{\sigma} \sigma_2 k}{CD_{\kappa \omega} d^2} \right]$$  \hspace{1cm} (2.62)

where $d$ is the distance to the nearest wall, and $CD_{\kappa \omega}$ is the positive component of the cross diffusion term.

$$CD_{\kappa \omega} = \max \left( 2 \bar{\rho} \sigma_2 \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}, 0 \right)$$  \hspace{1cm} (2.63)

Eddy viscosity is defined by

$$\mu_t = \frac{a_1 \bar{\rho} k}{\max(a_1 \omega, \Omega F_2)}$$  \hspace{1cm} (2.64)

where $a_1 = 0.31$ and $\Omega = \sqrt{2 \bar{\Omega}_{ij} \bar{\Omega}_{ij}}$, the magnitude of the vorticity. While $F_2$ is,

$$F_2 = \tanh(\text{arg}_2^3)$$  \hspace{1cm} (2.65)

$$\text{arg}_2 = \max \left( \frac{2 \sqrt{k}}{0.09 \omega d}, \frac{500 \nu}{d^2 \omega} \right).$$  \hspace{1cm} (2.66)
An essential feature of a useful industrial turbulence model is an accurate and robust near wall treatment. In addition, the solutions should be largely insensitive to the near wall grid resolution. For complex industrial flows, the requirement $y^+ < 1$ is excessive and in most cases cannot be satisfied for all walls [1]. Consequently, the SST model developed by Mentor is formulated such that the incorporation of wall functions is straightforward. Wall functions ease the near wall grid resolution requirement. Subsequently, the computational expenditures are less restrictive. For this research, wall functions have been used and more detail regarding the formulation will be given in the next chapter describing boundary conditions.

2.3 Transport Properties

High-temperature, chemically reacting viscous flows can be characterized by the molecular transport of species, momentum, and energy in a multi-component gaseous mixture. Evaluation of these properties includes evaluation of diffusion coefficients, viscosities, thermal conductivities, and thermal diffusion coefficients. Various models derived from standard kinetic theory exist to enable the determination of these properties. Care must be taken to compute the pure species properties coupled with proper methods to determine the mixture-averaged properties.

However, efforts again must be made to minimize computational requirements. In light of this methodology, species viscosity is computed using Sutherland’s law, a relatively simple yet accurate approximation for air which can be defined as,

$$\mu_i = \frac{A_s \sqrt{T}}{1 + T_s/T}$$

(2.67)
in which the constant $A_s$ is determined by

$$A_s = \frac{\mu_{\text{ref}}}{T_{\text{ref}}^{3/2}} \left( T_{\text{ref}} + T_s \right) \quad (2.68)$$

The reference values and Sutherland’s constant, $T_s$, can be found in tabular form [11]. Species thermal conductivity is calculated using a modified Eucken formula [4],

$$\kappa_i = \mu \left( c_p + \frac{5}{4} \frac{R}{W_i} \right) \quad (2.69)$$

where $R$ is the universal gas constant and $W_i$ is the species molecular weight. The mixture viscosity and thermal conductivity are determined using a weighted average of species viscosities and thermal conductivities. Finally, density is determined from the perfect gas equation of state

$$\bar{\rho} = \frac{p}{RT} \quad (2.70)$$

2.4 Chemical Kinetics

Chemical kinetics are critical for an accurate combustion simulation. Once ignition is achieved, reactions are the primary driving mechanism pushing combustion towards completion. Consequently, chemical kinetic reaction mechanisms directly impact the accuracy of the simulation. As a result, a reduced, yet detailed reaction mechanism consisting of ten species and twenty-one reactions has been used for this research. Description of the reaction mechanism can be found in Appendix A.

Considering a mixture of $n$ chemically reacting species, a species mass fraction transport equation must be used. After Favre decomposition, the transport equation
can be expressed as

\[
\frac{\partial}{\partial t}(\overline{pY_i}) + \frac{\partial}{\partial x_j}(\overline{\rho u_i Y_i}) = \frac{\partial}{\partial x_j}(j_i - \overline{\rho u_j Y_i''}) + \omega_i \tag{2.71}
\]

where \( Y_i \) is the species mass fraction defined as,

\[
Y_i = \frac{W_i}{W} X_i \tag{2.72}
\]

in which \( W_i \) is the species molecular weight, \( W \) is the mean molecular weight, and \( X_i \) is the mole fraction. Equation 2.71 contains the final remaining correlation term, \( \overline{\rho u_j'' Y_i''} \). Once again using the gradient-diffusion hypothesis, Equation 2.71 can be re-written using [9]

\[
\overline{\rho u_j'' Y_i''} = - \frac{\mu_t}{S_{ct,i}} \frac{\partial Y_i}{\partial x_j} \tag{2.73}
\]

resulting in

\[
\frac{\partial}{\partial t}(\overline{pY_i}) + \frac{\partial}{\partial x_j}(\overline{\rho u_i Y_i}) = \frac{\partial}{\partial x_j}\left( j_i + \frac{\mu_t}{S_{ct,i}} \frac{\partial Y_i}{\partial x_j} \right) + \omega_i . \tag{2.74}
\]

Here, \( S_{ct,i} \), represents the turbulent Schmidt number. Simplification of Equation 2.74 can be achieved by assuming the species viscous diffusion and mass diffusion rates are equal. This assumption results in a Schmidt number of one and consequently \( \overline{\rho D} = \mu \).
Subsequently Equation 2.74 can be rewritten

\[
\frac{\partial}{\partial t}(\bar{p}Y_i) + \frac{\partial}{\partial x_j}(\bar{p}\bar{u}_i Y_i) = \mu_{eff} \frac{\partial^2}{\partial x_j^2}(Y_i) + \omega_i
\]  

(2.75)

where \( \mu_{eff} = (\mu + \mu_t) \).

A more elegant turbulence/chemistry model can be formulated by implementing multi-component species transport and diffusion models. By assuming unity Lewis and Schmidt numbers, the effects of thermal diffusion and viscous diffusion have been set equal to mass diffusion. In many cases, the availability of computational resources practically eliminates the possibility of using multi-component transport and diffusion models. Incorporation of a multi-component diffusion model also requires special care when writing the program to insure global species mass conservation. The second term on the right hand side of Equation 2.75 is the chemical source term for a given species resulting from the potential imbalance between the forward and reverse reaction rates. The rate of reaction \( k \) in a mechanism containing \( r \) chemical reactions is defined as [2]

\[
w_k = k_{f,k} \prod_{j=1}^{N_s} \left( \frac{\bar{p}Y_j}{W_j} \right)^{\nu'_{jk}} - k_{b,k} \prod_{j=1}^{N_s} \left( \frac{\bar{p}Y_j}{W_j} \right)^{\nu''_{jk}}
\]  

(2.76)

where \( k_{f,k} \) and \( k_{b,k} \) are the reaction rate coefficients of the forward and backward reactions respectively. The rate coefficients are sensitive to temperature and pressure and are determined using Arrhenius parameters. The Arrhenius equation, remarkably accurate in predicting the temperature dependency of reaction rates is expressed as,

\[
k = AT^{\beta_k}e^{-E_a/(RT)}
\]  

(2.77)
The pre-exponential factor is denoted $A$, and has the units of $s^{-1}$. While $E_a$ is the activation energy with units of energy per mole and $\beta_k$ is the temperature exponent. In Equation 2.76, the exponents $\nu'_{jk}$ and $\nu''_{jk}$ are the stoichiometric coefficients of reaction $k$ in both forward and backward directions respectively. Subsequently, the chemical source term can be expressed as,

$$\omega_i = W_i \sum_{k=1}^{N_r} (\nu''_{jk} - \nu'_{jk}) w_k . \quad (2.78)$$

The sum over all chemical source terms vanishes [4],

$$\sum_{i=1}^{n} \omega_i = 0 . \quad (2.79)$$

If a third-body is required for a reaction because an energy surplus or deficit exists as a result of splitting molecules, Equation 2.78 takes the form

$$\omega_i = W_i \sum_{k=1}^{N_r} (\nu''_{jk} - \nu'_{jk}) [M_i] w_k \quad (2.80)$$

and $[M_i]$ can be expressed as

$$[M_i] = \sum_{i=1}^{N_s} \alpha_{ik} [X_i] \quad (2.81)$$

where $\alpha_{ik}$ is the third-body efficiency factor for species $i$.

Pressure dependent reactions are governed by different parameters compared to their temperature dependent counterparts. Pressure dependent reaction rate con-
stants are given by [4]

\[
k = k_\infty \left( \frac{p_r}{1 + p_r} \right) F
\]  
(2.82)

where the reduced pressure is defined as [4]

\[
p_r = \frac{k_0 [M_i]}{k_\infty} .
\]  
(2.83)

At the high and low pressure limits, pressure dependent Arrhenius equations take the form

\[
k_\infty = A_\infty T^{\beta_\infty} e^{(-E_\infty/RT)}
\]  
(2.84)

and

\[
k_0 = A_0 T^{\beta_0} e^{(-E_0/RT)}
\]  
(2.85)

In Equation 2.82, the function \( F \) is presented as [4]

\[
\log(F) = \left\{ 1 + \left[ \frac{\log(p_r) - 0.4 - 0.67\log(F_{\text{cent}})}{0.75 - 1.27\log(F_{\text{cent}}) - 0.14(\log(p_r) - 0.4 - 0.67\log(F_{\text{cent}}))} \right]^2 \right\}^{-1} \log(F_{\text{cent}}) .
\]  
(2.86)

where
\[ F_{\text{cent}} = (1 - \alpha) \exp\left(-\frac{T}{T_3}\right) + \alpha \exp\left(-\frac{T}{T_1}\right) + \exp\left(-\frac{T_2}{T}\right) \] (2.87)

The four parameters, \( \alpha, T_1, T_2, \) and \( T_3 \) are presented for the pressure dependent reactions in Appendix A. In fact, all constants found in Equations 2.77 and 2.81 as well as Equations 2.82 through 2.87 can be found in Appendix A.

2.5 Combustion Model

During turbulent combustion, turbulence has a direct impact on the homogeneity of the multi-component reactive mixture which in turn affects the chemical kinetics and subsequently the chemical source term. Care must be taken to accurately simulate the interchange between the turbulence and chemical kinetics. However, great simplification is needed to avoid issues with computational costs and data storage. Considering the size of the computational domain, a direct numerical simulation is not realistic as the various time scales needed to accurately simulate turbulent combustion of a reactive mixture far exceed current capabilities. As a result, the Partially Stirred Reactor (PaSR) combustion model has been introduced to avoid such complications [12].

Further development of the perfectly stirred reactor (PSR) model has given rise to the partially stirred reactor model. Using the PaSR approach, a computational cell is divided into two different zones. In one zone, the chemical reactions occur under the assumption of a perfectly mixed reactive mixture. This assumption permits the exclusion of fluctuations when calculating the chemical source terms [12]. While in the other zone there are no chemical reactions taking place. Therefore the species concentration change via a mass exchange between zones.
The PaSR model regards the combustion process as a series of separate processes. First, the species concentration is adjusted to the reactive mixture within the reaction zone. Second, through turbulence, the reacted mixture is mixed with the non-reacted mixture giving the new species concentration. Next, the reaction rate modifier is then determined by the final species concentration. Due to the formulation of the PaSR model, reaction rates are proportional to the ratio of the chemical time scale to the total conversion time in the reactor [12]. The total conversion time is the sum of both the chemical time scale and micro-mixing time scale. This ratio can be defined as

\[ RR = \frac{\tau_c}{\tau_c + \tau_{mix}} \]  

(2.88)

where

\[ \tau_{mix} = C_{mix} \sqrt{\frac{1}{\omega}} \]  

(2.89)

Equation 2.89 represents the micro-mixing time scale, and \( C_{mix} \) is a tuning constant. The reaction rate modifier, \( RR \), is then used to scale the reaction rate and through the reaction rate modifier the turbulence/chemistry interaction is captured.
CHAPTER 3
SOLUTION METHODOLOGY

Chapter Three will begin with an introduction to OPENFOAM®, the CFD application used for this research. In addition, following the introduction are detailed formulations of the discretization schemes, solution methods, and boundary conditions.

3.1 Introduction to OPENFOAM®

OPENFOAM® was created as a C++ library with the intent of being used primarily to create executable files known as applications. The applications can be divided into two categories: solvers, which are designed to solve a specific problem in continuum mechanics; and utilities, which are designed to perform tasks that involve data manipulation. OPENFOAM® is an open-source software application, in other words, complete access to source files enables the user to modify files in order to create customized applications suited to the users needs, which consequently is the greatest strength of OPENFOAM®. Users are supplied with pre- and post-processing environments and the interface to the pre- and post-processing environments are themselves OPENFOAM® utilities, essentially ensuring consistent data handling across all environments.

OPENFOAM® also provides the user the ability to run applications within a parallel computing framework using a utility referred to as OpenMPI, (Open Message Passing Interface). Applications can be executed on a high-powered computing cluster
or laptop with parallel computing capabilities. Computing resources used for this analysis are as follows.

**System-76 Gazelle Professional** (laptop)

- Operating System: Ubuntu 14.04 1 LTS 64 bit
- 4th Generation Intel Quad Core i7-4810MQ Processor (2.8 GHz 6MB L3 Cache-4 Cores plus Hyperthreading) - Hyperthreading provides 4 additional virtual processors for a total of 8 processors.
- 8 GB Dual Channel DDR3 SDRAM at 1600MHz - 2x4 GB
- 240 GB Intel 730 Series Solid State Drive

### 3.2 Mesh Generation

Computational fluid dynamics is an extremely powerful tool used across many engineering platforms to resolve fluid flow physics. Validity of a CFD analysis depends directly on the ability of the user to build a representative model of the circumstances being analyzed, starting with mesh generation. A mesh is the geometrical discretization of the computational domain, by extension the governing equations, and is intended to capture the problem geometry. Having a rudimentary idea of the flow physics being modeled facilitates the choice of mesh construction. Options for grid arrangement also exist, and pressure-velocity-density coupling needs to be addressed in order to prevent spurious oscillations. For this reason in addition to minimal non-orthogonality as well as velocity aligned CV placement, a co-located grid arrangement has been chosen. As a result of the simple geometry describing the Multi-Mode Ejector-Augmented Pulsed Detonation Rocket Engine, a structured mesh has been utilized. In order to complete a grid convergence study, three suc-
cessively refined grids have been created with an axis of symmetry along the bottom boundary, see APPENDIX B.

3.3 Finite Volume Method

Since time is a parabolic coordinate, the solution is obtained by marching in time from prescribed initial conditions [13]. Therefore, prescribing the size of the time-step is sufficient for temporal discretization. A condition typically used to determine appropriate time-step size is the Courant-Friedrichs-Lewy condition where

\[
CFL = \frac{\Delta t u_x}{\Delta x} = 1 .
\] (3.1)

However, for turbulent reactive flow it is common to use a much more restrictive CFL condition, present code uses CFL < 0.1. The discretization of space for the finite volume method used here requires a subdivision of the domain into control volumes. No overlapping of control volumes is permissible and the computational domain is completely filled with control volumes. A control volume is bounded by a set of faces and each face is shared with only one neighboring control volume.

Cell faces can be divided into two groups; internal faces which are the faces between two control volumes and boundary faces which coincide with boundaries of the computational domain. The face area vector \( \mathbf{S}_f \) is constructed such that the vector points outwards from the control volume with a lower label, is normal to the face, and the magnitude equals the face area. OPENFOAM® uses a notation in which the cell with a lower label is called the “owner” of the face and its label is stored in the “owner” array. The label for the other cell is “neighbor” and is stored
in the “neighbor” array. Boundary face area vectors point out of the computational
domain and are “owned” by the adjacent cells.

3.4 Transport Equation Discretization

Standard form of the scalar transport equation is

\[
\frac{\partial}{\partial t} (\rho \phi) + u_j \frac{\partial}{\partial x_j} (\rho u_i \phi) = \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial \phi}{\partial x_j} \right) + S_\phi(\phi)
\]  

(3.2)

where \( \phi \) is a scalar property, \( D \) is the diffusion coefficient, and \( S_\phi(\phi) \) represents the
source terms. This is a second-order equation, as a second derivative exists within the
diffusion term. For good accuracy, it is necessary for the order of the discretization
to be equal to or higher than the order of the equation being discretized [14]. The
discretization practice adopted in this study is second-order accurate in both space
and time and is the subject matter in the remaining sections of this chapter.

In certain regions of the discretization, relaxation of the accuracy requirement
is necessary in the presence of steep gradients in order to preserve the boundedness of
the solution. Deviation from the prescribed order of accuracy creates numerical error
on the order of the other terms in the original equation and disappears only in the limit
of excessively fine mesh [14]. However, as will be explained in later sections, the use of
total variation diminishing schemes mitigates this problem with the implementation of
flux limiters. In the presence of steep gradients, an “anti-diffusion” term, proportional
to the limiter, is added to maintain accuracy which is higher than first-order. This
creates an opportunity to use Richardson \( h^2 \)-extrapolation to extrapolate what is
thought to be a fourth order accurate solution [15], whereby the extrapolated value
can be used for simulation validation.
Accuracy of the discretization method depends on the variation of the scalar property of Equation 3.2, $\phi = \phi(x, t)$, in space and time around the cell center point value. In order to obtain a second-order accurate method, this variation must be linear in both space and time. For example,

$$
\phi(x) = \phi_{cp} + (x - x_{cp}) \cdot (\nabla \phi)_{cp} \tag{3.3}
$$

$$
\phi(t + \Delta t) = \phi_t + \Delta t \left( \frac{\partial \phi}{\partial t} \right) \tag{3.4}
$$

where $\phi_{cp} = \phi(cp)$ and $\phi_t = \phi(t)$.

Starting with a Taylor series expansion of the scalar function around point $x_{cp}$

$$
\phi(x) = \phi_{cp} + (x - x_{cp}) \cdot (\nabla \phi)_{cp} + \frac{1}{2} (x - x_{cp})^2 : (\nabla \nabla \phi)_{cp}
+ \frac{1}{3!} (x - x_{cp})^3 :: (\nabla \nabla \nabla \phi)_{cp}
+ ... + \frac{1}{n!} (x - x_{cp})^n ::: (\nabla \nabla \cdots \nabla \phi)_{cp} \tag{3.5}
$$

Comparison of Equation 3.3, the assumed variation of $\phi$, and Equation 3.5, the Taylor series expansion of $\phi$, the first term of the truncation error scales with $| (x - x_{cp})^2 |$. Therefore, the spatial variation is second-order accurate.

Using Equation 3.4 in conjunction with a Taylor series expansion in time, a similar result is derived for the temporal term

$$
\phi(t + \Delta t) = \phi_t + \Delta t \left( \frac{\partial \phi}{\partial t} \right) + \frac{\Delta t^2}{2!} \left( \frac{\partial^2 \phi}{\partial t^2} \right) + \frac{\Delta t^3}{3!} \left( \frac{\partial^3 \phi}{\partial t^3} \right) + \cdots + \frac{\Delta t^n}{n!} \left( \frac{\partial^n \phi}{\partial t^n} \right) \tag{3.6}
$$

Again, making the comparison with Equation 3.4, the assumed variation of $\phi$ with
time, the first term of the truncation error scales with $\Delta t^2$. Thus the temporal
discretization is second-order accurate in time.

Using the finite volume method requires Equation 3.1 to be satisfied over all
control volumes around the center point cell value

$$
\int_{t}^{t+\Delta t} \left[ \frac{\partial}{\partial t} \int_{V_{cp}} \rho \phi dV + \int_{V_{cp}} \nabla \cdot (\rho u \phi) dV \right] - \int_{t}^{t+\Delta t} \left( \int_{V_{cp}} \nabla \cdot (\rho D \nabla \phi) dV \right) dt
$$

$$
= \int_{t}^{t+\Delta t} \left( \int_{V_{cp}} S_{\phi}(\phi) dV \right) dt \tag{3.7}
$$

The next few subsections are a description of the term-by-term discretization of Equation 3.7.

3.4.1 Spatial Discretization

Using Equation 3.7 as a framework and remembering Equation 3.3, the linear
variation of $\phi(x)$ over a control volume follows,

$$
\int_{V_{cp}} \phi(x) dV = \int_{V_{cp}} [\phi_{cp} + (x - x_{cp}) \cdot (\nabla \phi)_{cp}] dV . \tag{3.8}
$$

However, the computational point $cp$ is located at the centroid of the control volume
such that [14],

$$
\int_{V_{cp}} (x - x_{cp}) dV = 0 . \tag{3.9}
$$

This is a result of a discretization technique referred to as the mid-point integration
rule. As a result, Equation 3.8 can be rewritten as,

\[
\int_{V_{cp}} \phi(x) dV = \int_{V_{cp}} \phi_{cp} dV + \left[ \int_{V_{cp}} (\mathbf{x} - \mathbf{x}_{cp}) \cdot (\nabla \phi)_{cp} dV \right] = \phi_{cp} V_{cp}
\]  \hspace{0.5cm} (3.10)

where \(V_{cp}\) is the volume of the cell. Gauss’ theorem may be used to evaluate terms with the divergence operator,

\[
\int_{V_{cp}} \nabla \cdot \phi dV = \int_{\partial V_{cp}} \phi_f dS_f = \sum_f \left( \int_f \phi_f dS_f \right).
\]  \hspace{0.5cm} (3.11)

No sources or sinks within the volume is implied, however, there are discontinuities (i.e., shock and detonation waves). Using Equations 3.8, 3.9, 3.10, and applying the linear variation assumption to Equation 3.11, a second-order accurate discretized form of Gauss’s theorem is obtained,

\[
(\nabla \cdot \phi) V_p = \sum_f \phi_f S_f.
\]  \hspace{0.5cm} (3.12)

The subscript \(f\) implies values of the variable \(\phi\) at the face center. Applying this methodology to a CFD analysis, the face area vector \(S_f\) points outward from the center point \(cp\) only if \(cp\) is the centroid of an “owner” cell. For neighboring faces, \(S_f\) points inwards, which needs to be taken into account in the sum of Equation 3.12 [14].
Consequently, Equation 3.12 is split into sums over the “owned” and “neighboring” faces

\[ \sum_f \phi_f S_f = \sum_{\text{owner}} \phi_f S_f - \sum_{\text{neighbor}} \phi_f S_f \quad (3.13) \]

The necessity to sum across “owner” and “neighbor” cells applies to all discretized equations henceforth.

3.4.1.1 Convection Terms

Using Equation 3.12, the convection term is discretized as follows

\[ \int_{V_{cp}} \nabla \cdot (\rho u \phi) dV = \sum_f S_f (\rho u \phi)_f \]

\[ = \sum_f F \phi_f \quad (3.14) \]

where \( F = S_f (\rho u)_f \), the flux through the face. In order for Equation 3.14 to be calculated, the value of \( \phi \) on the control volume face must be determined using the value at the cell center. This task is accomplished using the chosen convection differencing scheme.

A myriad of differencing schemes exists. When using a differencing scheme to represent the true solution, consideration of the differencing scheme solution accuracy and solution boundedness are important. However, schemes tend to exhibit either solution accuracy or solution boundedness but not both. In the presence of solution discontinuities, i.e., shock waves or detonation waves, obtaining both solution accur-
acy and boundedness is particularly difficult due to the extreme gradients present. The ability of a differencing scheme to capture such phenomenon and mesh refinement are directly correlated. In the limit of infinite computational node density, excessively steep gradients can be accurately represented regardless of scheme. However, as is often the case, computational limitations make excessively refined meshes impractical. As a consequence, efforts have been made to develop schemes utilizing both the solution accuracy of higher order central differencing schemes as well as the solution boundedness typical of upwind schemes.

Flux limiting is a procedure that creates a differencing scheme which is higher than first-order accurate, but without the spurious oscillations associated with the classical second-order schemes. This has proven to be the most promising approach [14]. Harten [16] introduces the notion of total variation diminishing (TVD) to characterize oscillation-free flux-limited schemes.

It is well known an estimate involved in convergence proofs of differencing schemes is a bound on the variation of the solution (Sweby [18], Harten [16]). For this research, a flux limiting TVD scheme is used and the total variation of the solution is defined by

$$TV(\phi^n) = \sum_f |\phi^N_N - \phi^P_P|$$

(3.15)

where $P$ and $N$ are the points around the face $f$. The total variation diminishing schemes satisfy the following condition for every time-step,

$$TV(\phi^{n+1}) \leq TV(\phi^n)$$

(3.16)
The TVD criterion starts with the derivation of semi-discrete schemes for the unsteady convection problems by Osher, named the “E-schemes” [18]. Weak solutions are not unique and the correct physical solution is assured as a result of satisfying the entropy condition.

TVD criterion is applied to the higher-order flux-limited schemes in a way suggested by Sweby [18]. The higher-order differencing scheme is written as a sum of the first-order bounded upwind differencing scheme (UD) and a “limited” higher-order correction

\[ \phi_f = (\phi)_{UD} + \Psi_{FL}[(\phi)_{CD} - (\phi)_{UD}] \]  \hspace{1cm} (3.17)

where \((\phi)_{UD}\) represents the face value for the first-order upwind differencing scheme, \((\phi)_{CD}\) represents the face value for the second-order central differencing scheme, while \(\Psi_{FL}\) is the flux limiter. Next is a description of both the central and upwind differencing schemes.

The central differencing scheme used to determine the face value of \(\phi\) is calculated according to

\[ (\phi)_{CD} = f_x \phi_P + (1 - f_x) \phi_N. \]  \hspace{1cm} (3.18)

Again, \(P\) and \(N\) are the center points of adjacent cells in which \(P\) is the center point of the “owner” cell and \(N\) is the center point of the “neighbor” cell as described in Section 3.3. The face in this instance is between points \(P\) and \(N\). Using a Taylor series expansion of \(\phi_N\) about point \(x_p\), Ferziger and Perić [19] show that Equation
3.18 is second-order accurate in space and this is consistent with the overall accuracy of the method [14]. The interpolation factor can be defined as the ratio of distances,

\[ f_x = \frac{x_N - x_f}{x_N - x_P}. \quad (3.19) \]

As mentioned, it has been noted that the central differencing scheme causes unphysical oscillations in the solution for convection-dominated problems, thus violating the boundedness of the solution [13].

The upwind differencing scheme used in Equation 3.17 is formulated as follows

\[
\phi_f = \begin{cases} 
\phi_f = \phi_P & \text{for } F \geq 0. \\
\phi_f = \phi_N & \text{for } F < 0.
\end{cases} \quad (3.20)
\]

where \( F \) is the face flux. Boundedness of the solution is guaranteed through the sufficient boundedness criterion for systems of algebraic equations. Boundedness of the upwind differencing scheme is effectively insured at the expense of accuracy, by implicitly introducing numerical diffusion [13].

Total variation diminishing schemes employ limiter functions \( \Psi_{FL} \) as can be seen in Equation 3.17. Part of the TVD criterion requires the limiting function to be a function of \( r \), the ratio of gradients between successive grid points. Because the notation is compact, notation from Sweby [18] is used where the convention is defined as \( [\Delta_+ y_k = \Delta y_{k+1/2} = \Delta_- y_{k+1} = y_{k+1} - y_k] \) and \( [u^k \equiv u^{n+1}_k, u_k \equiv u^n_k] \). The ratio of successive gradients is

\[ r = \frac{u_k - u_{k-1}}{u_{k+1} - u_k}. \quad (3.21) \]
Figure 3.1: Sweby Diagram

The Sweby diagram [18] gives the necessary and sufficient conditions for a scheme to be TVD, see Figure 3.1. In the figure, the grey area represents the admissible TVD region. However, not all limiter functions are second-order. To be consistent with notation, \( \Psi_{FL}(r) = \Phi(r) \) as indicated on the figure. To maximize the anti-diffusive flux while simultaneously increasing the accuracy of the scheme, the limiter function needs to be maximized subject to the TVD constraints. Subsequently a first choice limiter function could be

\[
\Psi(r) = \min(2r, 2), \quad r > 0
\]  

(3.22)

which is the upper bound of the grey region in Figure 3.1 [18]. A TVD scheme should be second-order accurate whenever possible, which leads to additional constraints on the preferred regions of Figure 3.1 where the limiter function must exist. Two second-order schemes provide the additional necessary bounds for the preferred domain in which the limiting function remains second-order accurate. First, the Lax-Wendroff second-order scheme for hyperbolic conservation laws is used where \( \Psi_{FL}(r) = 1 \) [18].
The LW scheme can be defined as follows,

$$
u^k = u_k - \nu \Delta u_{k-1/2} - \Delta \left\{ \frac{1}{2}(1 - \nu)\nu \Delta u_{k-1/2} \right\} \tag{3.23}$$

where here

$$\nu = \frac{a \Delta t}{\Delta x}. \tag{3.24}$$

Second, the second-order upwind scheme of Warming and Beam, where $$\Psi_{FL}(r) = r$$, provides the final boundary of the preferred domain [18]. The WB scheme can be written as

$$u^k = u_k - \nu \Delta u_{k-1/2} - \Delta \left\{ \frac{1}{2}(1 - \nu)\nu \Delta u_{k-1/2} \right\} \tag{3.25}$$

These schemes provide the boundaries with which the limiting function must abide by to remain second-order accurate. Although beyond the scope of this research, Van Leer’s approach of using Fromm’s scheme, the arithmetic average of these two schemes frame the bounds of the desired domain [18].

$$\Psi_{FL}(r) = (1 - \theta(r))\Psi_{FL}^{LW}(r) + \theta(r)\Psi_{FL}^{WB}(r) \tag{3.26}$$

which reduces to
\[ \Psi_{FL}(r) = 1 + \theta(r)(r - 1) \] (3.27)

where \( \Psi_{FL}^{LW}(r) \equiv 1 \), \( \Psi_{FL}^{WB}(r) \equiv r \), and \( 0 \leq \theta \leq 1 \). Now \( \Psi_{FL}(r) \) is confined to lie within the region of the Sweby diagram in which the limiter function remains globally second-order accurate. For this research, a modified Sweby limiter is used,

\[ \Psi_{FL}(r) = \max[\min(\beta r, 1), 0] \] (3.28)

where \( \beta = 2 \).

3.4.1.2 Diffusion Terms

Similar to the convection term, using Equation 3.14, the diffusion term can be discretized assuming a linear variation of \( \phi \). Because the mesh is minimally non-orthogonal, no non-orthogonality corrections to the code were made. As a result, the following expressions are used,

\[
\int_{V_{cp}} \nabla \cdot (\rho D \nabla \phi) dV = \sum_{f} S_f (\rho D \nabla \phi)_f \\
= \sum_{f} (\rho D)_f S_f (\nabla \phi)_f 
\] (3.29)

and

\[
S_f (\nabla \phi)_f = |S| \frac{\phi_N - \phi_P}{|d|} 
\] (3.30)
where $|\mathbf{d}|$ represents the vector pointing from $P$ to $N$, again the notation given to adjacent cell centers.

### 3.4.1.3 Source Terms

Any term not considered a convection, diffusion or temporal term is treated as a source term. The source term, $S_\phi(\phi)$, can be a general function of $\phi$ [14]. Before discretization, the source term needs to be linearized and can be done so by separating into two parts

$$S_\phi(\phi) = S_u + S_p \phi$$

Using Equation 3.10, the volume integral is evaluated as

$$\int_{V_{cp}} S_\phi(\phi) dV = S_u V_{cp} + S_p V_{cp} \phi_{cp} .$$

### 3.4.2 Temporal Discretization

Referring back to Equation 3.7 and using Equations 3.14, 3.29, and 3.32, the transport equation can be written as,

$$\int_{t}^{t+\Delta t} \left[ \left( \frac{\partial \rho \phi}{\partial t} \right)_{cp} V_{cp} + \sum_{f} F_{\phi_f} - \sum_{f} (\rho D)_{sf} S_f (\nabla \phi)_f \right] dt$$

$$= \int_{t}^{t+\Delta t} (S_u V_{cp} + S_p V_{cp} \phi_{cp}) dt .$$
Temporal discretization has been achieved using the Crank-Nicholson method. Remembering Equation 3.6, the time integrals and derivatives follow directly:

$$
\left( \frac{\partial \rho \phi}{\partial t} \right)_{cp} = \frac{\rho_{cp} \phi_n^p - \rho_{cp}^0 \phi_0^p}{\Delta t}
$$

(3.34)

and

$$
\int_{t}^{t+\Delta t} \phi(t) dt = \frac{1}{2}(\phi^0 + \phi^n) \Delta t
$$

(3.35)

where $\phi^0 = \phi(t)$ and $\phi^n = \phi(t + \Delta t)$. Finally Equations 3.33, 3.34, and 3.35 give,

$$
\frac{\rho_{cp}^n \phi_n^p - \rho_{cp}^0 \phi_0^p}{\Delta t} + \frac{1}{2} \sum_f F \phi^n_f - \frac{1}{2} \sum_f (\rho D)_f S_f (\nabla \phi)_f^n + \frac{1}{2} \sum_f F \phi^0_f - \frac{1}{2} \sum_f (\rho D)_f S_f (\nabla \phi)_f^0
$$

$$
= S_u V_{cp} + \frac{1}{2} S_p V_{cp} \phi_n^p + \frac{1}{2} S_p V_{cp} \phi_0^p .
$$

(3.36)

This is an implicit formulation and the Crank-Nicolson method is a combination of both the backward and forward Euler method.

With each time step, a new value of $\phi_P$ is determined. Since both $\phi_f$ and $(\nabla \phi)_f$ depend on the values in the neighboring cells, Equation 3.36 can be written as an algebraic equation,

$$
A_P \phi_P^n + \sum A_N \phi_N^n = R_P .
$$

(3.37)
One equation of this form is assembled for every control volume. Because $\phi^n_P$ depends on values in the neighboring cells, a system of algebraic equations is created,

$$A\phi = R$$

(3.38)

where $A$ is a matrix with coefficients $A_P$ on the diagonal and coefficients $A_N$ off the diagonal; $\phi$ is the flow variable vector for all control volumes and $R$ is the source term vector. The off diagonal coefficients above and below the diagonal correspond to the faces in the mesh. While the source term includes all terms which can be determined without knowing $\phi$, namely the terms corresponding to the old time values including the $S_u$ term of Equation 3.31. Once this system of equations is solved, a new set of $\phi$ values are computed for the new time-step.

3.5 Boundary Conditions

Proper boundary conditions are necessary to ensure realistic and accurate simulations. Three different flow configurations have been studied, each with different inlet boundary conditions based on freestream Mach numbers 0, 2, and 4.

3.5.1 Inlet Conditions

Dynamic pressure is a design parameter for flight vehicles, particularly hypersonic flight vehicles. High-performance aircraft designs have structural limits that are globally specified in terms of dynamic pressure. Simple calculation methods for the behavior of inviscid hypersonic flows along surfaces involve dynamic pressure [20]. As a result of the local pressure being a function of dynamic pressure, integrals over the entire body surface are functions of dynamic pressure as well [20]. Consequently, dy-
Dynamic pressure impacts the structural design of hypersonic aircraft, explaining why hypersonic aircraft end up being designed to operate within a fairly narrow range of dynamic pressure. Because dynamic pressure is proportional to freestream mass flow per unit area, hypersonic aircraft are flown along trajectories of their highest allowable dynamic pressure in an effort to maintain engine thrust. Inlet conditions are uniquely determined by

\[ q_0 = \frac{\gamma p_0 M_0^2}{2} \]  

(3.39)

where \( q_0 \) is the dynamic pressure, \( p_0 \) is the ambient pressure, \( M_0 \) the freestream Mach number and \( \gamma \) is the ratio of specific heats. Equation 3.39 can be rewritten to determine the ambient pressure necessary given a dynamic pressure and Mach number.

\[ p_0 = \frac{2q_0}{\gamma M_0^2} \]  

(3.40)

For this study, a dynamic pressure of 47,880 N/m\(^2\) was chosen. Following determination of the pressure, the ambient temperature and altitude can be calculated using standard atmospheric relations. Once the ambient conditions are known, inlet conditions to the computational domain can be computed.

Due to the presence of wall friction and shock waves, supersonic inlet losses arise resulting in a reduction in total pressure across the inlet system. Total pressure has an exponential dependency on entropy. In supersonic flight, within the inlet system, both wall friction and shock waves serve as mechanisms which cause an increase in entropy. The inlet’s overall total pressure loss is the product of the ram pressure
ratio and the diffuser pressure ratio [21]

\[ \pi_d = \pi_{max} \eta_r \]  \hspace{1cm} (3.41)

where \( \pi_{max} \) is wall friction loss and \( \eta_r \) is the portion of \( \pi_d \) due to ram recovery. For subsonic and supersonic flow, a useful reference for the ram recovery \( \eta_r \) is Military Specification 5008B [21], which is expressed as

\[
\eta_r = \begin{cases} 
1 & M_0 \leq 1 \\
1 - 0.075(M_0 - 1)^{1.35} & 1 < M_0 < 5 \\ 
\frac{800}{M_0^3 + 935} & 5 < M_0 
\end{cases} . \hspace{1cm} (3.42)
\]

Next, the wall friction portion is determined using a table of component efficiencies from [21]. For a supersonic aircraft with the engine integrated into the airframe, level 4 technology dictates a wall friction pressure ratio of \( \pi_{max} = 0.96 \).

The process to determine the computational domain inlet conditions is fairly straightforward. Using Equation 3.40 and the standard atmospheric relations to find temperature, the total temperature is found by

\[ T_{t0} = T_0 \left(1 + \frac{\gamma - 1}{2} M_0^2 \right) . \hspace{1cm} (3.43) \]

If flow within the computational domain (mixing chamber) remains subsonic, the inlet system exit temperature \( T_3 \) should be less than the freestream total temperature. Typically \( T_3 \) is between eighty to ninety percent of the freestream total temperature. Assuming the inlet system to be adiabatic, \( T_{t0} = T_{t3} \).
A value of $T_3 = 0.85T_{10}$ has been chosen for this research. Once the inlet system exit temperature is determined (note: The inlet system exit temperature is also the computational domain’s inlet boundary temperature), the inlet system exit Mach number can be determined. Resulting from the assumption of an adiabatic inlet and remembering the total temperature is constant, the inlet system exit Mach number can be determined by,

$$M_3 = \sqrt{\frac{2}{\gamma-1} \left( \frac{T_{10}}{T_3} - 1 \right)} .$$  \hspace{1cm} (3.44)

Next, using the calculated value for $T_3$ and $\pi_d$, $p_3$ can be computed as [20]

$$p_3 = \psi (p_0 \pi_d)^{(\gamma-1)/\gamma}$$ \hspace{1cm} (3.45)

where $\psi = T_3/T_0$. Finally, knowing $p_3$, $T_3$, $M_3$ and using the relation $a = \sqrt{\gamma RT_3}$, $u_3$ can be found. See Table 3.1 for a summary of the inlet flow conditions.

Mixing chamber inlet flow remains subsonic for all cases studied. With the exception of the case with a freestream Mach number $M_\infty = 0$, a Neumann boundary condition has been applied to pressure. As a result the mixing chamber inlet pressure gradient is defined by

$$\frac{\partial p_3}{\partial x} \bigg|_{\text{inlet}} = 0 .$$  \hspace{1cm} (3.46)

Precautions had to be taken for a freestream Mach number $M_\infty = 0$ because the detonation wave propagates out of both the inlet and outlet. As a consequence, a wave transmissive boundary condition was applied to both the inlet and outlet. A full
description of the wave transmissive boundary condition will be given shortly. While inlet velocity and temperature are set by Dirichlet boundary conditions at the inlet:

\[ \mathbf{u}(x, t) \rightarrow \mathbf{u}(0, t) = \alpha \]
\[ T\big|_{x=0} = \beta \]  

(3.47) \hspace{1cm} (3.48)

where Alpha and Beta are some value.

Inlet conditions for the turbulent parameters, \( k \) and \( \omega \) are important given the turbulence model’s dependence on freestream values of the turbulent variables. Directly estimating the turbulence model variables, like turbulent energy, dissipation or Reynolds stresses, is often difficult. Instead it is easier to think in terms of variables like the incoming turbulent intensity and turbulent length scale or eddy viscosity ratio [1]. These variables are more intuitive to understand and are more easily related to the physical characteristics of the problem. The turbulent energy can be computed as,

\[ k = \frac{3}{2}(u_x I)^2 \]  

(3.49)

where \( I \) is the turbulent intensity and for moderate turbulence can be between 0.07-0.1 percent [1]. Using the turbulent length scale, the specific turbulent kinetic energy dissipation value is calculated as

\[ \omega = \frac{\sqrt{k}}{l} \]  

(3.50)

where the turbulent length scale is proportional to the grid resolution \( (l \approx 0.002\text{m}) \).
Table 3.1: Mixing Chamber Inlet Flow Properties \((g_0 = 47,888 \text{ N/m}^2)\)

<table>
<thead>
<tr>
<th>Freestream Mach number</th>
<th>(p_3 \text{ (N/m}^2))</th>
<th>(T_3 \text{ (K)})</th>
<th>(u_3 \text{ (m/s)})</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>101325.00</td>
<td>298.15</td>
<td>0.00</td>
</tr>
<tr>
<td>2</td>
<td>67117.52</td>
<td>330.74</td>
<td>342.36</td>
</tr>
<tr>
<td>4</td>
<td>348729.49</td>
<td>780.04</td>
<td>553.90</td>
</tr>
</tbody>
</table>

Temperatures within the inlet system are such that the species mass fractions remain constant. Consequently, the species mass fraction gradients are zero. The species mass fraction at the domain inlet is expressed using a Neumann boundary condition.

\[
\left. \frac{\partial Y_i}{\partial x} \right|_{\text{inlet}} = 0 \tag{3.51}
\]

### 3.5.2 Solid Wall Boundary Conditions

Flow velocity adjacent to any solid wall in viscous flow is assumed to be zero,

\[
u_x = u_y = 0 \text{ at } y = 0 \tag{3.52}
\]

which also means turbulent kinetic energy is zero. Because all solid wall boundaries in the domain are adiabatic, meaning there is no transfer of heat through the surface of the wall, the temperature gradient normal to the wall is defined by

\[
\left. \frac{\partial T}{\partial y} \right|_{y=0} = 0 \tag{3.53}
\]
At solid wall boundaries, the species mass fraction are found to be

\[ \frac{\partial Y}{\partial y} \bigg|_{y=0} = 0 . \]  

(3.54)

Turbulence variables require special care in their near-wall treatment. Formulation of turbulence models begins with proper descriptions of turbulent variables throughout the boundary layer. All turbulence models adhere to some form, either incompressible or compressible, of the “law of the wall”. The boundary layer is broken into two regions with three distinct layers. First, there is the viscous sublayer where molecular diffusion as well as energy flux through the boundary play a prominent role. Next, there is the log layer, which is essentially an overlap between the viscous sublayer and defect layer regions developed through matched asymptotic expansions. Here turbulent kinetic energy production and dissipation are nearly balanced [6]. The third layer is the defect layer and velocity gradients are small in this layer as the velocity approaches the free-stream value. The incompressible law of the wall is expressed as,

\[ u^+ = \frac{1}{\kappa_{VK}} \ln(y^+) + C \]  

(3.55)

where \( \kappa_{VK} \) and \( C \) are turbulent model constants and \( y^+ = u_\tau y/\nu \), while \( u^+ = U/u_\tau \). The dimensionless velocity \( u^+ \) and distance \( y^+ \) are both functions of the friction velocity \( (u_\tau) \). A compressible analog has been derived and is known as the Van Driest transformation. However, for low Mach numbers coupled with an adiabatic wall boundary, the transformation collapses and generates a velocity profile similar to the incompressible law of the wall. Hence, an incompressible law of the wall formulation has been used. In order to appropriately capture the physics, significant
mesh resolution is required to achieve $y^+ < 1$, which is preferred. However, most CFD applications allow for the use of wall functions in high Reynold’s number flow and wall functions are indeed used for this research. Wall functions require the first computational node to be placed within the log layer. The boundary layer is then calculated rather than resolved by a sufficiently refined mesh. Significant computational overhead is saved thus drastically decreasing computational time. For this research, $7 \leq y^+ \leq 30$. A description of the wall functions used follows.

The $\omega$-equation is well suited for wall functions as it provides analytical solutions for both the viscous sublayer and the log layer [10].

\[
\omega_{\text{vis}} = \frac{6}{0.075y^2} 
\]

\[
\omega_{\text{log}} = \frac{1}{0.3\kappa_V K} \frac{u_T}{y} 
\]

Using the definition of $y^+$, Equations 3.56 and 3.57 can be reformulated as functions
of \( y^+ \). The wall function defines \( \omega \) as [10],

\[
\omega = \sqrt{\omega(y^+)_{vis}^2 + \omega(y^+)_{log}^2}.
\]

(3.58)

A similar formulation is used for the friction velocity profile near the wall [10];

\[
\begin{align*}
u_{vis}^\tau &= \frac{U}{y^+} \\
u_{log}^\tau &= \frac{U}{\frac{1}{n} \ln(y^+) + C}
\end{align*}
\]

(3.59) \hspace{1cm} (3.60)

where

\[
u^\tau = \left[ (u_{vis}^\tau)^4 + (u_{log}^\tau)^4 \right]^{0.25}.
\]

(3.61)

3.5.3 Outlet Boundary Conditions

The outlet boundary was spaced sufficiently far from the “flow action” to use Neumann boundary conditions,

\[
\left. \frac{\partial \phi}{\partial x} \right|_{outlet} = 0
\]

(3.62)

where \( \phi \) is a flow variable, for all flow variables except pressure. A wave transmissive boundary condition was chosen for pressure to prevent the reflection of waves at the outlet (and inlet for case 1). Application of an eigenvalue analysis is used to separate out decoupled waves and work directly on these waves, to either upwind or use a zero-gradient at the outlet. The sign of the wave speed indicates whether or not the
Table 3.2: Summary of Boundary Conditions

<table>
<thead>
<tr>
<th>M_∞-Re</th>
<th>Boundary</th>
<th>p_3 (N/m^2)</th>
<th>T_3 (K)</th>
<th>u_3 (m/s)</th>
<th>k (m^2/s^2)</th>
<th>ω (1/s)</th>
<th>Y_i</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 Re = 0.00</td>
<td>Inlet</td>
<td>WT</td>
<td>298.15</td>
<td>ZG</td>
<td>0.00</td>
<td>0.00</td>
<td>ZG</td>
</tr>
<tr>
<td></td>
<td>Wall</td>
<td>ZG</td>
<td>ZG</td>
<td>0.00</td>
<td>0.00</td>
<td>WF</td>
<td>ZG</td>
</tr>
<tr>
<td></td>
<td>Outlet</td>
<td>WT</td>
<td>298.15</td>
<td>ZG</td>
<td>0.00</td>
<td>0.00</td>
<td>ZG</td>
</tr>
<tr>
<td></td>
<td>Int.</td>
<td>101325.00</td>
<td>ZG</td>
<td>0.00</td>
<td>0.00</td>
<td>ZG</td>
<td>ZG</td>
</tr>
<tr>
<td>2 Re = 9.4e^6</td>
<td>Inlet</td>
<td>ZG</td>
<td>330.74</td>
<td>342.36</td>
<td>1758.16</td>
<td>20965.20</td>
<td>ZG</td>
</tr>
<tr>
<td></td>
<td>Wall</td>
<td>ZG</td>
<td>ZG</td>
<td>0.00</td>
<td>0.00</td>
<td>WF</td>
<td>ZG</td>
</tr>
<tr>
<td></td>
<td>Outlet</td>
<td>WT</td>
<td>330.74</td>
<td>ZG</td>
<td>0.00</td>
<td>0.00</td>
<td>ZG</td>
</tr>
<tr>
<td></td>
<td>Int.</td>
<td>67117.52</td>
<td>ZG</td>
<td>0.00</td>
<td>0.00</td>
<td>WF</td>
<td>ZG</td>
</tr>
<tr>
<td>4 Re = 4.2e^6</td>
<td>Inlet</td>
<td>ZG</td>
<td>780.04</td>
<td>553.90</td>
<td>3037.05</td>
<td>27554.74</td>
<td>ZG</td>
</tr>
<tr>
<td></td>
<td>Wall</td>
<td>ZG</td>
<td>ZG</td>
<td>0.00</td>
<td>0.00</td>
<td>WF</td>
<td>ZG</td>
</tr>
<tr>
<td></td>
<td>Outlet</td>
<td>WT</td>
<td>780.04</td>
<td>ZG</td>
<td>0.00</td>
<td>0.00</td>
<td>ZG</td>
</tr>
<tr>
<td></td>
<td>Int.</td>
<td>348729.49</td>
<td>ZG</td>
<td>0.00</td>
<td>0.00</td>
<td>ZG</td>
<td>ZG</td>
</tr>
</tbody>
</table>

wave is outgoing or incoming. See Table 3.2 for a summary of each case and the associated boundary conditions.

In the boundary column, the interior boundary conditions are denoted by (Int.), (WF) represents the wall function, (WT) represents the wave transmissive boundary condition, and (ZG) is zero-gradient. Additionally, in column one the inlet Reynolds number is shown, Case Two and Three are clearly turbulent flows. Gas species concentrations were initialized in two zones, zone one included the initiator and detonation tubes while all other areas make up the second zone. Within the initiator and detonation tubes gas species mass fractions were initialized to $N_2 = 0.745$, $O_2 = 0.226$, and $H_2 = 0.029$. All other areas, the gas species mass fractions were initialized to be $N_2 = 0.7552$, $O_2 = 0.2315$, and $Ar = 0.0133$.

3.6 Ignition Mechanism

Yi [22] has confirmed the notion that properties of a detonation eventually converge to the same values regardless of the conditions in the ignition zone. Ignition
of the fuel/oxidizer mixture was achieved by an explicit enthalpy injection source written into the code. Deflagration-to-detonation transition was avoided by direct detonation. The ignition zone is 2 by 9mm on the far left boundary of the initiator tube. An explicit injection source of 1500 J occurs for a duration of $5.5 \times 10^{-6}$ seconds. In addition to the enthalpy injection, a high temperature, high pressure patch was coded into the ignition zone. Within the ignition zone, $p = 30$ atm and $T = 3000$ K, which is equivalent to an energy density of 5.437 MJ/m$^3$. The primary focus of this research was to gain understanding of how the primary and secondary flow streams mix during the detonation cycle. Consequently, no precautions were taken to prevent over-driving the reaction as the detonation properties converge to the same values regardless of the ignition zone conditions, as previously mentioned. The same ignition mechanism was used across all cases, eliminating any possible variance from one case to another.

3.7 Solution Procedure

In this section a thorough description of the solution procedure follows, including solution steps, a derivation of the pressure equation, and an explanation of the PISO algorithm.

3.7.1 Step One: Internal Field and Boundary Condition Initialization

Set up initial conditions. The initial conditions consist of all boundary conditions as well as internal field conditions. Boundary conditions are automatically set. However, in OPENFOAM®, all internal conditions have to be initialized using the OPENFOAM® command “setFields”. If the simulation is running in parallel, the next step is to decompose the domain according to the chosen decomposition method. This is accomplished by using the OPENFOAM® command “decomposePar” A sim-
ple decomposition method was chosen for this research as a result of the simplicity of the mesh. The domain was decomposed into eight equally sized domain partitions.

3.7.2 Step Two: PISO Loop

Calculation of the new time-step values begins. First the momentum predictor equation is assembled and solved using the available face fluxes. The momentum equation takes the form

\[ A_P U_P = H(U) - \nabla p. \tag{3.63} \]

The first term on the right hand side of Equation 3.63, \( H(U) \), consists of two parts; the “transport part”, including the matrix coefficients for all neighbors multiplied by the corresponding velocities and the “source part” including the source part of the transient term and all other source terms \( (f) \) apart from the pressure gradient [14]

\[ H(U) = -\sum_N A_N U_N + \frac{U^0}{\Delta t} + f. \tag{3.64} \]

A solution to Equation 3.63 is obtained. However, the exact pressure gradient term is not known at this stage because the pressure field from the previous time-step is used. Finding a solution to Equation 3.63 provides an approximation of the new velocity field. The \( H(U) \) term can be re-assembled and the pressure gradient equation can now be formulated. The approximated velocity field can be represented by

\[ U_P = \frac{H(U)}{A_P} - \frac{1}{A_P} \nabla p. \tag{3.65} \]
Equation 3.65 is interpolated to the face and is computed by

$$U_f = \left( \frac{H(U)}{A_P} \right)_f - \left( \frac{1}{A_P} \right)_f (\nabla p)_f.$$ \hspace{1cm} (3.66)

The discretized continuity equation is

$$\nabla \cdot U = \sum_f S_f U_f = 0.$$ \hspace{1cm} (3.67)

Substituting Equation 3.66 into Equation 3.67 yields the pressure equation

$$\sum_f S_f \left[ \left( \frac{1}{A_P} \right)_f (\nabla p)_f \right] = \sum_f S_f \left( \frac{H(U)}{A_P} \right)_f.$$ \hspace{1cm} (3.68)

Using the solution to Equation 3.68 provides the first estimate of the new pressure field. Next, the face fluxes consistent with the new pressure field are determined using,

$$F = S_f U_f = S_f \left[ \left( \frac{H(U)}{A_P} \right)_f - \left( \frac{1}{A_P} \right)_f (\nabla p)_f \right].$$ \hspace{1cm} (3.69)

If Equation 3.68 is satisfied, the face fluxes are guaranteed to be conservative [14]. Finally the velocity is adjusted based on the new pressure field. This process is repeated until Equation 3.67 is satisfied to within a predetermined tolerance. At this point a new set of conservative fluxes are also obtained. The linearized system of algebraic equations is solved using an interative method.
3.7.3 Step Three: Turbulence and Chemical Kinetics

Using the newly obtained conservative fluxes, all other equations in the system are solved. Because the system includes a turbulence model, effective viscosity is computed from the turbulence variables and then turbulence model equations are solved. In addition to the turbulence model equations, species transport equations, and the chemical kinetic reaction mechanism equations must be solved. The reaction mechanism is represented by a system of ordinary differential equations. Operator splitting techniques are employed to navigate the potential vast differences between the chemical reaction characteristic time scales and all other characteristic time scales. The reaction mechanism system of equations is solved using an extrapolation method based on a linearly implicit Euler method used for stiff differential equations. These steps are repeated until the final time-step is reached.

3.8 Verification and Validation

3.8.1 Mesh Convergence

Because the computational domain is discretized, error is inherently introduced into the solution which is directly correlated to the computational node density. As the node density approaches infinity, the error approaches zero. Starting with a coarse mesh, each successive refinement is potentially accompanied by an increase in solution accuracy. Mesh refinement will reach a point at which the solution ceases to become more accurate, reaching what is termed as a “grid independent” solution. Using Richardson $h^2$-extrapolation, an estimation of the exact solution can be computed. Once the estimation to the exact solution is obtained, the extrapolated solution can be compared with other data sources, thus formalizing an error.
Yi [22] conducted research in which he developed a transient numerical simulation of the same propulsion concept studied in the present work. Yi’s objectives included simulations of a detonation within a tube having mixing chamber secondary flow Mach numbers of 0 and 2.5. These conditions are representative of modes 1 and 4 of the Multi-Mode Ejector-Augmented Pulsed Detonation Rocket Engine. While only mode one is the focus of this research, building on Yi’s work is accomplished by the addition of a turbulence model in addition to an analysis of the blowdown process. As a result of conducting a mesh independence study, Yi reached a grid independent solution with a von Neumann pressure spike of 23.150 atm. Figure 3.3 consists of pressure diagrams created from this study’s simulation, capturing the von Neumann pressure spike caused by the detonation wave. With each successive mesh refinement, the wave structure becomes more and more apparent. Table 3.3 is a summary of the pressure profiles from Figure 3.3 compared with the grid independent solution achieved by Yi [22]. Initial conditions in the detonation tube are the same conditions used by Yi, $p = 1$ atm and $T = 298.15$ K. Dimensions of the detonation tube are 0.20 m in length and 0.018 m in height, keeping in mind the bottom boundary is a symmetry boundary. Included in Table 3.3 is the detonation wave velocity, calculated using time-of-flight as well as the resolution used to obtain the measurements. Because there were no precautions to prevent over-driving the reaction, the detonation wave speeds are slightly higher than CJ theoretical values. Also in Table 3.3, values for the von Neumann pressure spike and left end wall pressures can be seen.
Figure 3.3: von Neumann Peak Pressure Profile at $t = 0.0001s$ for $M_\infty = 0$
Table 3.3: Pressure Profiles on Various Mesh Resolutions

<table>
<thead>
<tr>
<th>Number of grids</th>
<th>(\Delta x) (m)</th>
<th>(u_D) (m/s)</th>
<th>(p_{VN}) (atm)</th>
<th>(p_3) (atm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CJ</td>
<td>-</td>
<td>1965.10</td>
<td>15.586</td>
<td>-</td>
</tr>
<tr>
<td>Yi</td>
<td>(5.0 \times 10^{-5})</td>
<td>1965.57</td>
<td>23.150</td>
<td>5.878</td>
</tr>
<tr>
<td>(N_x = 38)</td>
<td>(5.3 \times 10^{-3})</td>
<td>1997.50</td>
<td>17.055</td>
<td>5.419</td>
</tr>
<tr>
<td>(N_x = 76)</td>
<td>(2.6 \times 10^{-3})</td>
<td>2047.50</td>
<td>20.295</td>
<td>5.637</td>
</tr>
<tr>
<td>(N_x = 152)</td>
<td>(1.3 \times 10^{-3})</td>
<td>2052.50</td>
<td>22.339</td>
<td>5.923</td>
</tr>
</tbody>
</table>

Richardson extrapolation, introduced by Richardson in 1910, assumes the discrete solutions \(\phi\) can be represented by a series expansion in the grid spacing \(h_R\).

\[
\phi = \phi_{\text{exact}} + g_1 h_R + g_2 h_R^2 + g_3 h_R^3 + \cdots + g_n h_R^n
\]  
(3.70)

Functions \(g_1, g_2, \) and so on are defined in the continuum and do not depend on any discretization scheme [15]. For a second-order method, \(g_1 = 0\). The objective is to combine two separate discrete solutions, \(\phi_1\) and \(\phi_2\), on two different grids with uniform discrete spacings of \(h_{R,1}\) (fine grid) and \(h_{R,2}\) (coarse grid) to eliminate the leading-order error terms in the assumed error expansion. Using the equations derived from the expansions on each discrete solution, solving for \(g_2\) in the first equation, then substituting the result into the second equation, a more accurate estimate of \(\phi(\text{exact})\) is obtained.

\[
\phi = \phi_{\text{exact}} + \frac{(h_{R,2}^2 \phi_1 - h_{R,1}^2 \phi_2)}{h_{R,2}^2 - h_{R,1}^2}
\]  
(3.71)

Higher-order terms have been dropped. The grid refinement ratio can be defined as

\[
r_R = \frac{h_{R,2}}{h_{R,1}}.
\]  
(3.72)
Equation 3.71 can be cast in the form

$$\phi_{\text{exact}} = \phi_1 + \frac{\phi_1 - \phi_2}{r^2 - 1}. \quad (3.73)$$

The grid spacing used for this research is a grid doubling, therefore $r = 2$. Equation 3.73 reduces to

$$\phi_{\text{exact}} = \frac{4}{3} \phi_1 - \frac{1}{3} \phi_2. \quad (3.74)$$

Using Equation 3.74 and the peak von Neumann pressure values obtained from Mesh 2 and Mesh 3 in Figure 3.3, an extrapolated approximation of the exact value can be computed.

$$\phi_{\text{exact}} = \frac{4}{3} (22.339) - \frac{1}{3} (20.295) = 23.02 \text{ (atm)} \quad (3.75)$$

The relative error between the result from Equation 3.75 and the grid independent solution obtained by Yi [22],

$$\epsilon_{\text{error}} = \frac{23.150 - 23.02}{23.150} = 0.5\% \quad (3.76)$$

The relative error between the value obtained by Yi [22] and the solution obtained from Mesh 3 is $\epsilon_{\text{error}} = 3\%$. The relative error between the Mesh 3 solution and the extrapolated solution is $\epsilon_{\text{error}} = 2.9\%$. It is often stated that Equation 3.74 is fourth-order accurate if $\phi_1$ and $\phi_2$ are second-order accurate [15]. The discrete solutions must be both globally and locally second-order. Total variation diminishing schemes
tend towards the upwind component in the presence of steep gradients, i.e., shocks. As a result, the local order of accuracy is less than second-order but greater than first-order. The Sweby limiter maximizes what is referred to as the “anti-diffusion” term to ensure the order of accuracy in smooth regions remains second-order. Consequently, the solution produced by Equation 3.75 is at most third-order accurate [15].

3.8.2 Iterative Convergence

Convergence of steady-state simulations can be ascertained by plotting the residuals from each iteration. Assuming a numerical simulation is developed properly, residuals are continually reduced with each outer iteration to below some predetermined tolerance. After some arbitrary number of iterations, residuals cease to change. When the residuals no longer change with successive iterations, while simultaneously having been reduced below the predetermined tolerance, the solution is thought to be converged. Similar principles apply to transient simulations. Transient simulations force convergence with each time-step while the residuals are reduced below some tolerance by an arbitrary number of inner iterations, typically machine tolerance. For this research, the tolerance threshold is $1 \times 10^{-12}$. The figure of importance here is the initial residual, which is also continually reduced over the total number of iterations. The initial residuals of both enthalpy and pressure are shown below.
Figure 3.4: Initial Residual Plots: $M_\infty = 0$
(a) Mesh 1

(b) Mesh 2

(c) Mesh 3

Figure 3.5: Initial Residual Plots: $M_\infty = 2$
Figure 3.6: Initial Residual Plots: $M_{\infty} = 4$
Upon review of the residual plots, the unsteady nature of the detonation wave is noticeable through the first 1000 iterations. Once the detonation is exhausted from the detonation tube and transitions to a non-reactive shock wave, the flow unsteadiness reduces significantly.

3.8.3 Chemical Kinetics Validation

The NASA computer program CEA (Chemical Equilibrium with Applications) calculates properties of complex mixtures and chemical reactions for various applications. These applications include thermodynamic states, theoretical rocket performance, Chapman-Jouguet detonations, and shock-tube parameters. CEA will be used to confirm the accuracy of post-shock species mass fractions computed by the present code.

Nitrogen has been excluded from Figure 3.7 because it is an inert species, however the nitrogen mass fraction can be viewed in the table comparison with CEA (Table 3.4). Figure 3.7 is a depiction of the change in species mass fraction as a detonation wave propagates through the fuel/oxidizer mixture. As can clearly be seen, the oxidizer O$_2$, is consumed rapidly while a brief and significant production of the hydroxyl radical (OH) occurs. Hyrdoxyl radical production is the driving force behind the reaction mechanism. As the radical is produced other elementary reactions within the overall mechanism consume and utilize the radical as a reactant. Differences between the present code and CEA are potentially attributed to the present code’s assumptions of equal thermal and mass diffusivities as well as equal viscous and mass diffusivities. Additionally, the present code utilizes a reduced reaction mechanism to save computational resources whereas CEA uses an equilibrium approach with a significantly larger species set.
Table 3.4: Species Mass Fractions

<table>
<thead>
<tr>
<th>Species</th>
<th>Present Code</th>
<th>CEA</th>
</tr>
</thead>
<tbody>
<tr>
<td>N$_2$</td>
<td>0.7452</td>
<td>0.7450</td>
</tr>
<tr>
<td>H$_2$O</td>
<td>0.2317</td>
<td>0.2250</td>
</tr>
<tr>
<td>OH</td>
<td>0.0099</td>
<td>0.0138</td>
</tr>
<tr>
<td>O$_2$</td>
<td>0.0103</td>
<td>0.0103</td>
</tr>
<tr>
<td>H$_2$</td>
<td>0.0021</td>
<td>0.0026</td>
</tr>
<tr>
<td>O</td>
<td>0.0012</td>
<td>0.0014</td>
</tr>
<tr>
<td>Ar</td>
<td>0.0005</td>
<td>0.0007</td>
</tr>
</tbody>
</table>

Figure 3.7: Species Mass Fractions Across the Shock Wave.
CHAPTER 4
RESULTS AND DISCUSSION

A brief review of the case set up follows. The geometry consists of the mixing chamber, which is 0.50 m in length by 0.09 m in height, and acts as a shroud around the pulsed detonation rocket. Within the pulsed detonation rocket is the initiation tube (0.04 by 0.009 m) and the detonation tube (0.20 by 0.018 m). Air is captured by the inlet, passes through the inlet system, then enters the computational domain through the left boundary. While in the mixing chamber, the entrained air mixes with the reaction products exhausted from the detonation tube by the detonation wave. Remembering Section 3.5.1, three cases were studied in which the freestream Mach numbers were 0, 2, and 4. Using the constant dynamic pressure trajectory constraint for hypersonic vehicles, Military Spec 5008b and isentropic relations along with standard atmospheric conditions were utilized to determine the inlet conditions for the mixing chamber. Hydrogen and air were chosen as the fuel and oxidizer in order to facilitate comparison with existing numerical simulation data.

4.1 Mode One Analysis

Figures 4.1 and 4.2 depict the pressure and temperature evolution resulting from the detonation wave. The detonation wave was ignited on the left within the initiator tube and immediately propagates towards the right through the detonation tube. As the detonation wave exits the detonation tube, it weakens and becomes a non-reactive shock wave. A low pressure area can be seen in Figures 4.1(a) and 4.1(b) emanating from the lip of the detonation tube resulting from vorticity and
wave diffraction. In Figure 4.1(c), and to a lesser extent in Figure 4.1(d), a Mach stem and triple point can be noticed. Figure 4.2 shows the temperature evolution, which is essentially the dispersion of the super-heated reaction products convected by the detonation wave. Although difficult to see, the temperature wave follows the pressure wave closely. Once the detonation wave is exhausted from the detonation tube and the fuel/oxidizer mixture is consumed, chemical reactions cease to occur. As a result the temperature decays rapidly. A quantitative color index is positioned just to the left of both Figure 4.1 and 4.2, pressure is measured in pascals where temperature is measured in units of kelvin. Figure 4.3 shows the progression of the detonation wave through the detonation tube. As the wave moves through the detonable mixture, significant compression occurs coupled with a considerable increase in temperature. In the reference frame of the detonation wave, flow immediately following the detonation wave is subsonic. Consequently, the energy released by the wave can propagate forward, continually reinforcing the wave. In the infancy of the detonation wave, some curvature exists at the wave front. However, eventually the wave fully develops into a planar detonation wave.
Figure 4.1: Pressure Evolution in Mixing Chamber at $M_\infty = 0$
Figure 4.2: Temperature Evolution in Mixing Chamber at $M_\infty = 0$
Figure 4.3: Detonation Wave Propagation Through the Detonation Tube.
Detonation wave propagation from case two and three has been excluded due to their propagation similarities within the detonation tube. Comparatively, the physics between cases is extremely similar, albeit with minor differences in temperature and pressure. The next set of figures represent the development of the detonation wave with a freestream Mach number \( M_\infty = 2 \). Keep in mind the flow entering the computational domain has just passed through the inlet system where the velocity is reduced to subsonic speeds. Figures 4.4 and 4.5 depict the evolution of pressure (pascals) and temperature (K) under different inlet conditions. In this case, the initial pressure and temperature in the internal domain are 67,117.52 N/m\(^2\) and 330.74 K respectively. The idea is to understand the evolution of the detonation wave during operational conditions. Section 3.5.1 gives a detailed methodology on how the internal pressure and temperature values were determined. Noticeably, inside the mixing chamber the non-reactive shock wave is not able to propagate upstream as quickly or as far when compared with case one. With an inlet velocity of 342.36 m/s (Mach = 0.94), a more complicated flow structure develops in the mixing chamber. Similarly to case one, a Mach stem and triple point form inside the mixing chamber and this can be seen in Figures 4.4(c) and 4.4(d). Starting with Figure 4.4(d), the rarefaction wave begins the purging process. Figure 4.5 indicates the high temperature air mass is transported downstream much more rapidly than case one. Once again, the temperature wave front propagates along with the pressure, however the temperature gradients make capturing the temperature wave front difficult. As will be discussed in the Future Work section, additional research of the flow interaction with nozzle geometry would provide a better understanding of the force augmentation caused by the high-pressure, high-temperature flow resulting from the detonation wave.
Figure 4.4: Pressure Evolution in Mixing Chamber at $M_\infty = 2$
Figure 4.5: Temperature Evolution in Mixing Chamber at $M_\infty = 2$
A major focus of this research is the mixing that occurs between the primary and secondary flow streams. Turbulent kinetic energy is a good indicator of turbulent mixing intensity and turbulence facilitates mixing between the flow streams. The specific turbulent energy dissipation and turbulent kinetic energy are shown in Figures 4.6 and 4.7 respectively. The turbulent parameter $\omega$ can build up near solid surfaces which is visible in Figure 4.6. Turbulence is known to form at the interface between two flow streams due to the momentum differences at high speeds. Instabilities are created and eventually the flow becomes turbulent. From both figures, the turbulent kinetic energy and dissipation can be observed to persist at the primary and secondary flow interface. Vortical flow structures can be noticed emanating from the lip of the detonation tube as well. During mode one operation, the primary objective of the Multi-Mode Ejector-Augmented Pulsed Detonation Rocket Engine is to transfer as much momentum to the secondary flow stream as possible. Turbulence is a good indicator of momentum transfer between two flow streams with unequal velocities.

Following figures 4.6 and 4.7 are figures for case three, with a freestream Mach number $M_\infty = 4$. Again, remember the flow coming into the computational domain has just passed through the vehicle inlet system. When compared to case two, case three has similar flow structures. However, in case three a more defined flow structure develops as evident by the pressure distribution. The detonation wave, as mentioned earlier, evolves into a non-reactive shock wave and is transported downstream very rapidly. Turbulence is again noticeable at the interface between the primary and secondary flow streams.
Figure 4.6: Specific Turbulent Energy Dissipation at $M_\infty = 2$
Figure 4.7: Turbulent Kinetic Energy at $M_{\infty} = 2$
Figure 4.8: Pressure Evolution at $M_{\infty} = 4$
Figure 4.9: Temperature Evolution at $M_\infty = 4$
Figure 4.10: Turbulent Specific Dissipation at $M_\infty = 4$
Figure 4.11: Turbulent Intensity at $M_\infty = 4$

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However turbulent production in case three is less than the turbulent production in case two. The primary and secondary (553.90 m/s, Mach = 0.99) flow velocities in case three are relatively close resulting in less turbulence, see Figures 4.7 and 4.11. Looking at Figures 4.10 and 4.11, there appears to be signs of vortex shedding from the lip of the detonation tube.

4.2 Blowdown Process

After a detonation is complete and the detonation wave has been exhausted from the detonation tube, high-temperature reaction products remain within the detonation tube. Before the next cycle begins, the high temperature reaction products must be removed to prevent auto-ignition of the fuel/oxidizer mixture required for the next detonation. From a practical stand-point, two methods exist for the successful removal of high-temperature gases. A pressurized system can be integrated into the structure of the hypersonic aircraft, consisting of a pressurized tank and relevant support structures. Air at sea-level conditions would be injected into the detonation tube through an injection system. A pressurized system will require more structural support, thus increasing the weight of the aircraft. Alternatively, air can be siphoned from the inlet system. Subsequently, the air injected into the detonation tube would have pressures and temperatures comparable to the secondary flow stream entering the mixing chamber.

Ultimately the system used will be determined by the mission profile of the aircraft. If the hypersonic aircraft has an assisted launch, a pressurized system may not be required. Alternatively, if the aircraft is designed to operate from runway conditions through the super/hypersonic regime, a combination of the pressurized system and siphoning from the inlet system would be necessary. At runway conditions
the pressure gradients necessary to initiate siphoned purging are not sufficient, thus a pressurized system is necessary. From the beginning, this research has focused on a hypersonic aircraft capable of operation extending from runway conditions through the hypersonic regime. Consequently, a pressurized system would be needed for purging under conditions relative to case one while purge gas is assumed to be siphoned under case three conditions. Case one and case three, in particular, are studied because they represent the extreme operational conditions under which purging would occur.

Two injection system configurations are studied. The first configuration will consist solely of an injection port on the left end wall of the initiation tube. As determined by [23], an injection velocity of 93 m/s will be used. Configuration two consists of five injection ports and the same injection velocity is used. From the first configuration, a left end wall injection port within the initiation tube will be retained in conjunction with four additional injection ports equally spaced along the length of the detonation tube. Remembering the symmetrical lower boundary, configuration two consists of nine total injection ports. This simulation is fundamentally simple and basic. No considerations were given to either injection port design or mechanical valve design and limitations. This study is an attempt to expose the physics which evolve during the blowdown process. Extreme conditions relevant to the mode one operational spectrum are examined, as a result, the blowdown process for case one and case three will be simulated (i.e. $M_\infty = 0$ and 4). Following is a description of the simulation set up.

A detonation was allowed to evolve over a period of two milliseconds. Each blowdown configuration is then simulated for an additional two milliseconds for a total of four milliseconds real time. Four milliseconds of real time in addition to the
time required to fill the detonation tube with a fuel/oxidizer mixture roughly translates to a 100 Hz cycle. A frequency of 100 Hz has long been the gold standard in pulsed detonation engine construction. Figures 4.11 and 4.12 are depictions of the temperature evolution during the blowdown process. Column one represents the multi-injection port configuration while the second column represents the left end wall injection port configuration.

4.2.1 Case One: $M_\infty = 0$

Figure 4.12: Temperature Evolution During Blowdown Process: $M_\infty = 0$
4.2.2 Case Three: $M_\infty = 4$

Multiple injection ports seem to remove the heated reaction products more rapidly than a single injection port located on the left end wall of the initiator tube. Although it does appear, to some degree, hot pockets of reaction products can be trapped and isolated between the injection port streams in the multi-injection port.
configuration. A systematic optimization study is needed to understand the most efficient injection port configuration.

4.3 Conclusions

A computational code has been developed into a tool to analyze the flow properties that exist within the mixing chamber during mode one operation of the Multi-Mode Ejector-Augmented Pulsed Detonation Rocket Engine. Detailed chemistry has been used. Although improvement is possible with a more robust reaction mechanism, especially when NO\textsubscript{x} production is a concern. A reduced mechanism developed at the University of California San Diego has been used in an effort to save computational effort. Important hydrogen-oxygen chain, recombination, hydroperoxyl, and hydrogen peroxide reactions have been retained to maintain accuracy. The $k$-$\omega$-SST turbulence model has been implemented to capture the turbulent parameters in an effort to better understand regions of the domain in which significant mixing occurs. This particular model was chosen for performance in bounded flow scenarios in addition to the model’s formulation which facilitates the use of wall functions. Using wall functions is another method utilized to save computational overhead. Mentor’s turbulence model blends the best attributes of both the $k$-$\epsilon$ and $k$-$\omega$ models with the implementation of blending functions, and thus far has preformed very well in flows with adverse pressure gradients. Pressure

Flow properties for the inlet boundary conditions were carefully developed using the constant dynamic pressure trajectory requirements for hypersonic aircraft, Military Spec 5008b, and isentropic relations. Three cases were studied to understand the full range of freestream Mach numbers the propulsion system would experience during mode one operation. The flow is assumed to be fully viscid, therefore appropriate so-
lid wall boundaries were used. A simple ignition mechanism was developed without concern to overdriving the detonation wave as Yi [22] has proven the detonation parameters settle to the Chapman-Jouguet conditions regardless of ignition conditions.

Code validation was achieved by comparison to a previously executed mesh independence study performed by Yi [22]. Using Richardson $h^2$-extrapolation, a third order accurate solution was computed and the solution was within reasonable relative error when compared to the grid-independent solution obtained by Yi [22]. Iterative convergence was demonstrated by initial residual plots of both pressure and enthalpy for each case. Chemical kinetics validation was accomplished by comparing species mass fraction histories with species mass fractions obtained by NASA CEA. The present code produced species mass fraction histories comparable to CEA, within an acceptable relative error.

The overall effectiveness of pulsed ejector-augmentation is clear. First and foremost there are significant weight savings by eliminating the rotational machinery common to turbine and compressor based propulsion systems. The Ejector-Augmented Pulsed Detonation Rocket Engine produces high pressure, high temperature flows which take advantage of detonation properties to increase propulsive efficiency. Geometrically simple, the design facilitates quick and easy production practices, reducing production costs. However, in order to have a complete understanding of the effectiveness of the propulsion system, a time history capturing multiple detonations is required to fully quantify a thrust profile. Research on pulsed flow passing through a nozzle is minimal.

4.4 Future Work

This research can serve as the foundation to other numerous research topics.
In particular, a more in depth study of the inlet system could provide more accurate mixing chamber inlet conditions, which in turn would serve as initial conditions for this present code. Nozzle effects are also an area of potential research. In fact, each operational mode could be studied in this manner, culminating in a comprehensive analysis of the entire Multi-Mode Ejector-Augmented Pulsed Detonation Rocket Engine operational profile. One could use the Numerical Propulsion Simulation System (NPSS) to design a fully integrated propulsion concept. NPSS has “zooming” capabilities which allow for the integration of higher fidelity simulation software, such as OpenFOAM or Fluent. Thus, essentially creating a working simulation of an entire propulsion system. Additionally, chemical reaction mechanisms can also be studied to understand their impact on the detonation parameters. OpenFOAM has a useful functionality which makes interchanging various reaction mechanisms effortless.

Another area of concern involves internal flow evolution after successive detonations. This study was limited to one detonation which occurs over a very small time interval. Unfortunately, other flow phenomena which take longer to develop are not noticeable. For instance, the process of vortex shedding appears to begin. Emanating from the lip of the detonation tube in both case two and three. Additionally, shock wave and detonation wave propagation within the detonation tube and mixing chamber will most certainly cause shock induced boundary layer separation. Areas of significant separation could exist within the detonation tube as a result of the unsteady detonation wave Mach number. Once the detonation wave exhausts from the detonation tube and begins to propagate upstream, the upstream velocity coupled with the mixing chamber inlet velocity could also generate shock induced boundary layer separation. Boundary layer separation can alter the flow depending on the magnitude of the separation. With the use of wall functions, the near wall resolution for this research was not sufficient to capture this behavior.
APPENDIX A

Hydrogen-Air Reaction Mechanism
Hydrogen-air combustion mechanism. The symbol ”M” stands for third body, meaning any species acting as a gas-phase catalyst. The default unit for the activation energy is cal/mol, for the pre-exponential factor mol-cm-s-K is the default.

A.1 Hydrogen-Air reaction mechanism

As expressed by Yi [22], the reaction for a stoichiometric hydrogen-air mixture produces water as a product of combustion processes.
Table A.1: Hydrogen-Air Combustion Mechanism

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>$A$</th>
<th>$B$</th>
<th>$E$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>$H + O = O + OH$</td>
<td>$k_f$</td>
<td>1.915$\times 10^{14}$</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>5.481$\times 10^{11}$</td>
<td>0.39</td>
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<tr>
<td>2.</td>
<td>$O + H_2 = H + OH$</td>
<td>$k_f$</td>
<td>5.080$\times 10^4$</td>
<td>2.67</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>2.667$\times 10^4$</td>
<td>2.65</td>
</tr>
<tr>
<td>3.</td>
<td>$OH + H_2 = H + H_2O$</td>
<td>$k_f$</td>
<td>2.160$\times 10^8$</td>
<td>1.51</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>2.298$\times 10^{11}$</td>
<td>1.40</td>
</tr>
<tr>
<td>4.</td>
<td>$O + H_2O = 2OH$</td>
<td>$k_f$</td>
<td>2.970$\times 10^6$</td>
<td>0.72</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>1.465$\times 10^5$</td>
<td>2.11</td>
</tr>
<tr>
<td>5.</td>
<td>$H_2 + M = 2H + M$</td>
<td>$k_f$</td>
<td>4.557$\times 10^{19}$</td>
<td>-1.40</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>1.146$\times 10^{20}$</td>
<td>-1.68</td>
</tr>
<tr>
<td>6.</td>
<td>$O_2 + M = 2O + M$</td>
<td>$k_f$</td>
<td>4.515$\times 10^{17}$</td>
<td>-0.64</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>6.165$\times 10^{11}$</td>
<td>-0.50</td>
</tr>
<tr>
<td>7.</td>
<td>$OH + M = O + H + M$</td>
<td>$k_f$</td>
<td>9.880$\times 10^{17}$</td>
<td>-0.74</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>4.714$\times 10^{18}$</td>
<td>-1.00</td>
</tr>
<tr>
<td>8.</td>
<td>$H_2O + M = H + OH + M$</td>
<td>$k_f$</td>
<td>1.912$\times 10^{23}$</td>
<td>-1.83</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>4.500$\times 10^{22}$</td>
<td>-2.00</td>
</tr>
<tr>
<td>9.</td>
<td>$H + O_2 (+M) = HO_2 (+M)$</td>
<td>$k_f$</td>
<td>1.475$\times 10^{12}$</td>
<td>0.60</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>3.090$\times 10^{12}$</td>
<td>0.53</td>
</tr>
<tr>
<td>10.</td>
<td>$HO_2 + H = H_2 + O_2$</td>
<td>$k_f$</td>
<td>1.660$\times 10^{13}$</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>3.164$\times 10^{12}$</td>
<td>0.35</td>
</tr>
<tr>
<td>11.</td>
<td>$HO_2 + H = 2OH$</td>
<td>$k_f$</td>
<td>7.079$\times 10^{13}$</td>
<td>0.00</td>
</tr>
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<td></td>
<td></td>
<td>$k_b$</td>
<td>2.027$\times 10^{10}$</td>
<td>0.72</td>
</tr>
<tr>
<td>12.</td>
<td>$HO_2 + O = OH + O_2$</td>
<td>$k_f$</td>
<td>3.250$\times 10^{13}$</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>3.252$\times 10^{12}$</td>
<td>0.33</td>
</tr>
<tr>
<td>13.</td>
<td>$HO_2 + OH + H_2O + O_2$</td>
<td>$k_f$</td>
<td>2.890$\times 10^{13}$</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>5.861$\times 10^{13}$</td>
<td>0.24</td>
</tr>
<tr>
<td>14.</td>
<td>$H_2O_2 + O_2 = 2HO_2$</td>
<td>$k_f$</td>
<td>4.634$\times 10^{16}$</td>
<td>-0.35</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>4.200$\times 10^{14}$</td>
<td>0.00</td>
</tr>
<tr>
<td>15.</td>
<td>$H_2O_2 + O_2 = 2HO_2$</td>
<td>$k_f$</td>
<td>1.434$\times 10^{13}$</td>
<td>-0.35</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>1.300$\times 10^{11}$</td>
<td>0.00</td>
</tr>
<tr>
<td>16.</td>
<td>$H_2O_2 (+M) = OH + OH (+M)$</td>
<td>$k_f$</td>
<td>2.951$\times 10^{14}$</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>3.656$\times 10^{08}$</td>
<td>1.14</td>
</tr>
<tr>
<td>17.</td>
<td>$H_2O_2 + H = H_2O + OH$</td>
<td>$k_f$</td>
<td>2.410$\times 10^{13}$</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>1.296$\times 10^{08}$</td>
<td>1.31</td>
</tr>
<tr>
<td>18.</td>
<td>$H_2O_2 + H = H_2 + HO_2$</td>
<td>$k_f$</td>
<td>6.025$\times 10^{13}$</td>
<td>0.00</td>
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<td></td>
<td></td>
<td>$k_b$</td>
<td>1.041$\times 10^{11}$</td>
<td>0.70</td>
</tr>
<tr>
<td>19.</td>
<td>$H_2O_2 + O = OH + HO_2$</td>
<td>$k_f$</td>
<td>9.550$\times 10^6$</td>
<td>2.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>8.660$\times 10^{3}$</td>
<td>2.68</td>
</tr>
<tr>
<td>20.</td>
<td>$H_2O_2 + OH = H_2O + HO_2$</td>
<td>$k_f$</td>
<td>1.000$\times 10^{12}$</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>1.838$\times 10^{10}$</td>
<td>0.59</td>
</tr>
<tr>
<td>21.</td>
<td>$H_2O_2 + OH = H_2O + HO_2$</td>
<td>$k_f$</td>
<td>5.800$\times 10^{14}$</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k_b$</td>
<td>1.066$\times 10^{13}$</td>
<td>0.59</td>
</tr>
</tbody>
</table>
The fundamental reaction can be written as

$$2\text{H}_2 + \text{O}_2 + 3.762\text{N}_2 \rightarrow 2\text{H}_2\text{O} + 3.762\text{N}_2$$

The fundamental reaction is completed through a series of elementary reactions, and together these elementary reactions form the chemical reaction mechanism. In addition, information is included in the reaction mechanism regarding the reaction rate expressions, third-body reactions and pressure-dependent reactions. Below are the necessary parameters to complete the hydrogen-air reaction mechanism in CHEMKIN format. CHEMKIN was used to input thermodynamic and chemical information.

1. Third-body efficiencies
   (a) Reaction 5: \( \text{H}_2/2.50/\text{H}_2\text{O}/12.00/ \)
   (b) Reaction 6: \( \text{H}_2/2.50/\text{H}_2\text{O}/12.00/\ AR/0.83/ \)
   (c) Reaction 7: \( \text{H}_2/2.50/\text{H}_2\text{O}/12.00/ \ AR/0.75/ \)
   (d) Reaction 8: \( \text{H}_2/0.73/\text{H}_2\text{O}/12.00/ \ AR/0.38/ \)
   (e) Reaction 9: \( \text{H}_2/1.30/\text{H}_2\text{O}/14.00/ \ AR/0.67/ \)
   (f) Reaction 16: \( \text{H}_2/2.50/\text{H}_2\text{O}/12.00/ \ AR/0.64/ \)

2. Lindemann Falloff parameters
   (a) Reaction Nine: LOW / \( 3.4820\times10^{16} -0.41100 -1.1150\times10^3 / \)
   (b) Reaction Sixteen: LOW / \( 1.202\times10^{17} 0.00 45500. / \)

3. Troe Falloff parameters
   (a) Reaction Nine: TROE / \( 0.5 1.0000\times10^{-30} 1.0000\times10^{30} 1.0000\times10^{100} / \)
   (b) Reaction Sixteen: TROE / \( 0.5 1.0000\times10^{-30} 1.0000\times10^{30} 1.0000\times10^{100} / \)

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APPENDIX B

Multi-Mode Ejector-Augmented PDR Mesh
This Appendix consists of the mesh images and the refinement ratio from Mesh 1 to Mesh 2 is 2, as is the mesh refinement ratio from Mesh 2 to Mesh 3. Mesh refinement ratio was determined using the Richardson extrapolation definition.

\[
h_R = \left[ \frac{1}{N} \sum_{i=1}^{N} (\Delta A_i) \right]^{1/2}
\]

(B.1)

Where \( h_R \) is the grid size, \( N \) number of cells, and \( A_i \) is \( i \)-th cell face area. The refinement ratio is defined as

\[
r = \frac{h_{R,coarse}}{h_{R,fine}}
\]

(B.2)
Figure B.1: Mesh Geometry

(a) 1954 Cells

(b) 7816 Cells

(c) 31264 Cells
REFERENCES


BIOGRAPHICAL STATEMENT

Joshua M. Dawson was born in Dallas, TX, on February 11, 1981. He received B.S. degree from Texas A&M University in 2004 in Psychology. From 2004 to 2010, he worked with Fidelity Investments as a Client Service Manager. While working at Fidelity he decided to return to school to obtain his Masters of Science degree in Aerospace Engineering. After completion of his undergraduate studies, in 2013, he was accepted into the aerospace graduate program at the University of Texas at Arlington. His current research interests include turbulence modeling and hypersonic propulsion system concepts for SSTO/TSTO applications.