The Pennsylvania State University
The Graduate School
Department of Mechanical and Nuclear Engineering

LARGE-EDDY SIMULATION OF

SUPERCritical FLUID FLOW AND COMBustion

A Dissertation in
Mechanical Engineering

by
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Submitted in Partial Fulfillment
of the Requirements
for the Degree of

Doctor of Philosophy

May 2011
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Abstract

In liquid-propellant rocket engines, the chamber pressure and temperature are well above supercritical conditions, and the propellants undergo a series of physicochemical processes that are dramatically different from the low-pressure processes. Although extensive experimental studies and many numerical simulations have been performed on propellant mixing and combustion in the context of liquid rocket engines, the current understanding of the flow and combustion dynamics under supercritical conditions is not sufficient to support the engine design and optimization. The present study focuses on the modeling and simulation of injection, mixing, and combustion of real fluids at supercritical conditions. The objectives of the study are: (1) to establish a unified theoretical framework that can be used to study the turbulent combustion of real fluids; (2) to implement the theoretical framework and conduct numerical studies with the aim of improving the understanding of the flow and combustion dynamics at conditions representative of contemporary liquid-propellant rocket engine operation; (3) to identify the key design parameters and the flow variables which dictate the dynamics characteristics of swirl- and shear-coaxial injectors.

The resulting theoretical and numerical framework accommodates the full conservation laws and includes real-fluid thermodynamics and transport phenomena over the entire temperature and pressure regimes of concern. Thermodynamic properties, such as enthalpy, internal energy, and heat capacity, are directly calculated from fundamental thermodynamics theories and a modified Soave-Redlich-Kwong (SRK) equation of state. The transport properties, such as viscosity and thermal conductivity, are estimated using Chung’s method. Mass diffusivity is obtained using the Takahashi method, which is calibrated for high-pressure conditions. Turbulence closure is achieved using a Large-Eddy-Simulation (LES) technique, in
which the large-scale structures are resolved and the effects of unresolved small-scale motions are modeled. The static and dynamic Smagorinsky models are incorporated to model the effect of the sub-grid scale motions. The steady flamelet and the extended flamelet/progress-variable models are used to handle turbulence/chemistry interactions. The resulting set of equations is solved numerically using a preconditioned, density-based finite volume method along with a dual-time stepping technique. Rigorous effort is made to ensure mass conservation and higher-order numerical accuracy. The robustness and the effectiveness of the resulting framework has also been validated. The framework utilizes a parallel computation scheme that involves the Message-Passing Interface (MPI) library and multi-block treatment.

The theoretical and numerical framework is validated by simulating the Sandia Flame D. The calculated axial and radial profiles of velocity, temperature, and mass fractions of major species are in reasonably good agreement with the experimental measurements. The conditionally averaged mass fraction profiles agree very well with the experimental results at different axial locations.

The validated model is first employed to examine the flow dynamics of liquid oxygen in a pressure swirl injector at supercritical conditions. Emphasis is placed on analyzing the effects of external excitations on the dynamic response of the injector. The high-frequency fluctuations do not significantly affect the flow field as they are dissipated shortly after being introduced into the flow. However, the lower-frequency fluctuations are amplified by the flow. As a result, the film thickness and the spreading angle at the nozzle exit fluctuate strongly for low-frequency external excitations.

The combustion of gaseous oxygen/gaseous hydrogen in a high-pressure combustion chamber for a shear coaxial injector is simulated to assess the accuracy and the credibility of the computer program when applied to a sub-scale model of a combustor. The predicted heat flux
profile is compared with the experimental and numerical studies. The predicted heat flux profile agrees very well with the experimental data.

The steady flamelet model and the flamelet/progress-variable have been used to study the LOX/methane flame stabilized by a splitter plate. Results show that the flame is always anchored in the recirculation zone that is immediately after the splitter plate. Turbulence is not strong enough to extinguish the non-premixed flame. The flame stabilization is found to be achieved through the recirculation zone and the vortex shedding processes in the near field of the splitter plate. The flamelet-progress-variable case further confirms that the artificially quenched flame can be re-established as long as the quenching distance is within the mean recirculation zone.
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ACKNOWLEDGMENTS

I would like to express my deepest gratitude and appreciation to my advisor, Dr. Vigor Yang, for his consistent support with his invaluable academic guidance, and spiritual encouragement during the development of this study. Working with him has been one of the most exciting experiences in my life. I would also like to thank Dr. Daniel C. Haworth, Dr. André L. Boehman, Dr. Robert J. Santoro, and Dr. Richard A. Yetter for providing their expert guidance, insightful comments, and for serving as my Ph.D. committee members.

I extend my sincere appreciation to Dr. Nan Zong for his guidance, advice, and suggestions. I am also grateful to Drs. Dongjun Ma, Jian Li, Tao Liu, Yanxing Wang, Fuhua Ma, Ying Huang, Shanwu Wang, Danning You, Hua Meng, Liwei Zhang, Puneesh Puri, and Piyush Thakre, as well as Prashant Khare, Dilip Sundaram, Huaguang Li, Xiaodong Chen, Xiaowei Wang, and Professor Wenpu Zhang, for the enlightening discussions with them, and the wonderful time we spent together in the past five years.

The research work reported in this thesis was sponsored in part by the Air Force Office of Scientific Research under Grant No. FA 9550-07-1-0111, and by NASA Constellation University Institutes Project under grant NO. NCC3-989.

My deepest gratitude goes to my parents, Zhiguo Huo and Xiangde Cui, for giving me my life and the wings so that I can fly; my elder brother, Hongling Huo, and younger sister, Guanying Huo, for their constant love and support.

The deepest love and gratitude belong to my wife, Jing Cheng, for her everlasting love, support, encouragement, and the happiness she brings to me. To her I dedicate this thesis.
Chapter 1

Introduction

1.1 Background and Motivation

One of the greatest accomplishments in human history can be attributed to space exploration and satellite technologies, which enable intercontinental communications, global live TV shows, long-range weather predictions, and scientific experiments on space stations to be part of today's reality. A high-thrust rocket launcher is one of the key enabling techniques that make all of these contemporary technologies possible. For future space exploration endeavors, including continual scientific researches on space stations, missions on Earth's moon, and Mars, and other even deeper space explorations, development of next generation of high-thrust, high-performance, reliable liquid rocket engines for these missions will be one of the key building blocks.

Table 1.1 lists propellants, operating conditions and performance data for three representative Liquid-propellant Rocket Engines (LRE). Those high-thrust lower-stage liquid rocket engines operate at hundreds of atmospheres and more than 3500 K, providing several hundred tons of thrust within a combustion chamber of much less than one cubic meter (for example, the volume of one main combustion chamber of the RD-170 engine is about one eighth cubic meters) in several minutes. Successful missions require very high engine reliability, energy
efficiency, and pose very severe challenges to the design of the Thrust Chamber Assembly (TCA). Of these challenges and difficulties encountered in the development of liquid rocket engines, combustion instability has been recognized as one of the most challenging difficulties, which has plagued almost all liquid rocket engine programs since the late 1930’s (Culick and Yang, 1995). On the one hand, within the almost entirely closed combustion chamber, it takes only an extremely small fraction of heat released from combustion to drive unsteady motions; on the other hand, the internal process to attenuate these unsteady motions is very weak, resulting in the prevalence of combustion instabilities in liquid rocket engines.

Table 1.1. Propellants and chamber operating conditions for selected LRE's.

<table>
<thead>
<tr>
<th>Engines</th>
<th>SSME</th>
<th>RD-170</th>
<th>Vulcain 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Propellants</td>
<td>LOX/H₂</td>
<td>LOX/Kerosene</td>
<td>LOX/H₂</td>
</tr>
<tr>
<td>Chamber Pressure (MPa)</td>
<td>22.6</td>
<td>24.5</td>
<td>11.5</td>
</tr>
<tr>
<td>Chamber Temperature (K)</td>
<td>3700</td>
<td>3676</td>
<td>3500</td>
</tr>
<tr>
<td>Thrust at sea level, (MN)</td>
<td>1.78</td>
<td>7.55</td>
<td>0.9</td>
</tr>
<tr>
<td>Specific Impulse (Vacuum)</td>
<td>452.5</td>
<td>338</td>
<td>431</td>
</tr>
<tr>
<td>Burning Time (seconds)</td>
<td>480</td>
<td>150</td>
<td>600</td>
</tr>
</tbody>
</table>

Many different methodologies, ranging from small-scale research experiments to full-scale tests, have been conducted to investigate combustion instability in liquid rocket engines. Although cost-prohibitive and typically measurement-limited, historically, full-scale trial-and-error tests have played a crucial role in the development of liquid rocket engines. Taking the F-1 engine as an example, over 2000 of a total of approximately 3200 full-scale tests were conducted to solve the combustion stability problems that were encountered (Oefelein and Yang, 1993). Alternative test beds, such as sub-scale chamber combustors, are employed in a significantly cheaper and less committed phase of engine development. Sub-scale combustion diagnostic tests
(which often run at lower pressures, lower flow rates, and for shorter durations), are more amenable to a variety of measurement tools, optical access, thermocouples, and pressure transducers, for example. Thus, they are more attractive and are used widely to predict full-scale engine performance. Most commonly used experimental technologies include (1) Shadowgraph, (2) light scattering, including elastic (Rayleigh and Mie scattering) and inelastic (e.g. Raman scattering) light scattering, (3) OH* and CH* chemiluminescence, (4) Laser Induced Fluorescence (LIF) of radicals, and (5) wall temperature and heat flux measurements using thermocouples. Although sub-scale experiments provide a wealth of physical data and help provide insight into the fundamental processes in propellant injection, mixing, atomization, vaporization and combustion, the experimental results, particularly quantitative data are limited to chamber pressure, wall temperature, heat-flux, and data extracted from images taken using the optical diagnostic technologies listed above. More detailed knowledge regarding spatial distributions of temperature, velocity, turbulence quantities, turbulence/chemistry interactions, are unavailable.

Nevertheless, most (if not all) engines were developed through a time-consuming and costly process of trial and error because the current knowledge of physicochemical processes in liquid rocket engines is not sufficient to establish a predictive tool for combustor design and optimization. A successful design for one application may fail in another due to subtle difference in operating conditions or other system characteristics. Thus, without enough understanding of a series of non-linear psychochemical processes in a real liquid rocket combustion device, a simple copy from a previous successful design experience combined with some small incremental changes does not guarantee the success of the new engine. Trial and error, although costly and time-consuming, becomes unavoidable.
With recent advances in numerical modeling and simulations of turbulent reacting flows, it is possible to evaluate various important physicochemical processes of a candidate design and provide guidance in design optimization, avoiding or minimizing the time-consuming and costly manufacture and test processes in the initial design iterations. With the assistance of appropriate numerical and analytical tools, substantial reduction in the costly sub-scale and full-scale tests could be made to develop the next generation of liquid rocket engines, with better performance, higher thrust, and reliability associated with more requirements/constraints, including toxicity and ease of handing, for example. Thus, there is a clear need to establish a unified theoretical and numerical framework within which the effects of all known processes and design attributes can be studied and assessed by means of advanced modeling and simulation techniques.

In a typical liquid-oxygen gaseous-fuel rocket engine, oxygen is injected at around 100 K and supercritical pressure, while gaseous H₂ (or CH₄) is injected at higher speed. The chamber pressure and temperature are well above the critical points of the propellants, such that when the liquid oxygen is injected into the combustion chamber, transition from trans-critical propellants to supercritical combustion products occurs, which is substantially different from subcritical injection, mixing, vaporization and subsequent combustion processes. Figure 1.1 shows the shadowgraphs of nitrogen jet injection at sub-critical and supercritical conditions (Mayer et al., 1996). It is clearly observed that the mixing process under sub-critical pressures is substantially different from mixing at supercritical pressures. At subcritical conditions, under the effect of surface tension and aerodynamic force, intrinsic surface instabilities develop along the liquid-gas interface and promote the formation of ligaments and droplets, and consequently the breakdown of the jet and subsequent mixing processes. However, at supercritical conditions, due to the vanishing of surface tension and the enthalpy of vaporization, the jet features a variable density gas-gas like mixing process, but is still characterized with rapid variation of thermodynamic
properties (e.g., density, specific heat capacity, and speed of sound). Since mixing is the dominant process in non-premixed flames, the difference in sub-critical and supercritical mixing processes dictates the difference in flame anchoring and combustion dynamics in liquid rocket thrust chambers.

Figure 1.1. Shadowgraphs of nitrogen jet injection at subcritical (left column: at 1 MPa) and supercritical conditions (right column: at 4 MPa). $T_{LN2} = 105$ K, $T_{GN2} = 300$ K, $u_{LN2} = 10$ m/s, $D_{nj} = 1.9$ mm, $P_{cr} = 3.4$ MPa, $T_{cr} = 126$ K (Mayer et al., 1996).

In numerical modeling of combustion dynamics in liquid rocket engines, aside from the classical difficulties in dealing with turbulent reacting flows, new phenomena and problems arise due to the departures of thermodynamic properties from their ideal-gas limit, the vanishing of surface tension and of the enthalpy of vaporization for supercritical fluids. Figure 1.2 shows the thermodynamic property variations for a laminar counter-flow diffusion flame of LOX/methane at 10.0 MPa. The strain rate is fixed at a near extinction limit, i.e., $1.7 \times 10^6$ sec$^{-1}$. From the low temperature oxygen stream to the hot combustion zone, there is an extremely thin layer, within which density decreases by two orders of magnitude; specific heat capacity, molecular viscosity
and speed of sound also experience very rapid variations within that thin layer. These effects on the mixing are tremendous, and the challenges posed to numerical schemes are also stringent.

Figure 1.2. Thermodynamic property profiles for a LOX/methane laminar counter-flow diffusion flame at 10.0MPa. $T_{\text{LOX}} = 120$ K, $T_{\text{CH}_4} = 300$ K.

Numerical simulations of the high-pressure physicochemical processes occurring at supercritical combustion, as described above, pose a variety of challenges, which involve all of the classical difficulties in simulating turbulent reacting flow, and the unique problems associated with thermodynamic non-ideality and transport abnormality for supercritical combustion as
discussed above. From the classical point of view, turbulent reacting flow is characterized with a broad range of length and time scales, including the time scales of chemical reactions and those of various turbulent motions. The scales of the former are dependent on the species concentration and temperature (and pressure) of the flow. They could be smaller than one nano second or approach infinity (as for chemically frozen flow). For the latter, the time scales are highly dependent on the local flow dynamics and can range from an even smaller time scale (infinitely large Reynolds number) to infinity (as for stagnant reacting flow). The length scales cover the smallest Kolmogorov scales, the flamelet thickness, and all the way to the characteristic length of a combustion chamber. Resolving/modeling turbulent reacting flows are themselves open research issues at atmospheric pressures. Secondly, thermodynamic properties and transport properties behave abnormally at trans-critical conditions as discussed above. As a result, compressibility effects (i.e., volumetric changes induced by pressure variations) and variable inertial effects (i.e., volumetric changes induced by heat addition and/or variable composition) play a dominant role in the flow evolution (Yang, 2000). Thirdly, Reynolds number increases and the flame thickness decreases with increasing pressure. The reduction in Kolmogorov scale and flame thickness may change the turbulence/chemistry interaction mechanism and thus the flow evolution. Finally, rapid variation of thermodynamic data needs extreme grid resolution to resolve, and the high density gradient also affects the turbulence anisotropy in this region and changes the flow characteristics. Comprehensive reviews of the knowledge on supercritical mixing and combustion were given by Yang (2000) and Bellan (2000).

The complexity of the problem outlined above is numerically demanding, and a variety of uncertainties exist with regard to closure. This study attempts to address key issues related to modeling and understanding unsteady fluid dynamics and physicochemical processes at supercritical conditions. The objectives are as follows: 1) to establish a unified theoretical
framework which could accommodate full conservation laws, turbulence closure, real-fluid thermodynamics, transport anomalies, and chemical reactions; 2) to conduct an integrated theoretical and numerical study to substantially improve the fundamental knowledge of the flow and flame dynamics under conditions representative of contemporary liquid-propellant rocket engine operation; 3) to develop a quantitative basis for identifying and prioritizing the key design parameters and flow variables that exert strong influence on the injector behavior in different environments; and 4) to examine the dynamic response of injectors to external excitations over a range of frequencies of practical concern in order to assess the combustion stability characteristics of the injector and the entire combustion device.

1.2 Review of Relevant Literature

Extensive studies have been conducted on the processes of propellant injection, atomization, mixing and the combustion of single jet injections, shear coaxial injectors, and pressure swirl coaxial injectors with propellants of gas-gas, gas-liquid, and liquid-liquid phase combinations under various pressure conditions. Table 1.2 and 1.3 summarize the recent experimental and numerical studies, respectively, with detailed information about the injector types, dimensions, propellants, injection temperatures and chamber pressures. For reference, the critical temperatures and pressures of some propellants are summarized in Table 1.4.
<table>
<thead>
<tr>
<th>Researchers</th>
<th>Combustion or not</th>
<th>Propellants</th>
<th>$p_c$ (MPa)</th>
<th>$D_i$ (mm)</th>
<th>$D_o$ (mm)</th>
<th>$D_f$ (mm)</th>
<th>$T_{inj}$ (K)</th>
</tr>
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<tbody>
<tr>
<td>Jet</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chehroudi et al., 2002a</td>
<td>No</td>
<td>LN$_2$ into GN$_2$ of room temperature</td>
<td>3.0-9.0</td>
<td>0.254</td>
<td>1.59</td>
<td></td>
<td>99-110</td>
</tr>
<tr>
<td>Chehroudi and Talley, 2002</td>
<td>No</td>
<td>LN$_2$ into GN$_2$ of room Temperature</td>
<td>1.5-4.9</td>
<td>0.254</td>
<td>1.59</td>
<td></td>
<td></td>
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<tr>
<td>Branam and Mayer, 2003</td>
<td>No</td>
<td>LN$_2$ into GN$_2$ of room temperature</td>
<td>4.0-6.0</td>
<td>2.2</td>
<td></td>
<td></td>
<td>120-140</td>
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<td>Shear Coaxial Injectors</td>
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<td>Snyder et al., 1997, Candel et al., 1998, Herding et al., 1998, Kendrick et al., 1999</td>
<td>Yes</td>
<td>LOX/GH$_2$</td>
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<td>70-80/300</td>
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<td>Singla et al., 2005, Singla et al., 2007a</td>
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<td>LOX/GH$_2$, LOX/GCH$_4$, LOX/LCH$_4$</td>
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<td>--</td>
<td>--</td>
<td>80/288, 85/288, 85/120</td>
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<td></td>
<td>Yes</td>
<td>LOX/GH$_2$</td>
<td>0.1-1.0</td>
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<td>Reference</td>
<td>Availability</td>
<td>Atmosphere</td>
<td>LOX/GH₂</td>
<td>LOX/GH₂</td>
<td>LOX/GH₂</td>
<td>LOX/GH₂</td>
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<td>Mayer and Tamura, 1996a</td>
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<td>1</td>
<td>1.6</td>
<td>2.5-3.9</td>
<td>100/150-300</td>
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<td>Mayer et al., 2000</td>
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<td>LN₂/GHe</td>
<td>2.0-4.0</td>
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<td>2.9</td>
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<td>Mayer et al., 2000</td>
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<td>LOX/GH₂</td>
<td>2.0-6.0</td>
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<td>90/100-370</td>
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<td>Mayer et al., 2001</td>
<td>No</td>
<td>LH₂/</td>
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<td>Mayer et al., 2001</td>
<td>Yes</td>
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<td>4</td>
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<td>6.5</td>
<td>127/125</td>
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<td>Mayer et al., 2001</td>
<td>Yes</td>
<td>LOX/GH₂</td>
<td>0.18</td>
<td>1.2</td>
<td>2</td>
<td>7</td>
<td>77/200</td>
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<td>Davis and Chehroudi, 2004, Davis et al., 2005, Davis and Chehroudi, 2006</td>
<td>No</td>
<td>LN₂/GN₂ into GN₂ at room temperature</td>
<td>1.5-4.9</td>
<td>0.508</td>
<td>1.59</td>
<td>2.42</td>
<td>120/140-190</td>
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<td>Habiballah et al., 2006</td>
<td>Yes</td>
<td>LOX/GH₂</td>
<td>0.1-6.7</td>
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<td>--</td>
<td>--</td>
<td>~100/300</td>
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<td>Woodward et al., 2006</td>
<td>Yes</td>
<td>LOX/GCH₄</td>
<td>2.1-8.3</td>
<td>5.7</td>
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<td>Salgues et al., 2006b</td>
<td>Yes</td>
<td>LOX/GCH₄</td>
<td>4.1</td>
<td>3.429</td>
<td>4.191</td>
<td>5.18</td>
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<td>Lux et al., 2006</td>
<td>Yes</td>
<td>LOX/GCH₄</td>
<td>4.0-7.0</td>
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<td>4.6</td>
<td>7.6-9.2</td>
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<td>Smith et al., 2007</td>
<td></td>
<td>LOX/GH₂</td>
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<td>4.6</td>
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<td>120/130-250</td>
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<td>Lux and Haidn, 2009b, a</td>
<td>Yes</td>
<td>LOX/GCH₄</td>
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<td>6.2</td>
<td>7-8</td>
<td>120/280</td>
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<td>Source</td>
<td>Swirl</td>
<td>Fuel</td>
<td>Temperature</td>
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<td>E</td>
<td>T</td>
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<td>Leyva et al., 2008</td>
<td>No</td>
<td>LN\textsubscript{2}/GN\textsubscript{2} into GN\textsubscript{2} of 213-235K</td>
<td>1.5-5.0</td>
<td>0.51</td>
<td>1.59</td>
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<td>109-137/145-199</td>
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<td>Inamura et al., 2001, Inamura et al., 2003</td>
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<td>H\textsubscript{2}O</td>
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<td>7</td>
<td>8</td>
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<td>Yoon et al., 2004</td>
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<td>H\textsubscript{2}O/H\textsubscript{2}O(kerosene) bi swirl</td>
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<td>Kim et al., 2005b</td>
<td>Yes</td>
<td>H\textsubscript{2}O/Kerosene LOX/kerosene bi-swirl</td>
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<td>--</td>
<td>--</td>
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<tr>
<td>Im et al., 2005</td>
<td>No</td>
<td>H\textsubscript{2}O/GN\textsubscript{2}</td>
<td>0.1</td>
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<td>4</td>
<td>7</td>
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<td>Kalitan et al., 2005, Salgues et al., 2006a</td>
<td>Yes</td>
<td>LOX/GCH\textsubscript{4}</td>
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<td>3.43</td>
<td>4.19</td>
<td>5.18-6.35</td>
<td>120/300</td>
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<td>Woodward et al., 2006</td>
<td>Yes</td>
<td>LOX/GCH\textsubscript{4}</td>
<td>2.1-8.3</td>
<td>5.7</td>
<td>--</td>
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<tr>
<td>Yang et al., 2008</td>
<td>No</td>
<td>Water/air</td>
<td>0.1</td>
<td>2</td>
<td>--</td>
<td>4.6</td>
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Table 1.3. Recent numerical simulation studies on jet, shear coaxial and swirl coaxial injectors.

<table>
<thead>
<tr>
<th>Researchers</th>
<th>Combustion or not</th>
<th>propellant and injector type</th>
<th>$p_c$ (MPa)</th>
<th>$D_t$ (mm)</th>
<th>$D_o$ (mm)</th>
<th>$D_f$ (mm)</th>
<th>$T_{inj}$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jet</td>
<td>Zong et al., 2004</td>
<td>No</td>
<td>LN$_2$ jet into GN$_2$ of 300K</td>
<td>4.3-9.3</td>
<td>0.254</td>
<td></td>
<td>120</td>
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<tr>
<td>Shear Coaxial Injector</td>
<td>Kim and Heister, 2004, Kim et al., 2005a</td>
<td>No</td>
<td>Recessed region of SSME MCC LOX/GH$_2$ injector</td>
<td>19.3</td>
<td>4.77</td>
<td>6.6</td>
<td>8.84</td>
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<tr>
<td>Shear Coaxial Injector</td>
<td>Liu et al., 2006</td>
<td>No</td>
<td>Recessed region of SSME preburner LOX/GH$_2$ injector</td>
<td>34.1</td>
<td>2.26</td>
<td>3.76</td>
<td>5.03</td>
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<td>Shear Coaxial Injector</td>
<td>Canino et al., 2006</td>
<td>No</td>
<td>LN$_2$/GN$_2$</td>
<td>5.0-10.</td>
<td>0.508</td>
<td>1.59</td>
<td>2.42</td>
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<td>Tsohas et al., 2007</td>
<td>No</td>
<td>gas/gas</td>
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<td>18.95</td>
<td>21.05</td>
<td>23</td>
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<td>Shear Coaxial Injector</td>
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<td>Yes</td>
<td>LOX/GH$_4$</td>
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<td>3.42</td>
<td>4.18</td>
<td>5.18</td>
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<td>Shear Coaxial Injector</td>
<td>Zong et al., 2008</td>
<td>Yes</td>
<td>LOX/GH$_4$ splitter</td>
<td>10</td>
<td>3.72</td>
<td>4.37</td>
<td>5.32</td>
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<td>Shear Coaxial Injector</td>
<td>Masquelet et al., 2009</td>
<td>Yes</td>
<td>LOX/GH$_2$</td>
<td>10</td>
<td>3.72</td>
<td>4.37</td>
<td>5.32</td>
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<td>Swirl Injectors</td>
<td>Schmitt et al., 2009</td>
<td>Yes</td>
<td>LOX/GH₂</td>
<td>6.0</td>
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<tr>
<td>Schmitt et al., 2010</td>
<td>Yes</td>
<td></td>
<td>LOX/CH₄</td>
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<tr>
<td>Kim and Heister, 2006</td>
<td>No</td>
<td></td>
<td>GOX jet/liquid swirl</td>
<td>2</td>
<td>3</td>
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<tr>
<td>Richardson et al., 2007</td>
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<td></td>
<td>Simplex swirl injector</td>
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<tr>
<td>Zong and Yang, 2008</td>
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<td>LOX simplex</td>
<td>10</td>
<td>4</td>
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Table 1.4. Critical points of some pure substances.

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<thead>
<tr>
<th>Propellants</th>
<th>O₂</th>
<th>H₂</th>
<th>CH₄</th>
<th>H₂O</th>
<th>CO₂</th>
<th>He</th>
<th>N₂</th>
<th>Kerosene</th>
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<tr>
<td>Tc (K)</td>
<td>154.59</td>
<td>32.97</td>
<td>190.45</td>
<td>647</td>
<td>304.25</td>
<td>5.19</td>
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<td>p_c (MPa)</td>
<td>5.04</td>
<td>1.29</td>
<td>4.60</td>
<td>22.06</td>
<td>7.38</td>
<td>0.23</td>
<td>3.39</td>
<td>2.34</td>
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High-pressure cryogenic propellant combustion in liquid rocket engines poses various technological and scientific difficulties, including injection optimization, ignition, flame stabilization, and combustion instabilities. The complete process is so complex that its mechanism cannot be thoroughly understood without extensive theoretical and experimental works conducted on simplified configurations under well-controlled conditions. In this subsection, a short discussion on free shear flow is presented, then the experimental and numerical work on high-pressure fluid injection and mixing is reviewed.

1.2.1 Free Shear Layer Flows

Free shear layer flows, including jets, wakes, plumes, and mixing layers, are very common in nature and engineering applications. For example, the smoke from a chimney, the plume from a smoldering cigarette, the fuel jet in combustion devices are all free shear flows. In the current study, the propellants issuing from the coaxial injectors form a wake region at the nozzle tip, and a free mixing layer downstream. A review on the shear layer flows is helpful to understand and explain the results.

The free shear flows are remote from walls, so that the development of three-dimensional vorticity is not constrained by the solids. Instability waves develop in the shear layer, and the flow must transit to turbulence if the Reynolds number is large enough. Helmholtz (1868) and Kelvin (1871) studied the linear stability of mixing layers. The instability mode they discovered is referred to as Kelvin-Helmholtz instability. The stabilities of mixing layers have been studied extensively since then. Linear instability theories are established to predict the onset of instability.
and transition to turbulence. A comprehensive review on the instability physics of incompressible mixing layer was conducted by Ho and Huerre (1984).

In turbulent free shear flows, mean velocity gradients exist perpendicular to the streamwise direction, and is generally orders-of-magnitude larger than the streamwise gradients. Boundary layer equations can be applied to these flows to predict mean flow quantities. In large Reynolds number flows, similarity exists after the development section. For example, similarity exists for \( x/d > 30 \) in high Reynolds number turbulent jet flows. The mean flow and mixing characteristics can be studied with these simplified analyses. More information about all kinds of turbulent free shear flows can be found in standard texts, for example, Schlichting (1968), Tennekes and Lumley (1972), and Pope (2000).

Although extensive studies have been made in turbulent shear flows, the spatially evolving flows are very much dependent on the specific characteristics of the flow, including the upstream conditions and the thermo-chemical characteristics of the flow. In the current studies, the two fluids are at dramatically different thermodynamic states, and extremely large gradients of thermodynamic properties exist in the mixing layer. Chemical reactions further complicate the situation, rendering the flows physics very complicated. In addition, in the near-field region of the injector, where flame anchoring and its subsequent development are very important, similarity has not been achieved, and boundary layer analysis is not relevant either. Bearing the similarity and difference between the flows in the current study and those canonical shear layer flows in mind help us understand the physics in the current study.
1.2.2 Experimental Studies of Cryogenic Fluid Injection and Mixing

Liquid injection into supercritical environments has been studied as early as in 1971 by Newman and Brzustowski (1971). In their studies, subcritical CO$_2$ at 295 K was injected into pure N$_2$ and also into N$_2$/CO$_2$ mixtures, which are preconditioned at sub-critical or supercritical pressures and temperatures. Based on the shadowgraph images they obtained, as chamber temperature increases from subcritical to supercritical values, the suppression of jet surface structures and spray formation was explained to be due to the reduction in surface tension and increase in CO$_2$ evaporation. They proposed the jet gasification could be treated as a variable-density, single-phase turbulent submerged jet, as far as the ambient temperature remained supercritical.

Since then, extensive experimental studies have been conducted to investigate supercritical fluid injection and mixing by many researchers, particularly for liquid rocket engine studies. The following paragraphs summarize their work and recent advances in supercritical fluid injection and mixing.

Mayer and his colleagues (Mayer et al., 1998, Mayer et al., 2000, Mayer et al., 2001, Ivancic and Mayer, 2002) have systematically studied the injection of liquid nitrogen jets, LN$_2$/GHe coaxial jets, and LN$_2$/GN$_2$ coaxial jets into chambers preconditioned at pressures ranging 1.0-6.0 MPa and at 300K. The liquid nitrogen velocity is set at 10 m/s (or less, as in the single jet study, Branam and Mayer, 2003), while the coaxial flow of gaseous nitrogen or helium is at a much higher velocity (on the order of 100m/s). Flow visualization and image processing techniques were used to study the injection, mixing characteristics. Similar cold flow shadowgraphs were also obtained for LOX/GH$_2$ coaxial injection and combustion (Mayer and Tamura, 1996a) at 1.0-10.0 MPa. The results consistently showed that the droplet and spray formation process, which is valid in sub-critical injection and mixing, was no longer appearing in
near- and super-critical conditions. Instead, the so-called "stringy" or "thread-like structures" developed, grew and rapidly dissolved due to the fade of surface tension; the atomization mechanism changed to shear-layer instability; and the mixing of the dense nitrogen fluid with the co-flow or ambient gas behaved like a variable density, turbulent shear-layer at near- and supercritical conditions.

Mayer and his colleagues (Ivancic and Mayer, 2002, Branam and Mayer, 2003) also investigated the length scales of the cryogenic injection of nitrogen at supercritical conditions, based on flashlight photography and high-speed cinematography. For pure nitrogen injection at a near critical temperature (104-132 K), the length scales in axial direction were found to be two to three times greater than the radial counterpart near the injector exit, due to the strong density gradient around the jet surface. This phenomenon became unpronounced as the fluid was convected downstream where the injection temperature exceeded the critical value of nitrogen. It was also found that the flow conditions (specifically density) seem to be most affected by temperature variations. The effect of velocity and pressure on the flow field was minimal, if there was any. The quantitative measurements in the jet study provide validation data for numerical studies of supercritical injection and mixing.

Chehroudi and colleagues have also systematically studied the supercritical injection of liquid nitrogen, with or without co-flow of gaseous helium, injected into gaseous nitrogen environment over a wide range of pressures (Chehroudi et al., 1999, Chehroudi et al., 2000 Chehroudi et al., 2002a, Chehroudi and Talley, 2002, Chehroudi et al., 2002b). Liquid nitrogen was injected at a subcritical temperature in all studies while the gaseous nitrogen environment is fixed at 300K and the pressure is ranging from 0.9 to 9.4 MPa. Flow visualization and image processing techniques, including shadowgraph imaging, fractal analysis, and Raman scattering measurement were employed to examine the jet and shear-layer structures between the liquid jet
and the gaseous ambience. The results were consistent with Newman and Brzustowski’s findings. Drastic changes in jet surface phenomena took place when the ambient pressure changed from sub-critical to supercritical values. The formation of ligaments and droplets disappeared at supercritical conditions, due to the vanishing of surface tension and the prevalence of turbulent motions. The authors also adopted fractal analysis to study the difference between sub-critical and supercritical jet surfaces. The results showed that the jet surface topology at supercritical pressure bore a strong resemblance to its gaseous counterpart but rapidly recovered to the surface topology of liquid spray as the pressure was reduced below the critical point.

Chehroudi and others quantitatively examined the initial growth rate of high-pressure cryogenic jets and compared it to the initial growth rates of various mixing layer flows, including atomized liquid sprays, turbulent incompressible gaseous jets, supersonic jets, and incompressible but variable density jets. The density ratio of the jets to the ambient gases of these mixing layers covered more than four orders of magnitude (Chehroudi et al., 2002b). The growth rate of the supercritical jet agreed well with that of the incompressible, variable density, gaseous mixing layers at low pressures. The result was claimed as the first time to define a quantitative parameter to demonstrate the similarity between those two flows beyond their physical appearance. A unified model for the initial growth rate of a jet was proposed, applicable to both the droplet gasification at low pressures, and the interfacial bulge formation/separation at high-pressure, that is, sub-critical and supercritical conditions (Chehroudi et al., 2002b). Its prediction showed agreement with the measured data.

Chehroudi et al. (Chehroudi and Talley, 2002, Davis and Chehroudi, 2004, Davis et al., 2005, Davis and Chehroudi, 2006, Leyva et al., 2008) also extended their studies on cryogenic jet injection and mixing under supercritical conditions to both LN₂ single jet injection and LN₂/GN₂ coaxial injection with acoustic forcing. They studied the effects of acoustic waves on the single
and coaxial jets over a wide range of chamber pressures (Chehroudi and Talley, 2002, Davis and Chehroudi, 2004). The Piezo-Siren acoustic driver was adopted to impose transverse acoustic forcing, and it was capable of producing sound pressure level (SPL) of up to 180 dB in an impedance tube at pressures up to 14 MPa. Acoustic forcing at the resonant frequencies of the assembly (2700 and 4800 Hz) was switched on/off to study the acoustic effect. The influence was substantial at subcritical conditions but became unnoticeable as pressure increased and exceeded the critical point. This phenomenon was attributed to the formation of high-frequency vortices in the shear-layer and to the weaker characteristics of acoustic impedances of injected fluids under supercritical pressure. In addition, the results also showed that the co-axial subcritical jets at higher velocity ratios were more apt to be influenced. Based on their argument, since the sensitivity of coaxial jet to the external acoustic oscillations might correspond to the causes of combustion instability in liquid rocket engines, the acoustic impedance of the central jet and the fuel/oxidizer momentum ratio were proposed as the key parameters to physically characterize different operating conditions. Chehroudi and his co-workers also investigated the dark core lengths of the LN₂/GN₂ coaxial injection under sub- to near- and supercritical conditions with acoustic forcing on/off. In addition to the aforementioned flow visualization techniques, calibrated thermocouples with a maximum estimated uncertainty of 0.8 K were used to measure the temperature radial and axial profiles downstream of the injector face. Root Mean Square (RMS) of the dark core lengths was found to decrease with an increase in velocity ratio, and it was suggested that the decrease in dark core length fluctuations could weaken a key feedback mechanism for the self-excitation process, which was attributed to drive the combustion instability in rocket engines, and was proposed as an explanation for the “temperature ramping” stability rating method. The dark-core length measurement was compared to all other core length data available in the literature versus the momentum ratio of over three orders of magnitude. It
was found that the subcritical dark core length is proportional to the power of -0.2 to the momentum ratio, versus -0.5 for near- and supercritical counterpart. The observations confirmed that the effect of the acoustic field was less pronounced under near- and supercritical pressures. However, the oscillations of the jet in the acoustic field under near- and supercritical conditions were observed from the consecutive frames from high-speed shadowgraph images in their later studies. The growth rate or spreading angle of the outer jet of a coaxial jet flow at sub-, near- and supercritical conditions were found to be fairly constant, with a mean of 0.19 and a standard deviation of 0.02. This was compared with theoretical predictions obtained from 2D shear layers of variable density flows for gaseous flows, and with other experimental data for single jets and coaxial gas-gas jets issuing into a gas. The growth rate was consistently lower than the theoretical predictions and the other experimental data for coaxial jets. The reason was attributed to the thickness of the inner jet tube. Through varying the phase angle between two acoustic sources that transversely excited the coaxial jet at sub-critical pressures, it was also found that maximum acoustic velocity gave rise to the greatest enhancements on mixing, resulting in enhanced decrease on the dark core lengths.

The spontaneous Raman Scattering technique was employed to qualitatively measure the species distributions in high-pressure experiments (Anderson et al., 1995). It was, then, applied to investigate the density and temperature distributions of supercritical nitrogen jets (Oschwald and Schik, 1999, Branam and Mayer, 2003). In general, the normalized density profiles in the downstream indicated a tendency towards the self-similarity solution observed for classical constant- and variable-density single-phase fluid jets at low pressures. This, again, confirmed the similarities of those two types of jet flows. The centerline density and temperature distributions of a cryogenic jet at a near critical pressure (4.0MPa) were acquired by Oschwald and Schlik (1999). They noted that the density decay speeded up as the fluid temperature increased from
sub- to supercritical values. The temperature, however, remained a relatively flat profile, even far downstream. This was attributed to the anomalous thermophysical property variations near the critical point of nitrogen. Those quantitative measurements, conducted at high pressures, provided an indispensable basis for CFD model validation.

In summary, the injection of single cryogenic jet, and the coaxial injection of liquid jet and a high speed gas into ambient gas pre-conditioned at various pressure conditions have been studied extensively. It was consistently found that the supercritical injection shows a variable-density, gas/gas-like mixing without the formation of sprays, ligaments or droplets as in sub-critical conditions. Quantitative data, such as the jet growth rates, length scales, potential core lengths, and density were measured, and these provided the basis for CFD model validation. However, most of the studies have been performed in a more qualitative manner, and are highly dependent on the images obtained using various flow visualization techniques. This lack of data for supercritical injection and mixing is probably a result of the difficulty of acquiring data under supercritical conditions. High-fidelity numerical schemes that are validated against these experimental studies could potentially provide more insight into the physical processes and deepen our current understanding of supercritical injection, mixing and combustion in liquid rocket engines.

1.2.3 Experimental Studies on High-Pressure Combustion of Cryogenic Propellants

In a typical cryogenic propellant rocket engine, such as Space Shuttle Main Engine (SSME), propellants are introduced into the combustion chamber through shear coaxial injectors. Liquid oxygen (LOX) is generally delivered through the inner LOX post at a low speed (typically
on the order of 10 m/s), while gaseous fuel (GH$_2$ or GCH$_4$) is fed through the outer annular duct at a much higher speed (typically on the order of 100 m/s).

The subcritical combustion of cryogenic propellants has been widely used to study the flame and combustion characteristics of the selected injector design (for example, Candel et al., 1998, Singla et al., 2007a). This preference is probably due to the fact that, at lower pressure, the experiments are easier to conduct, and measurement techniques are valid (for example, Singla et al., 2007a). However, as discussed in the previous section, the supercritical injection and subsequent mixing characteristics are totally different from those at sub-critical conditions. As studied by Mayer and Tamura (1996b) and discussed by Oefelein and Yang (1998), the physicochemical processes associated with subcritical and supercritical combustion are dramatically different from each other. Extreme care must be exercised to extrapolate the findings in one state to those in another. At subcritical pressures, the injected fluids undergo a cascade of processes associated with atomization. Atomization starts at the confluence of the liquid and gaseous streams, and the liquid core diminishes progressively as the spray is formed under the effect of surface tension and the aerodynamic force of the high-velocity co-flow gas. The initial ligaments are detached from the LOX jet, forming droplets, that break up into finer droplets and leads to the secondary atomization. The droplets then vaporize, mix with the gaseous hydrogen, and finally burn out. However, under supercritical conditions, no droplets can be observed. Instead, thread-like structures evolve from the liquid jet and diffuse rapidly within the turbulent mixing layer of oxygen and fuel. Having the difference between sub-critical and supercritical mixing and combustion in mind, in this section we discuss results at both conditions for further comparison.

At subcritical conditions, the momentum ratio $J$ of the fuel to oxidizer stream and Weber number are two important parameters for determining the atomization quality (Candel et al.,
1998). Snyder and colleagues (1997) concluded that the vaporization of LOX droplets controls the combustion process at sub-critical pressure through estimating and comparing the chemical, vaporization and mixing characteristic time scales. If the droplets are too large, they may escape the combustion chamber without fully vaporized. This indicates that combustion occurs only in thin reactive zones and that the regime of combustion is of the flamelet type.

Subcritical experimental studies on LOX/methane combustion have been conducted by several researchers (Cuoco et al., 2004, Singla et al., 2007b, Yang et al., 2007, Yang and Oschwald, 2007) (Cuoco, 0.15 MPa, Yang M3, 0.15 MPa and Singla 1.0-2.5 MPa). Optical diagnostic techniques, including shadowgraph, excited CH, OH chemiluminescence, and Planar Laser Induced Fluorescence (PLIF) of OH or O₂, were used to visualize the flow and flame structures. Qualitative images were obtained regarding variations of the LOX potential core, the atomization process, and the flame anchoring and spreading. In those subcritical studies, spray and atomization processes prevailed; momentum flux ratio and Weber number were varied to investigate their effects on the flow and the combustion dynamics. It was found that methane flame is relatively easier to be lifted off from the rim of the LOX post and less stabilized compared to LOX/H₂ flame. Even at higher pressure subcritical conditions (1.0-2.5 MPa), the OH LIF results of LOX/CH₄ combustion of a shear coaxial injector by Singla et al. (2007b) showed that the flame developed as a thin wrinkled layer spreading near the liquid oxygen jet. The flame started from a location away from the injector lip indicating the reactive region was sensitive to the flow perturbation. The result showed that the methane flame was less stabilized than liquid oxygen/hydrogen flames.

At near- and supercritical conditions, that is, when chamber pressure is near or above the critical points of the injected propellants, the surface tension and the enthalpy of vaporization approach zero. The injected fluids form a variable density, continuous fluid characterized with
exceedingly large density gradients. At these conditions, the LOX jet gasification rate is at least one order or magnitude greater than that of droplet vaporization at atmospheric pressure (Delplanque and Sirignano, 1994). Furthermore, the Reynolds number increases with pressure, leading to faster small-scale mixing. These two effects combine to suggest that large-scale turbulent mixing is the slowest and, therefore, it is the most influential process.

Candel and his colleagues at ONERA have systematically studied cryogenic propellant combustion of LOX/GH₂, LOX/GCH₄, and LOX/LCH₄ at various chamber pressures over the past decades (Snyder et al., 1997, Candel et al., 1998). In the study of LOX/GH₂ combustion of a coaxial injector at 0.1, 0.5, and 1.0 MPa, flow visualization techniques such as elastic light scattering, OH radical emission, and PLIF of OH were used to obtain flame structures, and study the flame stabilization and dynamics. The momentum ratios and Weber number were varied to study their effects on the combustion. No apparent lifted flames have been observed in any images. It was concluded that the flame was stabilized at the injector lip or very close to the injection plane at conditions considered therein. The flame expansion rate was larger for a larger momentum ratio.

In their later shear coaxial injector LOX/GH₂ combustion study (Candel et al., 1998) at the same pressures, similar momentum ratios, and Weber numbers, PLIF of O₂, as well as the aforementioned visualization techniques, were applied to obtain images of the flame zone. Temperature was also measured, using the Coherent Anti-Stokes Raman Spectroscopy (CARS). The results further confirmed the flame stabilized in the vicinity of the LOX post. It was also found that the wrinkling and flapping of the flame were low in the near field of the injector and increased with downstream location, where the temperature became more homogeneous after intense mixing. The authors argued that the combustion rate was faster than turbulent mixing in
the cryogenic jet flame, supported by the sharpness of O₂-PLIF images and the fact that the flame was always attached to the lips of the coaxial injector.

Kendrick and others (1999) also investigated the effect of recessing the LOX tube of the coaxial injector with respect to the injector plane on the flame stabilization improvement. The operating conditions were chosen from their previous subcritical studies. Only the test cases with a chamber pressure of 1.0 MPa were studied, corresponding to a subcritical jet flame study. OH emission images were obtained to assess the flame structure changes due to the LOX tube recess. It was found that the flame was stabilized inside the injector with an increased expansion angle and flame brush thickness. This phenomenon was attributed to the acceleration of the hydrogen stream and the resulting increment of the momentum ratio when the flame is inside the injector and combustion products occupy a fraction of the duct area.

Zurback et al. conducted a preliminary flow visualization of shear coaxial injection and combustion of LOX/methane at near-critical pressures on the Mascotte test facility at ONERA, France (Zurbach et al., 2002, Zurbach et al., 2003). Shadowgraph images revealed that the flame was attached to the LOX post and spread downstream along the oxygen jet boundary, which was quite similar to the phenomena observed for the LOX/hydrogen system.

Singla et al. (2005) performed a detailed experiment of subcritical LOX/GCH₄, transcritical LOX/GCH₄, and trans-critical LOX/LCH₄ combustion of a single coaxial injector, through examination of OH* and CH* emission images. The temperature of the oxygen stream remained at 85 K, whereas the methane injection temperature was set as 120 or 288 K, corresponding to trans- and supercritical injection conditions. The chamber pressure varied from 4.5 to 6.0 MPa. Emission images of exited OH and CH radicals indicated that the flame was stabilized in the vicinity of the LOX post tip under all flow conditions, similar to the behavior of the supercritical LOX/H₂ flames. They found that the subcritical LOX/GCH₄ flame was
atomization controlled and was greatly affected by the momentum ratio. At pressures above critical value, mixing became the slowest and most influential process. The trans-critical oxygen/trans-critical methane flames featured two conical emission regions, indicating two reaction layers. One reacting layer follows the boundary of the liquid oxygen jet, while the other one spread near the outer boundary of the liquid methane. This flame structure was very different from that of the cases in which only one of the reactants was injected in a subcritical or trans-critical state. In addition, they observed that the LOX droplets penetrated into the inner flame resulting in a secondary flame and a larger expansion angle, when both LOX and CH\textsubscript{4} were injected at trans-critical conditions. However, LOX droplet penetration was not observed when CH\textsubscript{4} was in a gaseous phase.

Singla et al. applied the PLIF of OH to both LOX/GH\textsubscript{2} and LOX/GCH\textsubscript{4} cryogenic flames (2006, 2007a, 2007b). High quality image data were obtained for LOX/GH\textsubscript{2} flames at both subcritical and supercritical pressures (3.6 MPa and 6.3 MPa). The PLIF images were shown to nearly match those deduced from Abel transformed averaged OH\textsuperscript{*} emission images. The results also confirmed that the supercritical jet flames were always stabilized in the vicinity of the liquid oxygen injector lip. The subcritical jet flame (3.6 MPa) showed a poorly stabilized flame that was not fully established in the combustion chamber. This result was explained by the argument that the momentum ratio was too low to atomize the liquid oxygen jet. The OH PLIF was also applied to LOX/Methane flames. However, due to the signal noise from other combustion products, meaningful image data were obtained up to only 2.5 MPa, which was still at a subcritical pressure of oxygen. The images showed that the flame edge stood a few LOX post lip sizes away from the injector plane and was less well stabilized, compared to LOX/GH\textsubscript{2} flames.

Habiballah et al. (2006) summarized the qualitative and quantitative measurements of high-pressure mixing and combustion of shear coaxial injectors conducted on the Mascotte
facility. Aside from high-speed photography, shadowgraph, and backlighting techniques, Coherent Anti-Stokes Raman Scattering (CARS) was also used for the temperature measurement in liquid rocket combustion, however the uncertainties with this method is generally very large.

Another notable and important work on high-pressure combustion was conducted by Mayer and Tamura (1996a), who also conducted research on the high-pressure combustion of LOX/\text{GH}_2 at various pressure conditions. Subscale shear coaxial injectors, with and without recess, were employed. Chamber pressures ranged from 1.5 MPa to 10.0 MPa. LOX was injected at 10-30 m/s at a temperature of 100K, while gaseous hydrogen was fed at 300K and 300m/s. Those conditions were comparable to the operating state of a liquid rocket engine. The flow visualization was achieved by shadowgraph imaging. Their results showed the flame was always attached instantaneously to the LOX post after ignition. A bright flame spot was observed close to the LOX-post tip, suggesting that a well-mixed flame with strong radiation was anchored in an intense recirculation zone. This flow pattern could be observed over the entire range of test conditions for injectors with and without recess and even for a post tip thickness of 0.3 mm.

The flame-anchoring mechanism is illustrated in Fig. 1.3. Several small recirculation eddies were generated in the vicinity of the LOX-post tip, which consisted of partly pre-burned, hydrogen-rich gas. As the evaporating LOX mixed and reacted with the hydrogen gas in these eddies, the hot product again mixed with the hydrogen stream and then circulated back. Since the flow velocities in this region were so low, stationary combustion was possible.
Non-intrusive optical measurement techniques, including light scattering, shadowgraph, OH and CH chemiluminescence, and OH PLIF were conducted in the Cryogenic Combustion Laboratory (CCL) at the Penn State University by Sauglas et al. (2006b) to investigate the swirl/shear coaxial injection and combustion of LOX/GCH\textsubscript{4} at a near critical chamber pressure (4.1MPa) and a mixture ratio of 3.0. Images were taken on spray and flame structures in the near field. The Abel de-convoluted images for the shear injector indicated that the flame was anchored in the vicinity of the LOX post. Woodward et al. (2006) conducted LOX/GH\textsubscript{2} combustion of a shear coaxial injector at very high momentum flux ratios (22-126) at pressures from 5.17 to 6.55 MPa. Strobe-lit and nanolamp-lit shadowgraph techniques were employed to visualize the flow evolution and to extract the liquid core breakup length data under combustion conditions. The visualizations showed that even for a high injection momentum flux ratio of larger than 20, the flow field was characterized by a long sinuous LOX core region that broke up into large LOX structures. This finding did not agree with the classical phenomenological breakup model stating that a liquid core quickly breaks up into a drop cloud. The liquid core breakup lengths were compared with those predicted by several correlations from the literature.

Figure 1.3. Schematic of flame-holding mechanism.
for predicting the liquid core breakup length for coaxial injectors. Existing correlations, none of which was developed under combustion conditions, did not predict the liquid core breakup length adequately, except for that of Woodward, who predicted reasonable core breakup lengths for the combustion tests described therein. However, a $\text{Ln}(J)$ scaling agreed with the experimental data, and therefore, further investigations were called for. Note that the measured LOX core breakup lengths were better matched with calculations from the subcritical two-phase correlations than with those of the single-phase coaxial jet correlations by Davis and Chehroudi (2006). Woodward et al. (2007) also studied the effect of recess and non-concentricity of the LOX tube on the LOX/GH$_2$ combustion of a shear coaxial injector. The chamber pressure was always supercritical (6.89-9.65 MPa), but the injection temperature of LOX was varied from subcritical to supercritical values. A rocket chamber with a contraction ratio of 2.86 associated with 1000 K pre-burner products coflow was used. Shadowgraph images showed the dense oxygen core exhibited a long sinuous structure, which eventually broke up into large structures. The core breakup lengths were found not sensitive to the LOX post recess or the LOX injection temperature, but were affected by the non-concentricity of the LOX tube.

Smith et al. (2007) conducted experiments of steady state LOX/H$_2$ combustion at sub-, near- and supercritical conditions. OH chemiluminescence and shadowgraph images were taken to visualize the combustion zone, and the flow field, respectively. The results confirmed the qualitative difference between sub-critical and supercritical injection, mixing and combustion processes. Flow unsteadiness tended to occur at subcritical pressures, but was not observed under near- and supercritical conditions.

Lux and Haidn (2009b) investigated the LOX/methane combustion of a shear coaxial injector at sub-, near- and supercritical conditions (chamber pressure ranging from 4 to 6 MPa). OH and CH emission images were taken to study the flame dynamics as well as the ignition
Transient. It was found that increases in the momentum flux ratio led to a constriction of the flame and a decreasing spreading angle for both subcritical and supercritical cases. Similar to LOX/H_{2} flames, the flame followed the liquid oxygen jet right after injection. At the location of about five to six times that of the LOX post diameter, the flame expanded due to the disintegration of the LOX jet and its high vaporization rate. The flame was anchored in the wake of the LOX-post tip at all of the studied operating conditions. They also studied the effect of LOX post recess on the flame stabilization of LOX/methane combustion of similar shear coaxial injectors under the same pressures but different mass flow rates (Lux and Haidn, 2009a). The same experimental techniques were used. The results showed an increased flame expansion with a recessed LOX post, but this effect decreased with increasing in momentum flux ratio. At low momentum flux ratio, the pressure drop across the injector increased with a recessed injector. A recessed injector led to a smoother combustion in general, but also showed additional resonant frequencies in the chamber acoustics.

In summary, high-pressure cryogenic combustion in shear coaxial injectors have been systematically studied. Various flow visualization techniques have been used to study the flame stabilization and flame structures. The experimental studies have consistently revealed the difference between subcritical and supercritical combustion. At supercritical pressures, flames are stabilized in the vicinity of LOX post, and the combustion is turbulent-mixing controlled. However, data are limited to shadowgraph, light scattering, OH PLIF, and OH/CH emission images. Quantitative data regarding the near field flow and flame dynamics are scarce. High-fidelity numerical studies may be necessary to improve the understanding of supercritical combustion.
1.2.4 Literature Survey on Swirl Coaxial Injectors

The literature survey for swirl coaxial injectors is presented separately in this section, considering the unique characteristics of swirl injector compared to those of shear coaxial injectors. Swirl injectors have been widely used in liquid-propellant rocket engines, especially those developed in Russia. Compared with jet injectors, a liquid swirl injector distinguishes itself in many aspects (Bazarov et al., 2004). First, swirl injectors can sustain a large capacity of flow rate, which enables a high thrust per injector element and features good throttling capability. The large passage in a swirl injector renders the atomization process less sensitive to manufacturing errors, and is also less sensitive to choking and cavitation. Second, swirl injectors feature good atomization and mixing efficiency, as the thickness of the liquid film becomes thinner as it swirls and spreads outward. Compared to jet injectors, the resultant mean diameter of droplets is 2.2-2.5 times smaller than that produced by a jet injector with the same pressure drop and mass flow rate. Propellant mixing can be significantly enhanced due to outward spreading of the liquid spray. This advantage prevails for high flow rates and abates when counter-pressure (that is, the sum of the combustion chamber pressure and the centrifugal pressure created by liquid swirling motion) grows. Third, swirl injectors also have low combustion instability and a wide operating range because of hydraulic spray characteristics. Finally, the central post of rocket swirl injectors features large aspect ratios (L/D up to 20), owing to propellant supply manifolding considerations. Viscous loss along the wall exerts significant influence on the flow evolution and consequently alters the spray distribution and atomization.

Figure 1.4 schematically shows the configuration of the inner tube of a typical swirl coaxial injector. Liquid oxygen is introduced from the tangential inlets into the center post, and then forms a swirling film attached to the tube due to centrifugal force. A hollow gas core exists
in the center region in accordance with the conservation of angular momentum. The film exits the nozzle in the form of a thin sheet and impinges on the surrounding fuel stream.

Figure 1.4. Schematic of swirl coaxial injector.

The fundamentals of inviscid swirl injector theory were established more than 60 years ago by Abramovich in 1944 and independently by Taylor in 1947. An up-to-date discussion of the classical theory and the injector design criteria was presented by Bayvel and Orzechowski (1993) and by Bazarov et al. (2004). Besides the theoretical analysis, a series of experiments have been conducted to provide an essential reference frame of swirl injector design, especially for liquid rocket applications. Similar to the experimental studies of shear coaxial injectors, cold flow tests of swirl injectors under atmospheric conditions have been commonly used to study the injector dynamics. These subcritical tests may not be appropriate to be used to study the true physics of supercritical injection, mixing and combustion processes of swirl injectors, due to the essential differences in the thermodynamic states of the injected propellants and the ambient fluid. However, subcritical studies may still provide insight into the injector flow characteristics to some extent. In this section we summarize experimental, theoretical, and numerical studies on swirl injectors, especially for liquid rocket engine applications.
Hulka et al. (Hulka et al., 1991, Hulka and Makel, 1993, Hulka and Schneider, 1993) conducted a series of cold-flow and firing tests of subscale swirl injector elements. In the cold flow tests, water and inert gases were used as stimulants of LOX and gaseous hydrogen. All the tests were conducted at atmospheric conditions. Spray angle, droplet size and their distribution were measured in water only as well as in water/nitrogen flows. Rupe mixing efficiency was measured using water/sucrose solution flows with a large grid patternator. A broad range of fuel/oxidizer mixture and velocity ratios was studied. Results indicated that the mixing efficiency could be greatly increased by increasing the oxidizer’s initial spreading angle, which was achieved by reducing the tangential inlet area or increasing the central post-exit diameter. The oxidizer mass flow rate had insignificant influence on the single element mixing efficiency, suggesting that a larger oxidizer swirl element with a mass flow rate greater than that of a shear coaxial injector could still obtain better intra-element mixing efficiency.

Rahman et al. (1995) visualized the water/air spray of a swirl injector at room conditions using the shadowgraph technique. The results indicated that in the absence of gas flow, a hollow conical liquid sheet was formed at the injector exit. The cone angle was effectively fixed by the injector geometry, whereas the breakup point of the liquid sheet moved closer to the injector exit as the mass flow rate increased. Due to the momentum loss along the injector wall, the conical sheet angle decreased with the increase in the aspect ratio of the post length to its diameter.

Sasaki et al. (1997) conducted cold flow experiments with water/nitrogen as propellant stimulants at room conditions. The effect of the central post recess distance was studied carefully. In a recessed injector, the spray angle narrowed with a deformed pattern, because the liquid sheet generated by the swirl motion impinged on the outer wall of the annular fuel passage. The liquid sheet, which blocked the annular passage, was blown off in the shape of a mushroom and with a screaming sound known as a self-pulsation phenomenon. The effect of recesses on the
spray characteristics of a swirl coaxial injector was also studied by Han et al. (2003). Water and kerosene were employed as stimulants for oxidizer and fuel, respectively. With the use of a phase Doppler particle analyzer (PDPA) and a mechanical paternator, the median droplet size, spray angle, and breakup length were measured. Their results indicated that an optimal recess length existed to obtain maximum mixing efficiency.

The dynamic characteristics of swirl injectors were thoroughly studied by Bazarov and Yang (1998). The overall response function of the swirl injector was represented in terms of the transfer characteristics of each individual element (tangential passage, vortex chamber, and discharge nozzle), analyzed independently and then combined together. The resultant amplitude-phase characteristics were very complicated; however, they guided the designers to obtain any desired pulsation characteristics by either suppressing or amplifying flow oscillations. Based on this work, it becomes possible to control engine combustion dynamics by changing injector dimensions alone—without modifying other parts of the combustion devices. In addition, various mechanisms for driving self-pulsations in both liquid and gas-liquid injectors were analyzed and discussed in detail. The self-pulsation boundary at different operating conditions was also illustrated. Those results are essential to the engineering design of swirl injectors.

Flow evolution in the center post of a swirl injector was investigated theoretically, using a boundary-layer theory by Inamura et al. (2001, 2003). The predicted film thickness at the post exit was compared with experimental results from measurements by means of a contact needle using water as a stimulant. The theoretical analysis showed good agreement with experimental data, except at low mass flow rates, where the measured film thickness increased rapidly compared to the theoretical predictions as the flow rate decreases. Empirical correlations for the sheet cone angle and breakup length were deduced for cases without gas stream injection. The comparison between the prediction and experiment agree very well, except at small mass flow
rates, at which point laminar flow dominated. The film thickness circumferential distribution at the injector exit showed three peaks corresponding to the tangential inlets. From the PDPA measurement, it was also found that the mean droplet size featured local maxima at the center and periphery.

Yoon and his colleague conducted systematic experimental studies on water/gaseous nitrogen swirl coaxial, water/water (kerosene) bi-swirl, and water simple pressure swirl injectors. The effect of recess and ambient pressure in the case of liquid-liquid bi-swirl coaxial injector was investigated by means of a shadowgraph for spray patterns, a PDPA for the droplet Sauter Mean Diameter (SMD), and a mechanical paternator for mass distribution and mixing (Yoon et al., 2004). The spray characterizes of liquid-liquid bi-swirl injector were more influenced by the interaction position of propellants in the recess. If the propellant interaction occurred inside the recess length, then as the recess length of the LOX post increased, the spray angle and breakup length also increased due to the formation and decay of the wave inside the recess region, while the droplet size increased due to the increase of the effective film thickness and the decrease of the spray angle. Mixing efficiency increased with recess length, but in the case of a very deep recess, the mixing efficiency decreased due to propellant separation caused by the density differences between water and kerosene. A high environmental pressure increased the aerodynamic force of the ambient gas significantly and resulted in shorter breakup lengths. Self-pulsation characteristics of a water/nitrogen gas swirl coaxial injector at various injection and geometric conditions were studied by Im et al. (2005). The increase of recess length and the decrease of the gap size tended to promote self-pulsation. Higher gas velocity enhanced the self-pulsation but had no influence on the pulsation frequency, while an increase of liquid velocity led to increases in inertia resistance and changes in the self-pulsation magnitude and frequency. The effect of the length of backhole on film thickness variations was investigated through film
thickness measurements using the conductance method (Kim et al., 2007). The results indicated
that optimum swirl injector design existed through the selection of a proper injector aspect ratio.
The spray and breakup characteristics of a swirling liquid sheet were investigated by measuring
the spray angle and the breakup length from photographic images and spray distributions from an
optical line patternator. The spray angle showed different tendencies before and after sheet
breakup. Before breakup, the spray angle increased as $We_i$ increased, while it remained almost
constant as the ambient gas density increased. After the liquid sheet broke up, the droplets
entrained ambient gas, and the spray angle decreased. The measurements of breakup length
according to the ambient gas density and $We_i$ were compared with the results using linear
instability theory. After the attenuation of the liquid sheet was considered in the linear instability
theory, the predicted results agreed well with the experimental data.

The spray characteristics of a recessed gas-liquid swirl-coaxial injector were studied both
theoretically and numerically by Yang et al. (2008), with pressure drops ranging from 0.2 MPa to
0.8 MPa. A high-speed photographic technique was used to measure the spray-field dynamics
and droplet size distribution. An expression was obtained for the calculation of the optimal recess
length.

The dynamic characteristics of an open-end swirl injector was studied by Fu et al. (2010)
with theoretical analysis and experimental tests. The formulations for the transfer function were
obtained for open-end swirl injectors. A series of experiments using conductance method were
conducted to validate the dynamics theory of open-end swirl injectors. The experimental results
showed agreement with the theoretical predictions.

A sheet breakup model using linear stability theory was improved by liquid viscous
theory for calculating initial liquid sheet properties as spray inlet conditions for numerical
program (KIVA in that study). The model was validated against experiments at various pressure
difference and ambient pressures. Long-wave and short-wave liquid sheet breakup regimes were observed for atmospheric and high ambient pressure cases, respectively. The computational model accurately calculated the sheet breakup length, the spray cone angle, the local Sauter Mean Diameter (SMD), and the overall spray shape compared with experimental results, and was proposed as a design tool for both atmospheric and high-pressure conditions.

An experiment study of a gas-centered, liquid-swirled coaxial single-injector element based on RD-170 injectors were conducted to investigate combustion instabilities (Miller et al., 2007). The chamber pressure ranged from 2.14 MPa to 2.38 MPa. Superheated water and oxygen mixture, and kerosene were used as oxidizer and fuel, respectively. The chamber length was varied to determine the dependence of combustion instabilities on resonant frequencies and mode shapes. Pressure fluctuations of magnitude of up to 50% of the chamber pressure were observed. A simplified acoustic analysis was conducted, and it predicted resonant frequencies with uncertainties of 4%-6%. A quasi one-dimensional computational method with full nonlinear Euler equations was developed later by Smith et al. (2008) to study the acoustic and combustion instabilities of the same single-element swirl injector. The combustion dynamics was represented by a response function. The computation started with a mean flow that corresponded to the experimental test conditions, and then perturbation was added by forcing the oxidizer flow rate. The computational predictions agreed well with the experimental results.

Most existing studies of swirl injectors were conducted at low pressures, and thus did not simulate many of the important scaling parameters of liquid rocket swirl injectors. Based on the cold flow experiments conducted at a moderate pressure (3.84MPa), Cox (1988) noted the importance of performing high-pressure experiments to match both the gas/liquid density and velocity ratios in real conditions. Strakey et al. (2001) studied the characteristics of a swirl coaxial gas-liquid injector over a wide range of gas/liquid momentum ratios from 0 to 100 at
elevated chamber pressure (2.97MPa), using water and helium/nitrogen as propellant simulants. For high momentum ratios, the spreading angle of the spray was much smaller than that reported in previous studies at one atmosphere of pressure. However, compared with the shear coaxial injector, the swirl spray did exhibit a smaller overall droplet size.

Besides cold flow testing, a number of hot-fire experiments were conducted for single- or multi-elements swirl injectors at both moderate (i.e., 2.6-3.5 MPa) and high chamber pressure (i.e., 10.3 MPa) (Elam, 1991, Tamura et al., 1997). The C* efficiency was found to increase with increasing mixture ratio. A major factor contributing to this phenomenon is the increased swirl cone angle as the fuel/oxidizer momentum ratio decreases. More details can be found in the cited works.

LOX/methane combustion studies of uni-element swirl coaxial injectors were conducted at near-critical chamber pressures at Penn State (Kalitan et al., 2005, Salgues et al., 2006a). Non-intrusive optical techniques, such as OH Planar Laser Induced Fluorescence (PLIF), OH* and CO₂* chemiluminescence, laser light scattering, and shadowgraph imaging, were employed to observe the injector near-field flow and flame structures. The C* efficiency analysis showed that swirl injectors were more efficient than shear coaxial injectors with the same injector geometry and mass flow rates, especially with higher momentum ratios, due to the faster atomization and mixing of the propellants. The visualizations of the injector near field indicated that the liquid core and flame for shear coaxial injectors did not expand radically as much as they do for swirl injectors.

Besides the theoretical analysis and experimental work on swirl coaxial injectors, attempts have also been made numerically to investigate the injector flow dynamics under sub- and supercritical conditions.
A fully nonlinear axisymmetric model was utilized to characterize the dynamic response of a classical swirl injector, compared with the linear results of Bazarov and Yang. An Inviscid, incompressible, two-dimensional axisymmetric flow was assumed, and a Boundary Element Method (BEM) model was developed to study the unsteady behaviors under periodic inflow conditions or with pulsating chamber pressures (Richardson et al., 2007). The governing equations were linear; nonlinearities entered through boundary conditions. The results indicated that the difference between pulsating either the inlet velocity or the chamber pressure was insignificant, as the height of the wave on the liquid surface in the vortex chamber was negligible, compared to the thickness of the liquid film. At low excitation frequencies, the results agreed well with the 1-D linear theory; at moderate frequencies, there was a substantial departure. A number of studies have been conducted to establish the cause of this departure from linear theory. The results ruled out the potential contributor of the channel width/location, vortex chamber length, and pulsation magnitude. It was proposed that the time and momentum exchange to create flow turning from a tangential to an axial direction played a role in determining the discrepancies. It was also concluded that the droplet size decreased as the oscillation amplitude increased, which was in agreement with Baranov’s study of self-pulsation (Bazarov, 1995).

Comprehensive numerical analysis was conducted recently by Zong and Yang (2008) to study the flow dynamics of LOX in a pressure swirl injector with tangential entry. The model is based on full-conservation laws and accommodates real-fluid thermodynamics and transport phenomena over the entire range of fluid states of concern. Turbulence closure was achieved by means of the Large-Eddy Simulation technique. LOX film thickness and spreading angle at the injector exit were compared to linear theory results. Influences of flow conditions and injector geometry on the injector flow were characterized systematically in terms of LOX film thickness and spreading angle. LOX film is intrinsically unstable and features 3D hydrodynamic instability
waves in both longitudinal and circumferential directions. The former propagates in a form similar to that of the shallow water wave for an incompressible flow, and the latter is convected downstream by the mean flow. When discharged to the combustion chamber, Kelvin-Helmholtz type instability emerges, breaks up, and forms droplets. Intrinsic unstable frequencies were identified as recirculating flow between inlet and head-end at 14 kHz, longitudinal wave of hydrodynamic instabilities at 0.55 kHz, acoustic oscillation at 3.2 kHz, and the central toroidal recirculation zone immediately downstream of the injector exit at 1.04 kHz.

The fundamental processes of injection, atomization, vaporization, and mixing in liquid rocket engines are the causes of various instability mechanisms, such as hydrodynamic wave on the liquid surface, acoustic fluctuations bouncing back and forth in the combustor and injector tubes, Kelvin-Helmholtz instabilities associated with the liquid breakup process, and the unsteady recalculation zone at various locations in the system. These instabilities may couple with the heat-release process, resulting in combustion instabilities. Injector designs dictate to a large extent the characteristics of these processes and play a vital role in the entire system. The dynamic characteristics of injectors are of great importance to the performance of the entire combustion system. However, unfortunately, there are very limited studies related to the dynamic response of swirling flows to external forcing. Several related studies are summarized in the following.

The dynamic response of swirling jets to external excitations was investigated by Panda and McLaughlin(1994) using flow visualization technique. When the air jet was excited at discrete frequencies by four acoustic speakers around the jet exit, organized structures evolved from the originally weak and irregular large-scale structures under conditions without acoustic forcing. Jet spreading was not affected by artificial excitation even at large excitation levels. The
overall growth rate of the instability waves at all modes was small, and the sub-harmonic formation through vortex pairing was suppressed due to the rapid growth of momentum thickness.

Cerecedo et al. (2004) studied the changes in co-flowing jet structures caused by acoustic forcing at the opposite end of the jet nozzle. When the forcing was imposed at its natural or sub-harmonic frequencies, large-scale coherent structures dominated the flow field, and altered the turbulence properties significantly. However, at a forcing of twice the natural frequency, the flow field behaved similarly to that of the natural jet.

In the experimental study of Gallaire et al. (2004), swirling water jet was excited at forcing frequencies less than 5 Hz using cam shaft controlling syringes. A strong response was observed only at frequencies about one order of magnitude higher than the natural frequency. The vortex breakdown process was found to be unaffected by the azimuthal forcing at the nozzle periphery, since this process was governed by the dynamics in the core region.

In contrast to the aforementioned studies on swirling jets, limited work focusing on the dynamic aspects of swirl injectors was reported in the literature. Bazarov and Yang (1998) reported a linear theory on the dynamic response of a swirl injector. Richardson et al. (2007) studied the dynamic response of a simple swirl injector using a boundary element method and compared their results with the linear theory reported by Bazarov and Yang. It was found that imposing external forcing by pulsating the inlet velocity or the chamber pressure did not bring about any significant difference. The height of the wave on the liquid surface in the vortex chamber was negligible compared to the thickness of the liquid film. At moderate excitation frequencies, the results deviated substantially from those predicted by the linear theory. The injector inlet location and inlet channel length, vortex chamber length, and pulsation magnitude were ruled out as potential contributors to the deviations. Rather, the injection velocity and the
time for the flow to direct from the tangential to axial direction were proposed as potential reasons for the deviations.

Wang and Yang (2005) investigated the flow evolution and dynamic response of a swirl injector to external excitations. It was found that the fluctuation of the instantaneous mass flow rate of a given frequency component at the injector exit can reach a magnitude substantially greater than that at the entrance, when the forcing resonates with the injector flow.

Most of the existing studies on the dynamic response of swirling flow to external excitations focus on flows at ambient conditions. Only recently, the effect of acoustic forcing on the flow dynamics of single jets, and shear coaxial jets were studied by Chehroudi and his colleagues (Chehroudi and Talley, 2002, Davis et al., 2005), as discussed before. Liu et al. (2006) numerically simulated the work performed by Davis et al. (2005). To the best knowledge of the author, the current study represents the first study on the effect of external forcing to swirl injectors under supercritical conditions.

1.2.5 Numerical Studies on High-Pressure Fluid Mixing and Combustion

Parallel to the experimental studies, attempts were made both theoretically and numerically to explore the underlying mechanisms of high-pressure fluid injection and combustion.

Oefelein and Yang (1998) established comprehensive numerical models for supercritical mixing and combustion. They studied the two-dimensional mixing and combustion of liquid oxygen and hydrogen streams at supercritical conditions by means of a Large-Eddy Simulation technique. All the thermophysical properties were evaluated directly from fundamental thermodynamics theories over the entire fluid states of concern. The focus was put on near-field
flow and combustion dynamics. The turbulence chemistry interaction was neglected and thus the numerical result is questionable when applied to LRE combustion. The results indicated that the density gradient dominated the evolution of the mixing layer, and that the mass diffusion rate greatly diminished near the critical point.

Oefelein (2005) also conducted quasi-2D direct numerical simulation of supercritical LOX/hydrogen combustion in a shear coaxial injector single element liquid rocket engine. Emphasis was placed on the near field of the injector. Results indicated the flame was anchored in the interfacial region of the high shear between LOX and hydrogen. The flame stabilization was attributed to the stagnation zone right after the LOX post.

The dominance of density gradients was observed in the direct numerical simulation (DNS) conducted by Bellan and colleagues (Miller et al., 2001, Okong'o et al., 2002, Okong'o and Bellan, 2002), where the temporal evolutions of heptane/nitrogen and oxygen/hydrogen mixing layers at supercritical conditions were treated, and several important characteristics of high-pressure transitional mixing processes were identified. Because emerging turbulent eddies were damped by strong density stratification, the layer was considerably more stable than a corresponding gaseous layer at standard pressure. During the entire evolution process, energy dissipation due to both the species-flux and heat-flux effects was dominant, whereas the viscous effect appeared to be minimal. This result suggested that turbulent models for supercritical fluids should focus primarily on duplicating the species mass flux rather than on the typical momentum flux.

The extinction limits of the flame generated around the LOX jet boundary were theoretically studied by Juniper et al. (2003a). A one-dimensional counter-flow diffusion flame model was constructed. The results indicated that the flame was very stable in the near injector region. It could not be extinguished by strain rate, even at a very low hydrogen stream
temperature. Since the typical strain rates encountered in rocket engines were insufficient to punch a hole in the flame, the edge of this diffusion flame sheet should be stabilized behind the lip of the LOX post. Following this suggestion, a two-dimensional simulation was performed to investigate the flame stabilization mechanism behind a step over a liquid reactant surface (Juniper and Candel, 2003b). It was reported that the most influential parameter regarding flame stabilization was the height of the step with respect to the flame thickness. If the flame was thicker than the step, it could not remain in the recirculation zone behind the step and was readily blown off.

A three-dimensional, incompressible, unsteady, viscous NS solver for two-phase flows based on the Locally Homogeneous Flow (LHF) assumption was developed for full three-dimensional simulations of the recessed region of shear coaxial injectors with geometries and operating conditions of the SSME main chamber combustor and the pre-burner (Kim and Heister, 2004, Kim et al., 2005a). High amplitude hydrodynamics were observed in the recessed region, exhibiting the self-pulsation mode theorized by Bazarov. Mass flow oscillated as much as 48% about the mean flow. The chamber pressure perturbation at various frequencies and amplitudes was forced at the exit boundary of the injector flow to investigate the acoustic perturbation effect. The resultant mass-flow pulsation is usually dominated by the frequency of the pressure oscillation. The pulsation magnitude is proportional to the pressure oscillation, but inversely proportional to its frequency. Forcing frequency higher than the natural frequency of the injector resulted in transient damp-out periods and settled into a steady-state oscillation of the liquid jet with phase shift. The liquid jet responded more radically to the lower frequency of perturbation than to the natural frequency and became unstable, even at small fluctuation amplitude.

Hydrodynamic instabilities within injector passages can couple to chamber acoustic modes and lead to unacceptable levels of combustion instabilities in liquid rocket engines.
Injector internal flow was studied numerically in order to explore the unforced injector response by Tsohas et al. (2007). It was indicated that the instability of vena-contracta regions and the mixing between fuel and oxidizer can serve as a fundamental source of unsteadiness produced by the injector, even in the absence of upstream or downstream pressure perturbations. Swirling the inner flow tends to increase the shedding frequency within the studies, while swirling the outer fluid produces a much more complex shedding process that does not show distinct shedding frequency. Under some combinations of the swirl and momentum ratio, a nearly steady flow was produced, which is desirable for rocket combustor applications.

The experimental studies of an LN$_2$/GN$_2$ shear coaxial injector injection with and without transverse acoustic forcing by Chehroudi et al. (Davis and Chehroudi, 2004, Davis et al., 2005, Davis and Chehroudi, 2006) was simulated by Liu et al. (2006). Again, the numerical method is based on full conservation laws and accommodates real-fluid thermodynamics and transport phenomena for the entire range of the fluid states of concern. The near-field flow evolution is characterized by three mixing layers originating from the rims of the two concentric tubes. Increasing the velocity ratio results in the enhancement of the entrainment of the outer stream into the inner region, and thus it shortens the length of the inner potential core, but increases the spreading angle. A higher chamber pressure also decreases the inner potential core, but produces a smaller spreading angle. The effect of transverse acoustic forcing on the jet flow evolution is apparent, even at the small amplitude of acoustic pressure oscillation of 0.3% of the mean chamber. The jet exhibits two-dimensional, sinuous-like structures in the slices, perpendicular to the acoustic velocity direction, but not in the parallel slices.

A comprehensive numerical study was conducted to investigate cryogenic fluid injection and mixing under supercritical conditions by Zong et al. (2004). As a result of intensive property variations, large density-gradient regions are formed, which act like a solid wall that amplifies the
axial flow oscillations but dampens the radial ones. The interfacial instability in the shear layer is effectively suppressed. The baroclinic torque arising from the density stratification plays an important role in determining the flow evolution. The jet dynamics are largely dictated by the local thermodynamic state of the fluid. The spatial growth rate of the surface instability wave increases as the ambient pressure increases, but it decreases significantly in the near-critical regime due to density stratification and increased mixing-layer momentum thickness.

Cryogenic propellant injection and combustion under conditions of actual liquid rocket engine operation were investigated recently by Zong et al. (Zong and Yang, 2007b, Zong et al., 2008) with several combustion models to account for the turbulence/chemistry interaction. The Laminar flamelet model, conserved scalar approach, and direct-closure approach were implemented to account for turbulence/chemistry interactions. The applicability of these models was carefully assessed by comparing the chemical and turbulence time scales at conditions typical for liquid-propellant rocket engine operation. The results indicated that the flamelet assumption is valid and the combustion process is mixing-dominant. The direct closure approach over-predicted the reaction rate and resulted in a thickened flame. The flame is stabilized by the wake recirculation zone with hot product, right behind the splitter plate, a result consistent with the other researchers’ findings (Mayer and Tamura, 1996a, Lux et al., 2006).

Masquelet et al. (2009) simulated the LOX/H₂ combustion in a subscale multi-injector liquid rocket engine. A simple EBU model was used to limit the chemical reaction rate. Heat flux along the chamber wall showed deviation from experiment measurements. Masquelet and Menon (2010) also studied the GOX/GH₂ combustion of a single-element shear coaxial injector. Chemical reactions were calculated directly from the resolved temperature and species, without consideration of turbulence/chemistry interactions. The calculated heat flux at the wall was compared with that of the experiment. The three-dimensional results captured the trend of heat
flux profile of the experimental data, and were much better compared to their two-dimensional cases.

Cutrone et al. (2010) conducted RANS simulations of the LOX/H\textsubscript{2} combustion using flamelet-progress-variable method. The numerical scheme was first validated against the Sandia flame D. Then the calculated OH distribution for LOX/H\textsubscript{2} combustion was compared to experiment emission images. Lacaze et al. (2009) conducted LES simulations of the flame ignition and propagation of LOX/H\textsubscript{2} in a rocket-like combustor, with focus placed on the transient ignition and flame propagation. The calculated transient chamber pressure and OH distributions were compared to the experimental pressure history and OH emission images, respectively.

Schmitt et al. (2009) conducted LES studies of nitrogen jet and LOX/H\textsubscript{2} combustion at supercritical pressures. The nitrogen jet studies showed good agreement with experiments for the low injection temperature case, but discrepancies were observed for the supercritical temperature injection. The predicted LOX/H\textsubscript{2} flames showed temperature distributions deviating from the experimental results. Recently, Schmitt et al. (2010) conducted large-eddy simulations of LOX/methane combustion under trans-critical conditions. The combustion model solved for species transport equations, but with the source term calculated based on steady flamelet concept. The numerical method was first validated against the "H3" flame. Then, numerical simulations of the experiment case by Singla et al. (2005) were conducted. The resulting flame structure was compared to the experimental images. Resemblance of flame structures was achieved.
1.3 Work Scope and Method of Approach

The present study investigates the high-pressure cryogenic fluid injection, mixing, and combustion by means of Large-Eddy Simulation. The flow evolution under consideration is extremely complicated, involving thermodynamic non-idealities, transport anomalies, and high Reynolds number turbulent reacting flows. A variety of uncertainties exist with regard to the closure problem. To address these difficulties in a manner consistent with current experimental efforts, this research focuses on detailed representations of fluid dynamic and thermophysical processes in simplified configurations and at well controlled experimental conditions. The approach follows three fundamental steps: 1) the development of a generalized and self-consistent theoretical framework with accurate property evaluation schemes, turbulence closure methodologies and turbulent combustion modeling; 2) the implementation of an efficient and robust numerical algorithm for general fluid mixture, in which the real-fluid thermodynamics are treated consistently with a full account of pressure effects; and 3) the systematic investigation of a series of cases associated with trans- and supercritical injection, mixing, and combustion dynamics.

Chapter 2 presents a generalized theoretical framework that accommodates high-pressure real fluid thermodynamics, transport anomalies, and turbulence. The governing equations are obtained using convolution integrals to filter out the small-scale dynamics from the resolved-scales over a defined set of spatial and temporal intervals. The subgrid-scale (SGS) terms are modeled using a compressible-flow version of the Smagorinsky model suggested by Erlebacher et al. (1992). Thermodynamic properties, including enthalpy, internal energy, heat capacity, and their related partial density properties, are directly calculated by means of fundamental thermodynamic theories (Moran and Shapiro, 2000) and a modified Soave-Redlich-Kwong (SRK) equation of state that is reasonably accurate and easy for implementation (Graboski and
Daubert, 1978a, b). Transport properties, such as viscosity and thermal conductivity, are estimated with the method of Chung et al., which fall into the category of corresponding state theories (Poling et al., 2001).

In Chapter 3, the governing system is discretized using a preconditioned, density-based, finite-volume methodology. The basic formulations are derived using fundamental thermodynamic theories, in which the definitions of partial mass and partial density properties are introduced. This framework takes into full account thermodynamic non-idealities and transport anomalies and also accommodates any arbitrary equation of state. The developed equations are coupled with the preconditioning scheme, which renders the numerical algorithm capable of solving all-Mach number fluid flows at any fluid state (Meng and Yang, 2003). Second-order dual-time stepping integration with the convergence acceleration techniques developed by Choi and Merkel (1993) and Buelow (1995) is adopted for temporal discretization. Spatial discretization employs the fourth-order accurate flux differencing methodologies developed by Rai and Chakravarthy (1993). A fourth-order scalar dissipation and matrix dissipation with a total-variation-diminish (TVD) switch developed by Swanson and Turkel (1992) and Jorgenson and Turkel (1993) is implemented to ensure computational stability and to prevent numerical oscillations in regions with steep gradients. A multiblock domain decomposition technique, along with static load balance, is used to facilitate the application of efficient parallel computation with message-passing interfaces at the domain boundaries.

In Chapter 4, the theoretical and numerical framework is validated by simulating the Sandia Flame D. The calculated axial and radial profiles of velocity, temperature, and mass fractions of major species are in reasonably good agreement with the experimental measurements. The conditionally averaged mass fraction profiles agree very well with the experimental results at different axial locations.
In Chapter 5, the validated model is first employed to examine the flow dynamics of liquid oxygen in a pressure swirl injector at supercritical conditions. Emphasis is placed on analyzing the effects of external excitations on the dynamic response of the injector. The high frequency fluctuations do not significantly affect the flow field as they are dissipated shortly after being introduced into the flow. However, the lower frequency fluctuations are amplified by the flow-field. As a result, the film thickness and the spreading angle at the nozzle exit fluctuate strongly for low-frequency external excitations.

In Chapter 6, the combustion of gaseous oxygen/gaseous hydrogen in a high-pressure combustion chamber for a shear coaxial injector is simulated to assess the accuracy and the credibility of the computer program when applied to a sub-scale model of a combustor. The predicted heat flux profile is compared with the experimental and numerical studies. The predicted heat flux profile agrees reasonably well with the experimental data.

In Chapter 7, the steady flamelet model and the flamelet/progress-variable have been used to study the LOX/methane flame stabilized by a splitter plate. Results show that the flame is always anchored in the recirculation zone immediately after the splitter plate. Turbulence is not strong enough to extinguish the non-premixed flame. The flame stabilization is found to be achieved through the recirculation zone and the vortex shedding processes in the near field of the splitter plate. The flamelet-progress variable case further confirms that the artificially quenched flame can be re-established as long as the quenching distance is within the mean recirculation zone.

Finally, the conclusions of the present work and recommendations for future studies are summarized in Chapter 8.
Chapter 2

Theoretical Formulation

2.1 Governing Equations

The conservation laws for mass, momentum, and energy are the basic principles of classic physics, regardless of the state of objects, solid or fluid, continuum or discrete, reacting or chemically frozen. In principle, these conservation laws can be applied to any system of interest to obtain mathematical formulations with different levels of approximation. These equations can be used to describe, explain and predict physical processes of interest. In fluid mechanics, with continuum hypothesis, and no body forces, the differential equations for mass, momentum, energy, and species in conserved forms are given by

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

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = \frac{\partial \sigma_{ij}}{\partial x_j}, \quad (i = 1, 2, 3) \tag{2.2}
\]

\[
\frac{\partial \rho E}{\partial t} + \frac{\partial [(\rho E + p)u_i]}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial (u_i \tau_{ij})}{\partial x_j}, \tag{2.3}
\]
\[
\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho Y_k u_j}{\partial x_j} = \dot{\omega}_k - \frac{\partial \left( \rho D_k \nabla Y_k \right)}{\partial x_j}, \quad (k = 1, \cdots, N-1)
\]  

where the repeated indices imply a summation of the indices.

The derivations of these equations can be made through applying conservation laws of mass, momentum, and energy to an infinitesimal control volume. Detailed derivation can be found in standard textbooks, for example, Kuo (1986).

In Eq. 2.2, the viscous stress tensor \( \sigma_{ij} \) for a Newtonian fluid, with Stokes' hypothesis to neglect the bulk viscosity, is given by

\[
\sigma_{ij} = -p \delta_{ij} + \tau_{ij} = -p \delta_{ij} + \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij}.
\]  

When evaluating the heat flux vector \( q_j \) in Eq. 2.3, the Dufour effect, which is the heat flux due to concentration gradient, is generally very small and neglected in the current study. Then \( q_j \) is defined as

\[
q_j = -\lambda \frac{\partial T}{\partial x_j} + \rho \sum_{k=1}^{N} h_k Y_k U_{k,j}.
\]

The specific total energy is defined as the sum of specific internal energy and kinetic energy, given by

\[
E = e + \frac{u_j u_j}{2}, \quad (2.7)
\]

where the specific internal energy is calculated from specific enthalpy, pressure, and density, given by

\[
E = e + \frac{u_j u_j}{2}, \quad (2.7)
\]
\[ e = h - \frac{P}{\rho} , \]  

where \( h \) is determined by the mixture concentration and partial-mass based enthalpies, \( \hat{h}_k \), for which the definition will be given later.

\[ h = \sum_{k=1}^{N} Y_k \hat{h}_k . \]  

The chemical source term in Eq. 2.4 is determined from the selected chemistry kinetics.

For an elementary reaction mechanism, with \( L \)-step reaction and \( N \) species,

\[ \sum_{k=1}^{N} \nu'_{ki} \chi_k \leftrightarrow \sum_{k=1}^{N} \nu''_{ki} \chi_k , \quad i = 1, 2, ..., L , \]  

the reaction rate constants of the forward and backward reactions, \( k_f \) and \( k_b \), may take the following form:

\[ k_f(T) = A T^b \exp\left(-E_f / R T\right) . \]  

The net production rate for each species in a multi-step mechanism is given by

\[ \dot{\omega}_k = W_k \sum_{i=1}^{K} \left( \nu''_{r'} - \nu'_{r} \right) \left[ k_f \prod_{k=1}^{N} \left( \chi_k \right)^{\nu''} - k_b \prod_{k=1}^{N} \left( \chi_k \right)^{\nu'} \right], \quad k = 1, 2, ..., N. \]  

For a global reaction mechanism, taking hydrocarbon oxygen combustion as an example:

\[ \nu'_F C_m H_n + \nu'_O_2 O_2 \rightarrow \nu'_{CO_2} CO_2 + \nu'_{H_2O} H_2O . \]  

The production rate for each species can be calculated by:

\[ \dot{\omega}_k = W_k A T^n \exp\left(-E_a / R T\right) [Fuel]^a [Oxi]^b , \]  

Where the constants \( a \) and \( b \) are obtained from experimental results.
In non-premixed combustion studies, mixture fraction is an important variable to describe combustion flames (Peters, 2000). However, the definition of mixture fraction is not unique. In a two feed system, mixture fraction is simply defined as the ratio of the local mass originating from the fuel (denoted by 1) to total mass (with mass from the oxidizer stream denoted by 2) (Peters, 2000),

\[ Z = \frac{m_1}{m_1 + m_2}. \] (2.15)

Although the definition based on Eq. 2.15 is straightforward and simple, it becomes ambiguous when there are multiple inlets. In such a case, a more general definition based on elemental conservation is used. If \( a_{ij} \) denote the number of atoms of element \( j \) in a molecule of species \( i \), then the mass of all atoms \( j \) in the system of interest is given by:

\[ m_j = \sum_{k=1}^{N} \frac{a_{ij} W_j}{W_i} m_i. \] (2.16)

Dividing Eq. 2.16 by the total mass, one has the mixture fraction of element \( j \) as:

\[ Z_j = \frac{m_j}{m} = \sum_{k=1}^{N} \frac{a_{ij} W_j}{W_i} Y_i. \] (2.17)

Clearly, \( Z_j \) is a linear function of species, \( Y_i \). Multiplying Eq. 2.4 by \( \frac{a_{ij} W_j}{W_i} \) and summing over all the species, we have:

\[ \frac{\partial \rho Z_k}{\partial t} + \frac{\partial (\rho u_j Z_k)}{\partial x_j} = -\frac{\partial}{\partial x_j} \left( \rho D_k \frac{\partial Z_k}{\partial x_j} \right). \] (2.18)

The source term vanishes because of the conservation of chemical elements. Further, it can be assumed that the mass diffusivity for all the species equal to \( D \) to obtain:
\[
\frac{\partial \rho Z_k}{\partial t} + \frac{\partial (\rho u_j Z_k)}{\partial x_j} = -\frac{\partial}{\partial x_j} \left( \rho D \frac{\partial Z_k}{\partial x_j} \right).
\] (2.19)

For hydrocarbon fuel as in Eq. 2.13, the coupling function can be defined as: (Burke and Schumann 1928):

\[
\beta = \frac{Z_c}{mW_c} + \frac{Z_H}{nW_H} - 2 \frac{Z_O}{v'_O \omega_O},
\] (2.20)

where \(\beta\) is a conserved scalar. It can be normalized so that it varies between 0 and 1 to get Bilger’s (1988) definition of the mixture fraction:

\[
f = \frac{Z_c / (mW_c) + Z_H / (nW_H) + 2(y_{O,2} - Z_O) / (v'_O \omega_O)}{Z_c / (mW_c) + Z_H / (nW_H) + 2Y_{O,2} / (v'_O \omega_O)}. \] (2.21)

From Eq. 2.18 and Eq. 2.21, one can get the transport equation for mixture fraction:

\[
\frac{\partial \rho f}{\partial t} + \frac{\partial (\rho u_j f)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial f}{\partial x_j} \right).
\] (2.22)

Progress variable, which is defined as the mass fraction of main products, i.e. \(\text{CO}_2\), \(\text{H}_2\text{O}\), and \(\text{CO}\) in the current study, is a linear function of the corresponding species. The transport equation for progress variable is given by:

\[
\frac{\partial \rho C}{\partial t} + \frac{\partial (\rho u_j C)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial C}{\partial x_j} \right) + \dot{\omega}_C,
\] (2.23)

where the reaction rate of progress variable is the sum of product reaction rates.
To close the governing equations listed in the previous section, equations of state and thermodynamic data should be defined. In the analysis of liquid rocket engine combustion, the propellants experience a broad range of temperatures at elevated pressures, which are generally well above the critical pressures of the propellants. Under these situations, the behavior of the propellants is far from the ideal-gas limit. An equation of state that can handle real fluid properties must be used. The thermodynamic properties have to be evaluated in a consistent manner to provide a unified treatment of real-fluid thermodynamics. In this section, the selected equation of state is first presented, then real-fluid thermodynamics treatment, including the derivatives appearing in the preconditioning matrix are summarized. Lastly, the methodology to evaluate real fluid mixture transport properties is discussed.

**2.2.1 The Modified Soave-Redlich-Kwong (SRK) Equation of State**

Due to their accuracy and fairly low computational cost, the cubic equations of state, such as Redlich-Kwong, Peng-Robinson (Peng and Robinson, 1976), and the modified Soave-Redlich-Kwong (Soave, 1972) equation of state, are the most commonly used equations of state for real-fluid properties (Poling et al., 2001). There are many other equations of state, such as the virial equation of state, BWR. The virial equation of state has a relatively small range of application (Poling et al., 2001). Although the Benedict-Webb-Rubin (BWR) equation of state is very accurate, it is non-analytical, and is generally used for pure substances (Reid et al., 1987).
The modified SRK equation of state, which is also capable of handling the quantum-gas behavior of hydrogen, is used in the current study. The consistent treatment of thermodynamic properties using this single equation of state leads to an efficient numerical algorithm.

The modified SRK equation of state takes the following form (Soave, 1972, Graboski and Daubert, 1978a, b):

\[
p = \frac{\rho R_u T}{(W - b \rho)} - \frac{a \alpha \rho^2}{W (W + b \rho)}.
\]  

(2.24)

In this equation of state, the molecule interactions, i.e. attractive and repulsive effects are accounted by ‘a’ and ‘b’, respectively. Unlike ‘a’ and ‘b’, which are functions of species mole fractions only, ‘α’ also depends on temperature and acentric factor. For mixtures, these parameters are evaluated as:

\[
\alpha a = \sum_{i=1}^{N} \sum_{j=1}^{N} x_i x_j \alpha_{ij} a_{ij},
\]  

(2.25)

\[
b = \sum_{i=1}^{N} x_i b_i.
\]  

(2.26)

The cross parameter \(\alpha_{ij} a_{ij}\) in Eq. 2. 25 is given by

\[
\alpha_{ij} a_{ij} = \sqrt{\alpha_i \alpha_j a_i a_j} \left(1 - \kappa_{ij}\right),
\]  

(2.27)

where \(x_i\) is the mole fraction of species \(i\), \(\kappa_{ij}\) is the binary interaction coefficient. The constants \(a_i, b_i\) and other parameters involved are calculated as:

\[
a_i = 0.42747 \frac{R_u^2 T_{ci}^2}{P_{ci}},
\]  

(2.28)
To account for the quantum-gas behavior, Eq. 2.30 for hydrogen is further established as (Soave, 1972, Graboski and Daubert, 1978a, b)

\[ \alpha_i = [1 + S_i (1 - \sqrt{T_n})]^2, \]  

(2.30)

\[ T_n = \frac{T}{T_{ci}}, \]  

(2.31)

\[ S_i = 0.48508 + 1.5517\omega_i - 0.15613\omega_i^2. \]  

(2.32)

This correlation is expected to be accurate for hydrogen at temperature higher than 83K. This is the case in liquid rocket applications. Note, \( \kappa \) involving hydrogen species should be set to 0.

### 2.2.2 Thermodynamic Properties

In addition to the equation of state, thermodynamic properties, which are functions of temperature, pressure, and species concentration, need to be evaluated to solve the equations listed before. Thermodynamic properties can be derived directly from fundamental thermodynamic relations, which are valid for all thermodynamic states. The thermodynamic properties are generally taken as the sum of the low pressure limit value, and a departure function,
which accounts for the pressure effects. Taking advantage of the path-independence of thermodynamic properties, specific internal energy, enthalpy, entropy, and specific heat capacity can be calculated as:

\[
e(T, \rho) = e_0(T) + \int_{\rho_0}^{\rho} \left[ \frac{p}{\rho^2} - \frac{T}{\rho^2} \left( \frac{\partial P}{\partial T} \right)_\rho \right] d\rho,
\]

\[
h(T, p) = h_0(T) + \int_{\rho_0}^{p} \left[ \frac{1}{\rho} + \frac{T}{\rho^2} \left( \frac{\partial P}{\partial T} \right)_\rho \right] dp,
\]

\[
s(T, \rho) = s_0(T, \rho_0) - \int_{\rho_0}^{\rho} \left[ \frac{1}{\rho^2} \left( \frac{\partial P}{\partial T} \right)_\rho \right] d\rho.
\]

\[
C_p(T, \rho) = C_{V0}(T) - \int_{\rho_0}^{\rho} \left[ \frac{T}{\rho^2} \left( \frac{\partial^2 P}{\partial T^2} \right)_\rho \right] d\rho + \frac{T}{\rho^2} \left( \frac{\partial P}{\partial T} \right)_\rho \left( \frac{\partial P}{\partial \rho} \right)_T.
\]

The subscript 0 refers to an ideal state at a low pressure and the integral terms are the departure functions. All the partial derivatives in these relations can be calculated from the given equation of state, here, the modified Soave-Redlich-Kwong equation of state:

\[
\left( \frac{\partial P}{\partial T} \right)_{\rho_j} = \frac{\rho R_u}{(M_w - b_\rho)} - \frac{1}{M_w} \left[ \frac{\partial}{\partial T} (\alpha) \right]_{\rho, Y_i} \frac{\rho^2}{(M_w + b_\rho)},
\]

\[
\left( \frac{\partial P}{\partial \rho} \right)_{T, Y_i} = \frac{M_w R_u T}{(M_w - b_\rho)^2} - \frac{a \alpha}{M_w} \frac{\rho (2M_w + b_\rho)}{(M_w + b_\rho)^2}.
\]
where the derivative \( \frac{\partial}{\partial T} (\alpha \alpha) \) is given in Appendix C.

### 2.2.3 Partial Molar and Partial Density Properties

For ideal gas mixtures, the mixture properties are simply the sum of molar-weighted properties. However, at high-pressure conditions, mixture properties, such as specific internal energy, specific enthalpy, and specific volume, are complex functions of temperature, pressure and chemical species. Partial molal properties for an extensive variable \( X \), is defined as:

\[
\bar{X}_i = \left( \frac{\partial X}{\partial n_i} \right)_{p,T,x,\rho,p_{x,\rho}}
\]  

(2.41)

where \( n \) is the mole number. Partial molar properties are defined as:

\[
\bar{\Phi}_i = \left( \frac{\partial \Phi}{\partial \chi_i} \right)_{p,T,x,\rho,p_{x,\rho}}
\]  

(2.42)

Early works in high-pressure droplet vaporization and combustion (Manrique and Borman, 1969, Hsieh et al., 1991) indicated that partial molar properties have to be used to get reliable results. This is easily understood by taking the mixture of water and ethanol at room
conditions as an example. The mixture volume (non-ideal mixture) of 1 mL water and 1 mL ethanol is less than 2 mL. In other words, the mixture property $V$, is not equal to the sum of molar-weighted volumes of water and ethanol. Partial molar properties have to be used to get accurate mixture properties in such situations.

However, unfortunately, in most CFD codes, all flow properties are based on mass or density instead of mole number, making the evaluation of partial molar properties inconvenient. The concept of partial mass and partial density properties were introduced by Lafon et al. (1995) and Meng (2001) to overcome these problems.

Any partial mass property $\phi$ in a mixture is dependent on pressure, temperature and species mass fractions:

$$m_\phi = m_\phi(p,T,m_i).$$  \hspace{1cm} (2.43)

Accordingly, the partial mass property is defined as

$$\hat{\phi}_i = \left( \frac{\partial m_\phi}{\partial m_i} \right)_{p,T,m_{\neq i}}.$$  \hspace{1cm} (2.44)

Partial density property, which is more convenient in fluid mechanics, is defined in a similar manner:

$$\bar{\phi}_i = \left( \frac{\partial \rho \phi}{\partial \rho_i} \right)_{T,\rho_{\neq i}}.$$  \hspace{1cm} (2.45)
Note the independent variables change from pressure, species mass fractions to species densities. The relation between a partial mass property and the corresponding partial density variable can be derived from fundamentals of thermodynamics (Meng, 2001), given by:

\[
\tilde{\phi}_i = \tilde{\phi}_i + \rho \left( \frac{\partial \tilde{\phi}_i}{\partial p} \right)_{T,Y_i} \left( \frac{\partial p}{\partial \rho_i} \right)_{T,\rho_i,\mu_i} .
\]  (2.46)

As an example of partial mass and partial density variable application, partial mass enthalpy is given by:

\[
\hat{h}_i = \hat{e}_i + T \left( \frac{\partial p}{\partial T} \right)_{\rho_i} \left( \frac{\partial p}{\partial \rho_i} \right)_{T,Y_i} .
\]  (2.47)

### 2.3 Transport Properties

Apart from the equation of state, transport properties are also needed to be evaluated accurately by taking into account the effect of pressure. Accurate calculation of transport properties, including dynamic viscosity, thermal conductivity, and binary mass diffusivity, is very important for fluid mixing and combustion prediction. They not only determine the flow dynamics, but also the heat and mass transfer rates (Vesovic and Wakeham, 1991).

As originally proposed by van der Waals in 1873, the law of corresponding states asserts that equilibrium properties can be related to the critical properties in a universal manner. (Poling et al., 2001). It expresses that the reduced \(P-V-T\) relationships are the same for all substances.
Based on the argument of the corresponding state theory, not only the reduced $P$-$V$-$T$ relationships are the same, any property of any fluid can be estimated by relating to its counterpart of a reference substance, whose properties can be easily obtained (Ely and Hanley, 1981). Chung et al.’s method (Poling et al., 2001), which also falls into the corresponding state theory category, is used in the current study for its fair accuracy, relative simplicity, availability of parameters, and consistency in evaluating dynamic viscosity and thermal conductivity of high-pressure fluid mixtures. As for the binary mass diffusivity, as discussed by Poling et al. (2001), there are few proposed methods to account for high-pressure effect on the diffusion coefficients, the Takahashi method is used in the current study to account for high-pressure effects.

2.3.1 Dynamic Viscosity and Thermal Conductivity

Chung et al.’s method (Poling et al., 2001) is used to calculate dynamic viscosity and thermal conductivity of mixtures at high pressures. This method finds its theoretical basis in the general formulations derived from elementary kinetic theory. Extensions were made to account for various effects that are not included in deriving the basic formulation. The resulting formulation provides a consistent procedure to estimate mixture dynamic viscosity and conductivity at high pressures.

Based on elementary kinetic theory, the transport coefficients, mass diffusivity $D$, dynamic viscosity $\eta$ and thermal conductivity $\lambda$ are all proportional to the average molecular speed $v$ and mean free path $L$ (Poling et al., 2001), as follows:
Assuming a rigid, no interacting sphere model for molecules, the viscosity relation is given by:

\[ D = \frac{vL}{3} = (\text{const}) \frac{T^{3/2}}{M^{1/2} \mu \sigma^2}, \]  

(2.48)

\[ \eta = \frac{m \rho vL}{3} = (\text{const}) \frac{T^{1/2} M^{1/2}}{\sigma^2}, \]  

(2.49)

\[ \lambda = \frac{vL \epsilon \eta}{3} = (\text{const}) \frac{T^{1/2}}{M^{1/2} \sigma^2}. \]  

(2.50)

Assuming a rigid, no interacting sphere model for molecules, the viscosity relation is given by:

\[ \eta = 26.69 \frac{T^{1/2} M^{1/2}}{\sigma^2}, \]  

(2.51)

where \( \eta \) = viscosity, \( \mu P \)

\( M \) = molecular weight, g/mol

\( \sigma \) = hard-sphere diameter, Å

If the effects of molecular interaction are taken into account, viscosity can be derived as:

\[ \eta = 26.69 \frac{T^{1/2} M^{1/2}}{\sigma^2 \Omega_v}, \]  

(2.52)

where \( \Omega_v \) is the collision integral, which can be calculated if the potential energy of interaction is given.

Chung et al. multiply Eq. 2.52 by a factor \( F_c \) to account for molecular shapes and polarities of dilute gases to get the expression for viscosity of low pressure gases:
\[ \eta = 26.69 \frac{F_c (MT)^{1/2}}{\sigma^2 \Omega_v} = 40.785 \frac{F_c (MT)^{1/2}}{V_c^{2/3} \Omega_v}, \]  

(2.53)

with \( \eta \) = viscosity, \( \mu P \)

\( M \) = molecular weight, g/mol

\( \sigma = 0.809 l_c^{1/3} \), har-sphere diameter, Å

\( T \) = temperature, K

\( V_c \) = critical volume, cm\(^3\)/mole

\( F_c = 1 - 0.2756 \omega + 0.059035 \mu^4 + \kappa \)

\( \Omega_p = A(T^*)^{-B} + C e^{-DT^*} + E e^{-FT^*} \), viscosity collision integral

\( A = 1.16145, B = 0.14874, C = 0.52487, D = 0.77320, E = 2.16178, F = 2.4378 \)

\( T^* = 1.2593 T_r \)

\( \omega \) = accentric factor

\( \mu_r = 131.3 \frac{\mu}{(V_c l_c)^{1/2}} \), dimensionless dipole moment

\( \kappa \) = special correction for high highly polar substances, like alcohols and acids

For gas mixtures at low pressures, mixture properties are used to evaluate viscosity:

\[ \eta_m = 26.69 \frac{F_c (MT)^{1/2}}{\sigma^2 \Omega_v} = 40.785 \frac{F_{cm} (M_m T)^{1/2}}{V_{cm}^{2/3} \Omega_{vm}}. \]  

(2.54)

Mixing rules to give mixture properties used in Eq. 2.54 are given by:

\[ \sigma_m^3 = \sum_i \sum_j \chi_i \chi_j \sigma_{ij}^3, \]  

(2.55)
The combining rules are:

\[
\sigma_{ii} = \sigma_i = 0.809 V_{ci}^{1/3},
\]

(2.62)

\[
\sigma_{ij} = \left(\sigma_i \sigma_j\right)^{1/2},
\]

(2.63)

\[
\frac{\varepsilon_{ii}}{k} = \frac{\varepsilon_i}{k} = \frac{T_{ei}}{1.2593},
\]

(2.64)
\[ \frac{\varepsilon_{ij}}{k} = \left( \frac{\varepsilon_i \varepsilon_j}{k} \right)^{1/2}, \quad (2.65) \]

\[ \omega_i = \omega_i, \quad (2.66) \]

\[ \omega_j = \frac{\omega_i + \omega_j}{2}, \quad (2.67) \]

\[ \kappa_i = \kappa_i, \quad (2.68) \]

\[ \kappa_j = \left( \kappa_i \kappa_j \right)^{1/2}, \quad (2.69) \]

\[ M_{ij} = \frac{2M_i M_j}{M_i + M_j}, \quad (2.70) \]

\[ F_{cm} = 1 - 0.275 \omega_m + 0.059035 \mu_r^m + \kappa_m, \quad (2.71) \]

\[ \mu_r^m = \frac{131.3 \mu_m}{\left( V_{cm} T_{cm} \right)^{1/2}}, \quad (2.72) \]

\[ V_{cm} = \left( \sigma_m / 0.809 \right)^3, \quad (2.73) \]

\[ T_{cm} = 1.2593 \left( \frac{\varepsilon}{k} \right)_m, \quad (2.74) \]

where \( T_c \) is in K, \( V_c \) is in cm³/mol, and \( \mu \) is in debyes.

To account for high-pressure effect on the viscosity of pure gas, a correction coefficient is added to Eq. 2.51 and is given by:
with the coefficients given by table 2.1.

Finally, for high-pressure mixtures, mixture properties are used in Eqns. 2.75-2.81 to calculate mixture viscosity.
Table 2.1. Coefficients to calculate $E_i$ in Eq. 2.81.

<table>
<thead>
<tr>
<th>$i$</th>
<th>$a_i$</th>
<th>$b_i$</th>
<th>$c_i$</th>
<th>$d_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6.324</td>
<td>50.412</td>
<td>-51.680</td>
<td>1189.0</td>
</tr>
<tr>
<td>2</td>
<td>$1.210 \times 10^{-3}$</td>
<td>$-1.154 \times 10^{-3}$</td>
<td>$-6.257 \times 10^{-3}$</td>
<td>0.03728</td>
</tr>
<tr>
<td>3</td>
<td>5.283</td>
<td>254.209</td>
<td>-168.48</td>
<td>3898.0</td>
</tr>
<tr>
<td>4</td>
<td>6.623</td>
<td>38.096</td>
<td>-8.464</td>
<td>31.42</td>
</tr>
<tr>
<td>5</td>
<td>19.745</td>
<td>7.630</td>
<td>-14.354</td>
<td>31.53</td>
</tr>
<tr>
<td>6</td>
<td>-1.900</td>
<td>-12.537</td>
<td>4.985</td>
<td>-18.15</td>
</tr>
<tr>
<td>7</td>
<td>24.275</td>
<td>3.450</td>
<td>-11.291</td>
<td>69.35</td>
</tr>
<tr>
<td>8</td>
<td>0.7972</td>
<td>1.117</td>
<td>0.01235</td>
<td>-4.117</td>
</tr>
<tr>
<td>9</td>
<td>-0.2382</td>
<td>0.06770</td>
<td>-0.8163</td>
<td>4.025</td>
</tr>
<tr>
<td>10</td>
<td>0.06863</td>
<td>0.3479</td>
<td>0.5926</td>
<td>-0.727</td>
</tr>
</tbody>
</table>

Table 2.2. Coefficients to calculate $E_i$ in Eq. 2.88.

<table>
<thead>
<tr>
<th>$i$</th>
<th>$a_i$</th>
<th>$b_i$</th>
<th>$c_i$</th>
<th>$d_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$2.4166 E + 0$</td>
<td>$7.4824 E - 1$</td>
<td>$-9.1858 E - 1$</td>
<td>$1.2172 E + 2$</td>
</tr>
<tr>
<td>2</td>
<td>$-5.0924 E - 1$</td>
<td>$-1.5094 E + 0$</td>
<td>$-4.9991 E + 1$</td>
<td>$6.9983 E + 1$</td>
</tr>
<tr>
<td>3</td>
<td>$6.6107 E + 0$</td>
<td>$5.6207 E + 0$</td>
<td>$6.4760 E + 1$</td>
<td>$2.7039 E + 1$</td>
</tr>
<tr>
<td>4</td>
<td>$1.4543 E + 1$</td>
<td>$-8.9139 E + 0$</td>
<td>$-5.6379 E + 0$</td>
<td>$7.4344 E + 1$</td>
</tr>
<tr>
<td>5</td>
<td>$7.9274 E - 1$</td>
<td>$8.2019 E - 1$</td>
<td>$-6.9369 E - 1$</td>
<td>$6.3173 E + 0$</td>
</tr>
<tr>
<td>6</td>
<td>$-5.8634 E + 0$</td>
<td>$1.2801 E + 1$</td>
<td>$9.5893 E + 0$</td>
<td>$6.5529 E + 1$</td>
</tr>
<tr>
<td>7</td>
<td>$9.1089 E + 1$</td>
<td>$1.2811 E + 1$</td>
<td>$-5.4217 E + 1$</td>
<td>$5.2381 E + 2$</td>
</tr>
</tbody>
</table>

Thermal conductivity is derived in a similar manner. The final expression for thermal conductivity is given by:
\[
\lambda = \frac{31.2 \eta' \Psi}{M'} \left( G_2^{-1} + B_b y \right) + qB_y y^{2-1/2}G_2 .
\]  

(2.82)

With \( \lambda \) = thermal conductivity, W/(m·K)

\( \eta' \) = low pressure gas viscosity, N·s/m

\( M' \) = molecular weight, kg/mol

\( q = 3.586 \times 10^{-3}(T_c M')^{1/2}/V_c^{2/3} \)

\[ \Psi = 1 + \alpha \left\{ \left[ 0.215 + 0.28288\alpha - 1.061\beta + 0.26665\omega \right] / \left[ 0.6366 + \beta\omega + 1.061\alpha\beta \right] \right\} , \]  

(2.83)

\[ \alpha = \frac{C_v}{R} - \frac{3}{2} , \]  

(2.84)

\[ \beta = 0.7862 - 0.7109\omega + 1.3168\omega^2 , \]  

(2.85)

\[ \omega = 2.0 + 10.5T_c^2 , \]  

(2.86)

\[ G_2 = \frac{(B_1 / y)\left[ 1 - e^{-R_b y} \right] + B_2 G_1 e^{R_b y} + B_3 E_i}{B_1 B_4 + B_2 + B_3} , \]  

(2.87)

\[ B_i = a_i + b_i\omega + c_i\mu^4 + d_i\kappa . \]  

(2.88)

with the coefficients listed in table 2.2.
2.3.2 Binary Mass Diffusivity

At low pressures, the product $Dp$ or $Dρ$ are almost constant, and are independent on species composition. However, it is not the case for high-pressure mixtures. Due to lack of experimental data for binary mass diffusivity, there are only a few estimation methods. In this study, lower-pressure values of binary mass diffusivity are evaluated with Fuller et al.’s empirical correlation, recommended by Poling et al. (2001). Then a very simple method, which is also a corresponding-state method, suggested by Takahashi is adopted in the current study to correct for high-pressure effect.

At low pressures, the binary mass diffusivity is given by Fuller et al. (Poling et al., 2001):

$$D_{ij} = \frac{0.00143T^{1.75}}{pM_{ij}^{1/2} \left[ \left( \Sigma_v \right)_i^{1/3} + \left( \Sigma_v \right)_j^{1/3} \right]^2},$$

(2.89)

where $D_{ij}$ is binary mass diffusivity with unit of cm$^2$/s, $\Sigma_v$ is found for each component by summing atomic diffusion volumes, which is tabulated in Poling et al. (2001, Table 11-1). The data of interest are listed in table 2.3.

Table 2.3. Diffusion volumes for selected atoms and molecules

<table>
<thead>
<tr>
<th>Atoms</th>
<th>Diffusion volume increments</th>
<th>Molecules</th>
<th>Diffusion volumes</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>15.9</td>
<td>O$_2$</td>
<td>16.3</td>
</tr>
<tr>
<td>H</td>
<td>2.31</td>
<td>Air</td>
<td>19.7</td>
</tr>
<tr>
<td>O</td>
<td>6.11</td>
<td>CO</td>
<td>18.0</td>
</tr>
<tr>
<td>N</td>
<td>4.54</td>
<td>CO$_2$</td>
<td>26.9</td>
</tr>
<tr>
<td>Aromatic Ring</td>
<td>-18.3</td>
<td>H$_2$O</td>
<td>13.1</td>
</tr>
</tbody>
</table>
Then high-pressure correction is evaluated based on Takahashi’s correlation, which is given by:

\[
\frac{D_y p}{(D_y p)^+} = f(T_r, p_r),
\]

(2.90)

where the superscript + indicates the low-pressure values given by Eq. 2.89. The function \( f(T_r, p_r) \) represents a pressure scaling factor, and is given by Fig. 2.1. The combining rules to calculate the reduced temperature and reduced pressure are given by:

\[
T_c = x_i T_{c,i} + x_j T_{c,j},
\]

(2.91)

\[
p_c = x_i p_{c,i} + x_j p_{c,j}.
\]

(2.92)

Figure 2.1. Correlation for high-pressure diffusivity using Takahashi method
2.4 Turbulence Closure: Large-Eddy Simulation

Although turbulence has been studied for more than one hundred years after Osborne Reynolds’ experiments, it is still a big challenge in fluid mechanics due to its strong nonlinear behavior (Piomelli, 1999). Numerical simulations of turbulent motions fall into three major categories, i.e., Direct Numerical Simulation (DNS), Reynolds-Averaged Navier-Stokes Equation (RANS), and Large-Eddy Simulation (LES) (Sagaut, 2001).

DNS is the most straightforward method. In DNS, the governing equations are discretized with enough resolution and solved numerically; it resolves the smallest scales of motion and does not need any modeling, thus giving accurate solution. This makes it possible to compute and visualize any quantity of interest, and it has been a very useful research tool to obtain insight on detailed kinematics and dynamics of turbulent flows (Moin and Mahesh, 1998). DNS has been applied to supercritical mixing layers (Miller et al., 2001, Okong’o et al., 2002) and combustion studies (Vervisch and Poinsot, 1998) to reveal physical and/or chemical processes that would not have been possible with other approaches. DNS also provides data for turbulent SGS model and combustion model validation. However, to resolve all scales of motion in three coordinate directions, the grid number is proportional to $Re_L^{3/4}$, and thus DNS is limited to small Reynolds number flows (typically, $Re_L=O(10^4)$) (Piomelli and Balaras, 2002), and is infeasible for industrial interested applications.

In contrast to DNS, RANS has been the most commonly applied method to solve turbulent flow problems, especially in engineering applications. In RANS, only statistical quantities, i.e., the ensemble or time-averaged mean quantities are predicted. The effect of all the scales of motion is modeled (except for Unsteady-RANS, in which coherent motions are partially resolved) (Sagaut, 2001). Even though RANS is inherently less expensive and has moderate
success in industrial applications, it suffers from one principal shortcoming that the model must account for a very wide range of scales. Based on Kolmogorov's hypothesis, at sufficiently high Reynolds number, the small-scale motions are statistically isotropic and tend to be universal to model (Pope, 2000). However, on the other hand, the large-scale motions are strongly dependent on the boundary conditions, (i.e. the device geometry), thus it is impossible to achieve a universal model that can cover all turbulent flows (Piomelli, 1999).

As a trade-off between the accuracy and computational cost of RANS and DNS, an intermediate technique known as Large-Eddy Simulation (LES) has been developed, which features higher accuracy than RANS, while requiring much less computational effort compared to DNS. In LES, energy-containing large-scale motions are fully resolved with the grid and filter employed, while the effect of the smallest-scale motions of turbulence is modeled (Piomelli, 1999). Since the small-scale motions are more isotropic and universal, they can be modeled in universal manner with much less adjustments in model coefficients, as compared with the turbulent models for RANS simulations. The demanding computational cost to resolve all scales of motions explicitly and accurately in DNS is avoided.

LES seems promising to solve turbulent flow problems. However difficulties arise near the wall. In the near-wall region, a series of important events occur. The production and dissipation of turbulent kinetic energy achieve peak values at less than 30 wall units (Pope, 2000). The energy-containing scales depend on Reynolds number, but the growth of the small scales is prohibited by the presence of the wall, making the exchange mechanisms between large and small scales different from unconstrained flows. To capture the important energy producing events in the near-wall layer, an extremely fine grid has to be used, especially for high Reynolds number flows. Based on Chapman’s estimate (1979), the boundary layer is divided into outer and inner layers; the number of grid points scales with \( \text{Re}^{0.4} \) for the outer layer; however, it scales with \( \text{Re}^{1.8} \)
for the inner layer. So for a boundary layer flow with a Reynolds number of $10^6$, 99% of the grid points are required to resolve the inner layer, whose thickness is only about 10% of the boundary layer. As pointed out by Piomelli (1999), the wall layer modeling is probably the most urgent challenge when it is intended to apply LES to industrially interested flows. Wall-modeled LES (WMLES) have been studied by many researchers. Cabot (1995) and Balaras et. al. (1996) used two-layer boundary layer equations to model the near-wall region in LES of wall bounded shear flows. Spalart (2009) proposed a Detached-Eddy Simulation (DES). It used Spalart-Allmaras turbulence model or k-omega SST model for the Reynolds stress and the sub-grid stress modeling. DES has been applied to massively separated flows and seems promising for wall bounded flows. More discussion on wall layer models can be found in review papers by Piomelli (1999) and Spalart (2009).

In the current work, the LES technique is used to achieve turbulent closure. The small-scale motions are not resolved in LES; however, based on the energy cascade analysis, it is in this range of scales where viscous dissipations drain kinetic energy to internal energy. This effect of turbulent motions has to be modeled with appropriate SGS models. The dissipation provided by SGS models is the only way for turbulent kinetic energy to leave the resolved flow motions. Commonly used SGS models include the Smagorinsky eddy viscosity model, and dynamic eddy viscosity model.

The Smagorinsky SGS model (Smagorinsky, 1963) has been the most widely used model because of its simplicity. With sufficiently fine grid, this model is fairly accurate. However, a constant model coefficient has to be given as an input to account for all sub-grid scale motions, which are actually dependent on the grid employed and the local flow conditions. For example, in laminar shear flow or viscous sub-layers close to the solid wall, in which the SGS stresses are zero, the Smagorinsky model with positive constants gives rise to non-zero residual stresses
In addition, the energy backscatter, representing the energy flux from small to large scales, is totally neglected with a constant model coefficient. Many *ad hoc* modifications are employed to avoid these drawbacks. For instance, van Driest damping (Van Driest, 1956) is introduced to correct the model behavior in the near-wall region and an intermittency function (Piomelli, 1999) is used to eliminate the non-zero residual stresses in the laminar flow region.

To improve the aforementioned algebraic Smagorinsky model, a dynamic eddy-viscosity model was proposed by Germano et al. (1991). Instead of using a constant input value, the Smagorinsky coefficient is dynamically determined from the resolved flow motions. This model assumes that the model coefficients are the same for the unresolved SGS motions and the sub-test-filter motions. Here a test filter, which is larger than the LES filter, is used to filter the resolved flow velocity. The dynamically calculated coefficient is not positive definite. When the model coefficient is negative, backscatter of energy is allowed.

In the next section, the filtered governing equations as well as the turbulence SGS models, i.e. the static and dynamic Smagorinsky models, are presented and discussed. The filtered governing equations, along with the thermodynamic property evaluation method and turbulence closure models, are ready to be solved with numerical method to study high-pressure mixing and combustion.

### 2.4.1 Filtering

In Large-Eddy Simulation, large-scale motions, which carry most of the kinetic energy are fully resolved, while small-scale motions, which are more universal and easier to model, are modeled with SGS models. To separate the large-scale motions from the small-scale ones, a low-
pass filtering operation is performed explicitly or implicitly. A filtered (or resolved) variable is defined as:

\[
\tilde{f}(x) = \int_{-\infty}^{\infty} f(x) G_f(x - x') dx',
\]

(2.93)

where \( G \) is the filter function and \( \int_{-\infty}^{\infty} G(x) dx = 1 \). The filter function determines the size and structure of the small scales. Leonard (1974) indicated that if \( G \) is only a function of \( x - x' \), the differentiation and filtering operations could commute with each other. Although for stretched grids, the commutation between filtering and differentiation is not strictly valid (Ghosal and Moin, 1995; Vanderven, 1995). The commutation error is usually neglected for moderately stretched grids, and can be accounted for by the SGS models (Le Ribault et al., 1999, Moin, 1997). The modeling error is found to be generally smaller than the discretization error (Le Ribault et al., 1999). One of the most commonly used filter functions, the box filter, which is also used in the current study, is defined as:

\[
\bar{f}(x) = \frac{1}{\Delta V} \int_{\Delta V} f(x) dx.
\]

(2.94)

With the box filter, any filtered quantity is simply its average in the control volume. A detailed description of properties of various filters can be found in standard textbooks (Pope, 2000).

### 2.4.2 Filtered Governing Equations

Based on the Favre-averaging (Favre, 1969), any instantaneous variable \( f \) can be expressed as the sum of a Favre-averaged filtered scale \( \tilde{f} \) and a sub-filter scale \( f^* \)
\( f = \tilde{f} + f^\prime. \)  \hspace{1cm} (2.95)

where

\[ \tilde{f} = \frac{\partial \tilde{f}}{\partial \tilde{\rho}}. \]  \hspace{1cm} (2.96)

Since \( \tilde{f}' \neq 0 \) and \( \tilde{f}^\prime \neq 0 \), the filter operation in LES is different from the conventional Reynolds average in time domain. The properties of Favre-averaging filter are shown in Appendix A.

The filtered Favre-averaged mass, momentum, energy, mixture fraction, and progress variable transport equations in conservative form can be written as

\[ \frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_i}{\partial x_i} = 0, \quad i = 1, 2, 3, \]  \hspace{1cm} (2.97)

\[ \frac{\partial \tilde{\rho} \tilde{u}_i}{\partial t} + \frac{\partial (\tilde{\rho} \tilde{u}_i \tilde{u}_j)}{\partial x_j} = -\frac{\partial \tilde{\rho}}{\partial x_i} + \frac{\partial (\tilde{\tau}_i - \tau_{i}^{SGS})}{\partial x_j}, \quad i = 1, 2, 3, \]  \hspace{1cm} (2.98)

\[ \frac{\partial \tilde{\rho} \tilde{E}}{\partial t} + \frac{\partial \left[ (\tilde{\rho} \tilde{E} + \tilde{\rho}) \tilde{u}_i \right]}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \tilde{q}_i + \tilde{u}_i \tilde{\tau}_j - Q_{i}^{SGS} - H_{i}^{SGS} + \sigma_{i}^{SGS} \right), \]  \hspace{1cm} (2.99)

\[ \frac{\partial \tilde{\rho} \tilde{f}}{\partial t} + \frac{\partial (\tilde{\rho} \tilde{u}_j \tilde{f})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \tilde{\rho} D \frac{\partial \tilde{f}}{\partial x_j} - \Phi_{j}^{SGS} \right), \]  \hspace{1cm} (2.100)

\[ \frac{\partial \tilde{\rho} \tilde{C}}{\partial t} + \frac{\partial (\tilde{\rho} \tilde{u}_j \tilde{C})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \tilde{\rho} D \frac{\partial \tilde{C}}{\partial x_j} - \Psi_{j}^{SGS} \right) + \tilde{\omega}_c. \]  \hspace{1cm} (2.101)

The SGS terms are defined as:
The SGS stress term $\tau_{ij}^{SGS}$, SGS energy flux term $H_i^{SGS}$, and SGS scalar flux terms $\Phi_i^{SGS}$, and $\Psi_i^{SGS}$, results from filtering the corresponding convective terms. The SGS viscous work term, $\sigma_{ij}^{SGS}$, comes from correlations of the velocity field with the viscous stress tensor. The resolved-scale progress variable production rate, $\overline{\omega_r}$, is also unclosed. The modeling of these SGS terms is discussed in detail in the following subsections.

In addition to the conservation equations, the equation of state must also be filtered. Filtering the equation of state gives us

$$
\tilde{p} = R_a \tilde{Z} \tilde{\rho} \tilde{T} + R_a (\tilde{Z} \tilde{\rho} \tilde{T}'' + \tilde{\rho} \tilde{Z}'' \tilde{T}'' + \tilde{T}'' \tilde{\rho}'') \, ,
$$

where $Z$ is the compressibility factor. For ideal gas without heat release, the correlations in the filtered equation of state can be neglected (Calhoon and Menon, 1996). This may not be true for high-pressure, real-fluid mixtures. However, due to the difficulty and uncertainty in modeling those correlations, they are neglected without any justification.
The filtered total energy $\tilde{E}$ can be approximated as

$$\tilde{E} = \tilde{h} - \frac{\tilde{p}}{\rho} + \frac{\tilde{u}_k^2}{2} + k^{\text{str}} = \tilde{\psi} + \int \left[ \frac{1}{\rho} \frac{T}{\rho^2} \left( \frac{\partial \tilde{p}}{\partial T} \right)_p \right] dp - \frac{\tilde{p}}{\rho} + \frac{\tilde{u}_k^2}{2} + k^{\text{str}}, \quad (2.109)$$

where $\tilde{\psi} = \sum_{k=1}^{N} Y_k h_k^0$ and $k^{\text{str}} = \frac{k^{\text{str}}}{2\tilde{\rho}} = \frac{1}{2} \left( \frac{\rho \tilde{u}_k \tilde{u}_k}{\tilde{\rho}} - \tilde{u}_k^2 \right)$.

### 2.4.3 Subgrid-Scale Models

In LES, as the sub-grid scales motions are not resolved, the energy that is transferred from integral length scales through energy cascade to the unresolved sub-grid motions, has to be dissipated with an appropriate SGS model, such that the energy is transferred to internal energy at correct dissipation rate. Most of the SGS models are based on an eddy-viscosity type model. In these models, the SGS stress $\tau_{ij}^{\text{str}}$ is related to the resolved strain-rate tensor $\tilde{\psi}_{ij}$ as follows

$$\tau_{ij}^{\text{str}} = -\frac{2}{3} \tau_{ik}^{\text{str}} = -2\nu_t \tilde{\psi}_{ij}, \quad (2.110)$$

where $\nu_t$ is the eddy viscosity and $\tilde{\psi}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right)$. In the following section, both the algebraic and dynamic Smagorinsky models are presented.

#### 2.4.3.1 Algebraic Smagorinsky Model

In this model, the eddy viscosity $\nu_t$ is obtained algebraically to avoid solving additional equations. To simplify the problem the equilibrium hypothesis is generally used, which assumes that small-scale motions, which have shorter time scales than the large, energy-carrying eddies, can adjust more rapidly to perturbations and recover equilibrium nearly instantaneously. Under
this assumption, a balance exists between the SGS kinetic energy production term and the viscous dissipation term: \(-\tau_{ij} \tilde{S}_{ij} = \varepsilon_v\). The Smagorinsky model based on the equilibrium hypothesis is given by:

\[
\nu_t = \left( C_s \bar{\Delta} \right)^2 |\tilde{S}| ,
\]

\[
|\tilde{S}| = \sqrt{2 \tilde{S}_{ij} \tilde{S}_{ij}} ,
\]

\[
\bar{\Delta} = \frac{\sqrt{\Delta_1 \Delta_2 \Delta_3}}{\bar{\Delta}},
\]

where \(\bar{\Delta}\) is the filter width, which is proportional to the grid size. The coefficient \(C_s\) can be specified from a priori test on decaying isotropic turbulence (Lily, 1967) with \(C_s = 0.16\). Erlebacher et al. (1992) extended the above model to include flow compressibility effects

\[
\tau_{ij}^{sgs} = -2\nu_t \bar{\rho} \left( \tilde{S}_{ij} - \frac{\tilde{S}_{ik} \delta_{kj}}{3} \right) + \frac{2}{3} \bar{\rho} k^{sgs} \delta_{ij} ,
\]

where \(\nu_t\) is the eddy viscosity.

\[
\nu_t = C_R (\Delta D)^2 |\tilde{S}| ,
\]

\[
k^{sgs} = C_I (\Delta D)^2 \tilde{S}_{ij} \tilde{S}_{ij}
\]

where the dimensionless quantities \(C_R\) and \(C_I\) represent the compressible Smagorinsky constants.

The Van-Driest damping function \((D)\) is used to take into account the inhomogeneities near the wall (Moin and Kim, 1982), and is expressed as
\[ D = 1 - \exp\left(-\left(\frac{y^+}{25}\right)^2\right), \]  

(2.117)

where \( y^+ = yu_\tau/v \) and \( u_\tau \) is friction velocity.

The subgrid energy flux term \( H_j^{sgs} \) is modeled based on the gradient transport assumption

\[ H_j^{sgs} = -\bar{\rho} \frac{v_j}{Pr_t} \left( \frac{\partial \tilde{h}}{\partial x_j} + \tilde{u}_i \frac{\partial \tilde{u}_j}{\partial x_j} + \frac{1}{2} \frac{\partial k^{sgs}}{\partial x_j} \right), \]  

(2.118)

where \( Pr_t \) represents the turbulent Prandtl number, and a standard value 1.0 is used. The SGS viscous work term, \( \sigma_j^{sgs} \), is neglected due to its small contribution to the total energy equation (Martin et al., 1999, Piomelli, 1999).

The convective mixture fraction flux term is usually approximated as

\[ \Phi_j^{mfv} = -\bar{\rho} \frac{v_j}{Sc_i} \frac{\partial f}{\partial x_j}, \]  

(2.119)

where \( Sc_i \) is the turbulent Schmidt number. However, the use of the gradient transport assumption for reactive species is questionable. The SGS species diffusive fluxes term, \( \Theta_k^{sgs} \), is usually neglected (Calhoon and Menon, 1996).

The algebraic Smagorinsky model described above is the most widely used model in LES. However, as pointed out by Germano et al. (1991), it has several limitations. First, the optimal model constant must be changed for a different class of flows. The model does not have the correct limiting behavior near the wall (Juneja and Brasseur, 1999). The SGS stress does not vanish in laminar flow and the model is found to be very dissipative in the laminar/transition region. The model does not account for the backscatter of energy from small to large scale, which has been shown to be of importance in the transition region.
In the current study, to ensure the aforementioned limitations have minimal effects on the current numerical simulations, the dynamic Smagorinsky model, as presented in the following section, is also used as a comparison basis.

### 2.4.3.2 Dynamic Smagorinsky Model

The dynamic model introduced by Germano et al. (1991) improves some of the aforementioned deficiencies in algebraic models. The dynamic model uses the assumption of scale invariance by applying the coefficient measured from the resolved scales to the SGS range. It calculates the model coefficients dynamically from the information already contained in the resolved velocity field during the simulation (rather than treating it as an adjustable parameter as in the standard Smagorinsky model). Apply the test-filter \( \tilde{G} \), with characteristic \( \tilde{\Lambda} > \Lambda \) (typically, \( \tilde{\Lambda} = 2\Lambda \)), to the equations of motion, one obtains filtered governing equations similar to Eqs. 2.97-2.101, but replacing \( \bar{f} = \frac{\rho f}{\overline{f}} \) with \( \bar{f} = \frac{\overline{f}}{\rho} \), yields the sub-testscale stress \( T_{ij} \), defined as:

\[
T_{ij} = \overline{\rho u_i u_j} - \overline{\rho \tilde{u}_i \tilde{u}_j} .
\]  
(2.120)

Formally, the dynamical procedure is based on the Germano identity (Germano, 1992)

\[
L_{ij} = T_{ij} - \tau_{s}^{SGS} = \overline{\rho \tilde{u}_i \tilde{u}_j} - \overline{\rho u_i u_j} .
\]  
(2.121)

The following expressions can be derived for the dynamic evaluation of \( C_R \) and \( C_I \) using the least square minimization approach of Lilly (1992) for the momentum SGS stress tensor.
The forms of $M_{ij}, \beta$ and $\alpha$ are given as follows

$$C_R = \frac{< L^{ij} M^{ij} >}{< M^{kl} M_{kl} >} - \frac{1}{3} \frac{< L^{mm} M_{mm} >}{< M^{kl} M_{kl} >} , \quad (2.122)$$

$$C_I = \frac{< L_{kk} >}{< \beta - \langle \alpha \rangle >} , \quad (2.123)$$

The forms of $M_{ij}, \beta$ and $\alpha$ are given as follows

$$M_{ij} = \beta_{ij} - \langle \alpha_{ij} \rangle , \quad (2.124)$$

$$\beta_{ij} = -2\hat{\Delta}^2 \langle \bar{\rho} \rangle |\bar{S}| (\bar{S}_{ij} - \frac{\delta_{ij}}{3} \bar{S}_{kk}) , \quad (2.125)$$

$$\alpha_{ij} = -2\hat{\Delta}^2 \bar{\rho} |\bar{S}| (\bar{S}_{ij} - \frac{\delta_{ij}}{3} \bar{S}_{kk}) , \quad (2.126)$$

$$\alpha = 2\bar{\rho} \hat{\Delta}^2 |\bar{S}|^2 , \quad (2.127)$$

$$\beta = 2 \langle \bar{\rho} \rangle \hat{\Delta}^2 |\bar{S}|^2 . \quad (2.128)$$

The same idea can be applied to model SGS turbulent stress so as to dynamically calculate the turbulent Prandtl number and Schmidt number in Eq. 2.118 and Eq. 2.119.

2.5 Turbulence Combustion Models

In large-eddy simulations, although the energy-carrying eddy motions are resolved with sufficient grid resolution, motions of scales smaller than the grid resolution, such as the Kolmogorov scale, are not resolved in LES, which plays a crucial role in mixing the reactants at
molecular levels. On the other hand, chemical reactions occur only at the molecular level. The chemical reaction rate is a very strong nonlinear function of local species concentration and temperature at the molecular level, which are highly dependent on the turbulent mixing. In return, chemical reactions release heat and alter species concentration and temperature gradients of the smallest turbulent eddies, which in turn change the turbulent mixing process. Chemical reaction occurring at different time scales may interact with turbulence eddies of different length/time scales, a situation which further complicates the picture. The interaction between these two processes occurring at length scales from the smallest turbulent scales to much larger inertial sub-range scales of motions, which, unfortunately, cannot be totally resolved in LES studies. The physical processes associated with these interactions are modeled with turbulent combustion models. This outlines the importance of the establishment of an accurate turbulent combustion model that can be used with enough accuracy in supercritical environment.

There are several combustion models for the LES of non-premixed turbulent combustion. The most straightforward way is to evaluate the filtered reaction rate from the filtered quantities, without consideration of the sub-grid interactions of turbulence and chemistry. This method has been used by several researchers due to the simplicity (Oefelein and Yang, 1998, Masquelet and Menon, 2010).

Conditioned Momentum Closure (CMC) was developed by Klimenko (1990) and Bilger (1993) independently for non-premixed turbulent combustion. Variables of interest are conditioned with mixture fraction before the Favre average is taken to obtain conditional moment equations. CMC has been used in homogenous and boundary layer flows. With those applications, CMC can be related to flamelet equations (Peters, 2000). However, this method solves conditional species equations for all species; thus the computational cost increases with the
number of species, which may become prohibitively costly when detailed chemistry kinetics is used.

The Linear-Eddy Model (LEM) was developed by Kerstein (1992b, a) and has been used by the author, Menon and colleagues (McMurtry et al., 1993, Sankaran and Menon, 2005). The one-dimensional laminar reactive scalar field is combined with stochastically independent rearrangement events to mimic turbulence/chemistry interactions. However, this model suffers from prohibitive computational costs in applications.

The Monte Carlo method for PDF transport equations has been developed by Pope and extensively tested in RANS and LES (Peters, 2000). However, the formulation is very complicated, and the computation cost is considerably high when even a moderate number of species is involved.

Recently dynamically thickened flame have been developed by Légier et al. (2000) for both premixed- and non-premixed combustion. This model can account for unsteady combustion such as extinction, re-ignition etc. However, it has similar difficulties when detailed chemistry is used.

Flamelet concept models have been studied extensively by Peters, Pitsch et al. (Peters, 2000). The steady flamelet model and the extended flamelet/progress-variable model fall in this category, and have been chosen for the current study to account for turbulence/chemistry interactions, and to identify the flame stabilization mechanism for supercritical combustion.

The flame stabilization mechanism and subsequent development of the flame plays an important role in dictating the combustion stability and are very important in injector design. The flame can either be anchored at or lifted-off from the oxidizer post. If the flame is anchoring at the LOX post in liquid rocket engines, it is important to ensure the heat compatibility of the injector head. If the flame is lifted-off from the LOX post, then the flame is susceptible to the
flow fluctuations. Consequently, it is crucial to identify the limit operating conditions and design parameters to assure the combustion stability in all possible operating conditions. However, unfortunately, even the flame stabilization mechanism at atmospheric conditions is not well understood (Peters, 2000). The stabilization of lifted flames can be explained with different mechanisms: the quenching of diffusion flames and premixed flame propagation (triple or edge flame) are possible mechanisms considered in the current study. Other mechanisms are not discussed here (for example, flame stabilization by large-scale turbulent structures). To identify the flame stabilization mechanism requires that the turbulent combustion model be able to account for those two mechanisms and turbulence/chemistry interaction in an appropriate manner. The flamelet model and the flamelet/progress-variable model are capable of resolving these two flame stabilization mechanisms, respectively. Thus, these two models have been used in the present work.

2.5.1 Laminar Flamelet Model

The basic assumption of the laminar flamelet model is that the chemical time and length scales are shorter than that of the Kolmogorov scales of turbulent flows. Consequently, a turbulent flame can be envisioned as a synthesis of thin reaction zones (i.e., flamelets) embedded in an otherwise inert turbulent flow field, and the inner structure of the flame can be handled separately from turbulent flow simulations. Instead of directly treating the reactive scalar (i.e., species concentration), the focus is placed on the identification of the flame surface in the flow-field, which can be obtained by solving the conservation equation of the mixture fraction together with the mass, momentum, and energy equations.
The flame thickness, however, is typically smaller than the grid size employed in LES and is not actually resolved. Therefore, the filtered species mass fraction of the \(i\)th species, \(\tilde{Y}_i(x,t)\), in each computational cell should be evaluated by convoluting the state relationships, \(Y_i(f,\chi_a)\), with the SGS Filtered Density Function (\(FDF\)) of mixture fraction, \(\tilde{P}(f)\), and the SGS \(FDF\) of scalar dissipation rate, \(\tilde{P}(\chi_a)\), as shown below:

\[
\tilde{Y}_i(x,t) = \int_0^1 \int_0^1 Y_i(f,\chi_a) \tilde{P}(\chi_a) \tilde{P}(f) d\chi_a df.
\] (2.129)

It should be noted that a statistical independence is intrinsically assumed in Eq. 2.129 between the SGS variations of mixture fraction and scalar dissipation. The unresolved SGS fluctuation of the mixture fraction is commonly represented by a presumed \(\beta\)-shaped Probability Density Function (PDF) parameterized by the filtered mixture fraction and its SGS variance, which takes the following form,

\[
P(f; \tilde{f}, f^{\ast 2}) = \frac{f^{\alpha - 1}(1-f)^{\beta - 1}}{\Gamma(\alpha)\Gamma(\beta)} \Gamma(\alpha + \beta),
\] (2.130)

where \(\Gamma\) is the \(\gamma\)-function. The parameters \(\alpha\) and \(\beta\) are defined as

\[
\alpha = \tilde{f} \left( \frac{\tilde{f}(1-\tilde{f})}{f^{\ast 2}} - 1 \right),
\] (2.131)

\[
\beta = (1 - \tilde{f}) \left( \frac{\tilde{f}(1-\tilde{f})}{f^{\ast 2}} - 1 \right).
\] (2.132)

The SGS variance of mixture fraction, \(f^{\ast 2}\), is modeled based on the scale similarity assumption (DesJardin and Frankel, 1998),
where $K_b$ is a model constant chosen as 3. It has been validated by many researchers that the $\beta$-function PDF provides an excellent estimation of the SGS mixture fraction distribution for non-premixed reacting turbulent flows (Cook and Riley, 1998). For simplicity, in the present work, the SGS FDF of the scalar dissipation rate, $P(\chi_o)$, which is typically assumed to be a lognormal, is considered as a Dirac peak at the filtered scalar dissipation rate. Further investigation is required to validate this assumption. The filtered rate of scalar dissipation, $\tilde{\chi}$, is modeled based on the eddy viscosity approach as suggested by Girimaji and Zhou (1996)

\[
\tilde{\chi} = 2\left(\frac{\nu}{Sc} + \frac{\nu_t}{Sc_f}\right)\left(\frac{\partial f}{\partial \chi} \cdot \frac{\partial f}{\partial \chi}\right).
\]  

(2.134)

The thermo-chemistry state relation is established through a steady-state flamelet approach. Taking advantage of the fact that the flamelet library only needs to be calculated once for every specified case, chemistry kinetics with any number of species and reaction steps can be used for the establishment of the flamelet library. The flamelet library should cover a broad range of strain rates, from near chemistry equilibrium to near-extinction limit. For all the calculations, the pressure is fixed at the same as the application; and the inlet temperatures of the fuel and oxidizer take the corresponding inlet temperature of the application cases. Consistent with the flamelet assumption, the corresponding scalar dissipation rate, $\chi$, for each solution is evaluated as a function of filtered mixture fraction. The solutions are then integrated based on Eq. 2.129 and tabulated as functions of $\tilde{\chi}$, $\tilde{f}$, and $f''$. The calculated filtered mixture fraction, mixture fraction variance, and the scalar dissipation rate from LES simulation are used to determine the appropriate entry in the table.
2.5.1.1 Steady vs. Unsteady Flamelets

Even if it has been justified that the flamelets are embedded in smallest turbulent eddies and retain laminar flame structures, and thus chemistry could be decoupled from local mixing such that chemical species can be looked up from a pre-evaluated table, another potential concern is that the flamelets may not be steady. For simplicity, a steady flamelet has been assumed in the current study. The flamelet library is generated from steady-state laminar counter-flow diffusion flames. Thus, the species profile does not include the history effect of the chemical reactions, i.e. the time taken to achieve the steady state flame profile. In a real turbulent flame, slow chemistry reactions, such as CO oxidation, take a much longer time compared to other reactions. Following Peters’ argument, if the scalar dissipation rate is changing slowly enough so that the change of chemical reactions can follow the pace of the local flow variations, the steady flamelet is valid (Peters, 2000). Otherwise, the unsteady effect may become important. Based on Pitsch's (2000) estimation, within the range of 30 nozzle diameter from the fuel nozzle exit, it is valid to assume a steady flamelet. Extreme caution must be exercised to use steady flamelet data further downstream, where the scalar dissipation rate becomes small and the chemistry may not be fast enough to follow the flow variations. In the current study, the focus is on the near field of the splitter plate and the unsteady effect is not expected to be significant.

2.5.1.2 Differential Diffusion Effect

In formulating the mixture fraction equation, unit Lewis number is assumed to achieve the current form of the mixture fraction equation (Peters, 2000). The effect of differential diffusion has been tested (Pitsch and Peters, 1998). Based on their discussion, the existence of a laminar region in the near field of the jet exit causes the differential diffusion effect. The
The differential diffusion effect is only important within a 10-diameter distance from the jet exit. However, the temperature and the species concentration distributions are influenced by the differential diffusion effect farther downstream from the nozzle exit. This is not assessed in the current study for several reasons. First, hydrocarbon fuels feature a Lewis number closer to unity, compared to hydrogen, which will make the differential diffusion less important than in hydrogen flames. Second, the differential diffusion effect itself is still an open research issue. There are model and numerical uncertainties associated with the evaluation of this effect; a simple inclusion of this model does not guarantee a better prediction of non-premixed turbulent combustion. For simplicity and ease of discussion of the model validity and its performance in supercritical applications, this effect is not addressed in the current study. Finally, in the process of building the flamelet library, the differential diffusion diffusivity is considered within the model used herein (Ribert et al., 2007). However, in the LES study, the unit Lewis number is assumed.

### 2.5.1.3 Evaluation of Scalar Dissipation

As pointed out by Poinset and Veynante (2005), the effect of external mixing (turbulent flow) is lumped into the scalar dissipation rate, while chemistry is decoupled from the flow and can be retrieved from the lookup table. Consequently, the scalar dissipation rate accounts for the effect of turbulent mixing as an external parameter on the laminar flamelet structures. The procedure to estimate this variable directly affects the chemical species distribution, the flame structure, and the combustion dynamics. Filtered quantities are used to look up the flamelet library. Although the fluctuation of the scalar dissipation rate has been taken into account by the PDF convolution with the laminar scalar dissipation rate, it may not represent the events that can occur in turbulent flames because it is the instantaneous, un-filtered scalar dissipation that acts on the laminar flamelets. Although the filtered scalar dissipation is not large enough to quench the
flame, independent individual events with large instantaneous values may quench the flamelets. However, it has been observed in experiments that flamelets can survive very large instantaneous scalar dissipation values without quenching. On the other hand, the quenching scalar dissipation rates in the present work are at least one order of magnitude larger than any resolved scalar dissipation rate at any time and any location. This means that the local strain (turbulence) is not strong enough to stretch the flame to extinction. Thus, the model predicts strongly burning flames everywhere in the flow field, resulting in an anchored flame attached to the splitter rim. It is the mixture-fraction conditioned instantaneous scalar dissipation rate that interacts with flamelets and promotes extinction and mixing; thus the time-averaged scalar dissipation rate is not evaluated.

Instead of assuming a pre-assumed shape of scalar dissipation as proposed by Peters, scalar dissipation as a function of the mixture fraction is calculated from the counter-flow laminar flamelets, which are generated in physical space using a one-dimensional code (Ribert et al., 2008). This is different from Pitsch's methods, which are conducted in the mixture fraction space, and the dependence of scalar dissipation on the mixture fraction is modeled by an exponential function of the mixture fraction.

2.5.1.4 Evaluation of the Variance of the Mixture Fraction

In evaluating the filtered variance of the mixture fraction, local equilibrium has been assumed instead of using a transport equation such as in RANS studies. The filtered variance of the mixture fraction is evaluated from filtering processes proposed by DesJardin and Frankel (1998). The variance is large where the gradient of the mixture fraction is large, its contribution to the species profile broadens the sampling space of species and thus results in less burned flames compared to the laminar case. This effect is important in the near field of the splitter
plate, where the gradient of the mixture fraction is large but decreases in downstream, where continual mixing has made the gradient of mixture fraction small.

2.5.2 Flamlet/Progress-Variable Approach

Although the laminar flamelet method is easy to implement and fairly inexpensive, it has several drawbacks. Firstly, the mixture fraction, which can be interpreted as a normalized equivalence ratio (Peters, 2000), essentially does not carry any information about the chemical reaction state. The flamelet method uses the scalar dissipation rate as an additional parameter to account for the flame stretching and quenching effect. However, the scalar dissipation rate does not provide a unique mapping from the mixture fraction to the corresponding chemical state. A pure mixing of fuel and oxidizer cannot be accounted for in the flamelet method if the local scalar dissipation is smaller than the quenching limit. This drawback is due to the lack of information regarding the local chemical state in the flow field. The Flamelet/Progress-Variable (FPV) method is used to overcome the limitations of the flamelet method by incorporating an additional transport equation for tracking a scalar in the form of a progress variable. This new method has been developed to account for extinction, ignition, and unsteady mixing effect (Pierce and Moin, 2004). In the FPV approach, similar to the flamelet model, to account for the sub-grid fluctuations in the mixture fraction and progress variable, filtered combustion variables are obtained by convoluting the state relationships, \( Y_i(f, C) \), with the joint SGS filtered probability density function of the mixture fraction and progress variable, \( \tilde{P}(f, C) \), as follows,

\[
\bar{Y}_i(x, t) = \int_0^1 \int_0^1 Y_i(f, C) \tilde{P}(f, C) dCdP. \tag{2.135}
\]
Following Pierce and Moin (2004), we assume a Delta function distribution for the PDF of the progress variable. More advanced modeling of the joint PDF will be addressed in the subsequent studies. With this assumption, the filtered mass fraction becomes

$$\tilde{Y}(x,t) = \int_0^1 \int_0^1 Y(f,C) \tilde{P}(f) \delta(C - \tilde{C}) dC df,$$  \hspace{1cm} (2.136)

where $\tilde{C} = \int_0^1 C(f, \chi_0) P(f) df$, and $\chi_0$ is a flame parameter. The filtered reaction rate of the progress variable is obtained in a similar manner.

$$\tilde{\omega}_c = \int_0^1 \int_0^1 \omega_c(f,C) \tilde{P}(f) \delta(C - \tilde{C}) dC df.$$  \hspace{1cm} (2.137)

The implementation of the FPV approach is similar to that of the flamelet method. The major difference is two-fold: (1) the parameterization of the flamelet library is based on the progress variable instead of the scalar dissipation; (2) the laminar counter-flow flame solutions which are used to build the library cover not only the stable burning and extinction branch of the S-shaped curve but also the unstable branch to account for the unsteady effects. Once the flamelet library is built, the filtered chemical variables can be easily looked up as a function of filtered mixture fraction, its variance, and the filtered progress variable.
Chapter 3

Numerical Methodology

Numerical studies of the physicochemical processes described in Chapter 1 bear a series of numerical difficulties. This chapter outlines the intrinsic challenges and the numerical methodologies used to handle these problems. The numerical scheme, with a unified treatment of real-fluid thermodynamic properties, treats the three dimensional governing equations in a general curvilinear coordinate, using finite volume approach, along with central differencing in space and backward differencing in physical time space. To obtain time accurate solutions, preconditioned dual-time-stepping technique, with a Runge-Kutta integration in pseudo time, is used to resolve the numerical difficulties associated with low-Mach number flows. The resulting numerical scheme is TVD-assured, fourth order accurate in space and second order accurate in time. MPI-parallelization is used to expedite the calculation and reduce the turnaround time.

3.1 Preconditioning Scheme for Real-Fluid Mixtures

The three-dimensional, unsteady, Favre-filtered governing equations listed in Chapter 2 can be re-written in vector form:
\[
\frac{\partial Q}{\partial t} + \frac{\partial (E - E_\gamma)}{\partial x} + \frac{\partial (F - F_\gamma)}{\partial y} + \frac{\partial (G - G_\gamma)}{\partial z} = H,
\]

where the vectors \( \mathbf{Q}, \mathbf{E}, \mathbf{F}, \mathbf{G}, \mathbf{E}_\gamma, \mathbf{F}_\gamma, \mathbf{G}_\gamma \) and \( H \) are defined as:

\[
\mathbf{Q} = \left( \rho, \rho \bar{u}, \rho \bar{v}, \rho \bar{w}, \rho \bar{E}, \rho \bar{f} \right)^T, \tag{3.2}
\]

\[
\mathbf{E} = \left( \rho \bar{u}, \rho \bar{u}^2 + \bar{p}, \rho \bar{u} \bar{v}, \rho \bar{u} \bar{w}, \left( \rho \bar{E} + \bar{p} \right) \bar{u}, \rho \bar{u} \bar{f} \right)^T, \tag{3.3}
\]

\[
\mathbf{F} = \left( \rho \bar{v}, \rho \bar{u} \bar{v}, \rho \bar{v}^2 + \bar{p}, \rho \bar{v} \bar{w}, \left( \rho \bar{E} + \bar{p} \right) \bar{v}, \rho \bar{v} \bar{f} \right)^T, \tag{3.4}
\]

\[
\mathbf{G} = \left( \rho \bar{w}, \rho \bar{u} \bar{w}, \rho \bar{w}^2 + \bar{p}, \left( \rho \bar{E} + \bar{p} \right) \bar{w}, \rho \bar{w} \bar{f} \right)^T, \tag{3.5}
\]

\[
\mathbf{E}_\gamma = \left\{ \begin{array}{l}
0, \bar{f}_x - \tau_{xx}^{\text{sgs}}, \bar{f}_y - \tau_{xy}^{\text{sgs}}, \bar{f}_z - \tau_{xz}^{\text{sgs}}, \bar{u} \bar{f}_x + \bar{v} \bar{f}_y + \bar{w} \bar{f}_z + \bar{q}_x - H_x^{\text{sgs}} + \sigma_x^{\text{sgs}},
\end{array} \right\}^T \nonumber
\]

\[
\begin{array}{l}
\bar{p} \bar{D} \bar{f}_x + \bar{p} \frac{V_x}{S_c} \bar{f}_x,
\end{array}
\]

\[
\mathbf{F}_\gamma = \left\{ \begin{array}{l}
0, \bar{f}_y - \tau_{xy}^{\text{sgs}}, \bar{f}_y - \tau_{yy}^{\text{sgs}}, \bar{f}_y - \tau_{yz}^{\text{sgs}}, \bar{u} \bar{f}_x + \bar{v} \bar{f}_y + \bar{w} \bar{f}_z + \bar{q}_y - H_y^{\text{sgs}} + \sigma_y^{\text{sgs}},
\end{array} \right\}^T \nonumber
\]

\[
\begin{array}{l}
\bar{p} \bar{D} \bar{f}_y + \bar{p} \frac{V_y}{S_c} \bar{f}_y,
\end{array}
\]

\[
\mathbf{G}_\gamma = \left\{ \begin{array}{l}
0, \bar{f}_z - \tau_{xz}^{\text{sgs}}, \bar{f}_y - \tau_{yz}^{\text{sgs}}, \bar{f}_z - \tau_{zz}^{\text{sgs}}, \bar{u} \bar{f}_x + \bar{v} \bar{f}_y + \bar{w} \bar{f}_z + \bar{q}_z - H_z^{\text{sgs}} + \sigma_z^{\text{sgs}},
\end{array} \right\}^T \nonumber
\]

\[
\begin{array}{l}
\bar{p} \bar{D} \bar{f}_z + \bar{p} \frac{V_z}{S_c} \bar{f}_z,
\end{array}
\]

\[
\tag{3.6}
\tag{3.7}
\tag{3.8}
\]
\( H = (0, 0, 0, 0, 0, 0)^T, \)  
(3.9)

where the superscript \( T \) stands for the transpose of the vector.

There are two severe numerical challenges in solving these equations for high-pressure mixing and combustion. First, at supercritical pressures, thermodynamic non-idealities and transport anomalies take place as the fluid transits from subcritical temperature to supercritical temperatures. Thus, treating these phenomena in a manner consistent with the intrinsic characteristics of a numerical algorithm presents a major obstacle. Second, the rapid variation of the fluid state and wide disparities in the characteristic time and length scales pose the well-known stiffness problem. The stiffness of the system results from: 1) ill-conditioned eigenvalues; 2) competing convective and diffusion processes; and 3) pressure singularities in the momentum equation.

In low Mach number flows, which is the case for the current study of supercritical mixing and combustion, convergence difficulties arise from the pressure singularity and the stiffness due to ill-conditioned system eigenvalues.

The dynamic pressure, defined as \( \frac{1}{2} \rho u^2 \), approaches zero as Mach number continues to decrease. The ratio of dynamic pressure to static pressure becomes negligible. Round-off error can overshadow the dynamic pressure and cause errors in momentum equations, the so-called pressure singularity problem. To overcome this difficulty, the static pressure is decomposed into a constant reference pressure and a gauge pressure (Choi and Merkle, 1993, Shuen et al., 1993),

\[ \bar{p} = \bar{p}_0 + \bar{p}_g. \]  
(3.10)

To optimize this method, the reference pressure should be chosen to account for majority of the mean pressure, while the gauge pressure is the dynamic pressure driving the flow motions. With this decomposition, \( \bar{p} \) is replaced with \( \bar{p}_g \) in the momentum equations.
To solve the ill-conditioned eigenvalue problem, let us look at the following equations:

\[
\frac{\partial \mathbf{Q}}{\partial t} + \mathbf{A} \frac{\partial \mathbf{Q}}{\partial x} + \mathbf{B} \frac{\partial \mathbf{Q}}{\partial y} + \mathbf{C} \frac{\partial \mathbf{Q}}{\partial z} = 0,
\]  

(3.11)

where \( \mathbf{A} = \frac{\partial \mathbf{E}}{\partial \mathbf{Q}} \), \( \mathbf{B} = \frac{\partial \mathbf{F}}{\partial \mathbf{Q}} \), and \( \mathbf{C} = \frac{\partial \mathbf{G}}{\partial \mathbf{Q}} \) are the Jacobian matrices. Analysis shows that the eigenvalues of matrix \( \mathbf{A} \) is:

\[
\lambda_1 = \bar{u} + \bar{c}, \lambda_2 = \bar{u} - \bar{c}, \lambda_{3,4,5,6} = \bar{u}.
\]  

(3.12)

In low Mach number flows, \( M \ll 1 \), the ratio of the largest eigenvalue to the smallest one is close to inverse of Mach number, indicating that the eigenvalues are order of magnitude different. However, the CFL number, which determines the maximum local time step is limited by the largest eigenvalue, and hence is extremely small, resulting in a very slow convergence. It becomes unacceptable for even lower-Mach number or time accurate simulations.

To cure the eigenvalue disparity problem, which is intrinsic in low Mach number flows, the time derivative preconditioning method (Turkel, 1993, Choi and Merkle, 1993, Shuen et al., 1993, Hsieh and Yang, 1997) has been used, associated with the methodologies developed by Meng and Yang (2003) for handling general fluid thermodynamics, to take full account of the thermodynamic non-idealities and transport anomalies in the whole fluid state of concern and accommodates any arbitrary equation of state.

Zong and Yang (2007a) made further improvement by changing primitive variable \( h \) to \( T \), getting rid of the cost intensive computation associated with iterative calculations to get temperature from enthalpy. In the current study, following Zong et al. (2008), the preconditioning method was applied to the mixture fraction equation for solution of supercritical combustion using flamelet approach. A unified treatment of thermodynamic properties and preconditioning matrix makes the numerical scheme accurate, robust and efficient.
The preconditioning method adds an additional pseudo time differential term in Eq. 3.1, by pre-multiplying it with a preconditioning matrix:

\[
\Gamma \frac{\partial Z}{\partial t} + \frac{\partial Q}{\partial t} + \frac{\partial (E-E_v)}{\partial x} + \frac{\partial (F-F_v)}{\partial y} + \frac{\partial (G-G_v)}{\partial z} = H, \tag{3.13}
\]

\[
Z = \left( \bar{p}, \bar{u}, \bar{v}, \bar{w}, \bar{T}, \bar{f} \right)^T. \tag{3.14}
\]

If we pre-multiply this equation by \(\Gamma^{-1}\), the new Jacobian matrices become \(\Gamma^{-1}A_v\), \(\Gamma^{-1}B_v\) and \(\Gamma^{-1}C_v\) with \(A_v = \frac{\partial E}{\partial z},\ B_v = \frac{\partial F}{\partial z}\), and \(C_v = \frac{\partial G}{\partial z}\). If \(\Gamma\) is chosen so that the eigenvalues of these matrixes are of the same order of magnitude, the resulting equations have well-conditioned eigenvalues and converge efficiently in all Mach number flows. When pseudo time approaches infinity, or in other words, steady state solutions are achieved with respect to pseudo time, the original governing equations are recovered. So the efficiency of preconditioning method is largely determined by the selection of the preconditioning matrix.

Following Zong (2005), the transfer matrix is derived as:

\[
T = \frac{\partial Q}{\partial Z}. \tag{3.15}
\]

In this matrix, a common term \(\left( \frac{\partial p}{\partial \rho} \right)_{T,Y_i}\) can be related to speed of sound and specific heat capacity ratio:

\[
\left( \frac{\partial p}{\partial \rho} \right)_{T,Y_i} = \frac{C_p}{C_v} \left( \frac{\partial p}{\partial \rho} \right)_{s,Y_i} = \frac{\gamma}{a^2}. \tag{3.16}
\]

\(a^2\) is replaced with \(\beta\) to define the preconditioning matrix,
\[
\Gamma = \begin{pmatrix}
\frac{\gamma}{\beta} & 0 & 0 & 0 & \rho_r & \rho_f \\
\frac{\gamma}{\beta} \ddot{u} & \tilde{\rho} & 0 & 0 & \ddot{u} \rho_r & \ddot{u} \rho_f \\
\frac{\gamma}{\beta} \ddot{v} & 0 & \tilde{\rho} & 0 & \ddot{v} \rho_r & \ddot{v} \rho_f \\
\frac{\gamma}{\beta} \ddot{w} & 0 & 0 & \tilde{\rho} & \ddot{w} \rho_r & \ddot{w} \rho_f \\
\frac{\gamma}{\beta} \ddot{h}_i + \frac{\tilde{T}}{\tilde{\rho}} \rho_r & \tilde{\rho} \ddot{u} & \tilde{\rho} \ddot{v} & \tilde{\rho} \ddot{w} & \tilde{\rho} c_p + \ddot{h}_i \rho_r & \rho_f E + \tilde{\rho} E_f \\
\frac{\gamma}{\beta} \ddot{f} & 0 & 0 & 0 & \rho_r \ddot{f} & \tilde{\rho} + \ddot{f} \rho_f
\end{pmatrix}, \quad (3.17)
\]

where \( \ddot{h}_i \) is the total specific enthalpy, \( \rho_r = \left( \frac{\partial \rho}{\partial T} \right)_{p, \gamma_r} \), \( \rho_f = \frac{\partial \rho}{\partial f} \), \( E_f = \frac{\partial E}{\partial f} \). \( \beta \) is defined as

\[
\beta = \frac{\gamma \varepsilon a^2}{1 + (\gamma - 1) \varepsilon}, \quad (3.18)
\]

where \( \varepsilon \) (\( 0 < \varepsilon \leq 1 \)) is the preconditioning factor. In contrast to the definition of preconditioning matrix by other researchers, all of the off-diagonal terms in Eq. 3.17 have been retained. By keeping these terms, the unaltered system is identically restored as \( \varepsilon \to 1; \)

\[
\lim_{\varepsilon \to 1} \Gamma = T. \quad (3.19)
\]

The conditioned governing equations, in the pseudo-time space, are characterized by the new Jacobian matrices \( \Gamma^{-1} A_p, \Gamma^{-1} B_p \) and \( \Gamma^{-1} C_p \), whose eigenvalues are given by:
\[
\lambda_1 = \frac{1}{2} [U (\varepsilon + 1) + \sqrt{U^2 (1 - \varepsilon)^2 + 4 \varepsilon \alpha^2}] ,
\]
\[
\lambda_2 = \frac{1}{2} [U (\varepsilon + 1) - \sqrt{U^2 (1 - \varepsilon)^2 + 4 \varepsilon \alpha^2}] ,
\]
\[
\lambda_{3,4,5,6} = U ,
\]

where \( U \) represents \( \tilde{u}, \tilde{v}, \) and \( \tilde{w} \) in x-, y- and z-direction respectively. If \( \varepsilon \) is small enough, the first two eigenvalues can be of the same order of magnitude as others. Note that since no assumption has been made to the form of the equation of state, it can be applied to any fluid state without loss of accuracy.

### 3.1.1 Determination of the Preconditioning Factor

From the definition of the preconditioning matrix, and the resulting system eigenvalues, it is clear that the effectiveness of the preconditioning method is totally determined by the choice of the preconditioning factor \( \varepsilon \). Appropriate criteria to determine the value of \( \varepsilon \) in each computational cell are crucial to get well-conditioned system eigenvalues and thus the rate of convergence of the numerical scheme.

Various competing time scales are associated with each computational cell in each coordinate direction, due to local flow convection, acoustic propagation, momentum, thermal and mass diffusion processes exist. These processes have to be taken into account when choosing the preconditioning factor, so as to maximize the convergence rate. The non-dimensional numbers characterizing the time scales associated with these physical processes are CFL number, Mach number, von Neumann number, cell Reynolds number, Prandtl number, and Schmidt number. Prandtl and Schmidt numbers correlate the rate of momentum, thermal and mass diffusion.
The CFL number, which characterizes the local convective propagation rates, for the three coordinate directions are defined as:

\[\text{CFL}_x = \frac{\rho(\lambda_x)\Delta \tau}{\Delta x}, \quad \text{CFL}_y = \frac{\rho(\lambda_y)\Delta \tau}{\Delta y}, \quad \text{CFL}_z = \frac{\rho(\lambda_z)\Delta \tau}{\Delta z},\]  

(3.21)

where \(\rho(\lambda_x), \rho(\lambda_y), \rho(\lambda_z)\) are the maximum eigenvalues in each direction, respectively.

The von Neumann number, which characterizes the diffusion propagation rates, is defined as:

\[V_{NN_x} = \frac{v\Delta \tau}{\Delta x^2}, \quad V_{NN_y} = \frac{v\Delta \tau}{\Delta y^2}, \quad V_{NN_z} = \frac{v\Delta \tau}{\Delta z^2},\]  

(3.22)

The cell Reynolds number, which indicates the ratio of local velocities to momentum diffusion velocity, is defined as:

\[\text{Re}_x = \frac{\overline{u}\Delta x}{\nu}, \quad \text{Re}_y = \frac{\overline{v}\Delta y}{\nu}, \quad \text{Re}_z = \frac{\overline{w}\Delta z}{\nu},\]  

(3.23)

If the respective quantities \(Re, Re_{Pr}\), and \(Re_{Sc}\) exceed unity in either of the coordinate direction, it means the convection velocity is larger than the corresponding velocity scale, thus convective effects dominant and the conservation equations exhibit a hyperbolic character. For this situation an inviscid criterion must be employed. If \(Re, Re_{Pr}, \text{or} Re_{Sc}\) are less than or equal to unity, diffusive effects dominate, a parabolic character is exhibited and a viscous criteria must be employed.

An additional criterion that must be considered for dual-time stepping methodology is the effect of the unsteady term on the pseudo time system. Stability analysis showed a limit exists
where preconditioning the pseudo-time derivative negates the favorable damping characteristics induced by the unsteady term, which promote favorable damping characteristics in time-marching schemes and accelerate convergence (Venkateswaran and Merkle, 1995). However, in the current study, the physical time steps are so small that this criterion almost always dominates and gives rise to an unconditioned degeneration. In the current work, no issues regarding stability are found, thus this criterion is neglected. The final preconditioning factor is selected based on methodologies developed by Choi and Merkel (1993), Buelow et al. (1995), and Venkateswaran and Merkel (1995). Optimal values are specified locally as:

$$\varepsilon = \min[1, \max(\varepsilon_{\text{inv}}, \varepsilon_{\text{vis}})].$$

(3.24)

The subscripts refer to the inviscid and viscous preconditioning factors, respectively. The criteria employed to evaluate these terms are discussed below.

### 3.1.1.1 Inviscid Preconditioning Factor

In the limit of infinitely large Reynolds numbers, or inviscid flows, following Choi and Merkle (1993), $\varepsilon$ is assigned a value proportional to the local Mach number to ensure that the pseudo acoustic speed and flow velocity are of the same order of magnitude. To achieve correct limiting behavior, as Mach number approaches zero (e.g. in stagnant region), a minimum value (typically, $1 \times 10^{-5}$) is used. The resulting preconditioning factor is defined as:

$$\varepsilon_{\text{inv}} = \begin{cases} 
\varepsilon^2, & M < \varepsilon; \\
2M^2, & \varepsilon < M < 1; \\
1, & M \geq 1. 
\end{cases}$$

(3.25)
In inviscid flows, this choice of $\varepsilon$ gives minimal disparity in system eigenvalues and optimal damping rates. The convergence rates are entirely dependent on the local pseudo CFL number, which is determined by the stability criterion.

**3.1.1.2 Viscous Preconditioning Factor**

In regions where diffusion processes are important, the effect of diffusion on the preconditioning factor has to be considered.

Buelow et al. (1994, 1995) have conducted a variety of studies to determine an optimal viscous preconditioning factor for the Navier-Stokes equations. Results from stability analysis indicate that three different requirements must be addressed in order to specify a generalized criterion. For high cell Reynolds numbers ($\text{Re} \gg 1$) the acoustic wave speeds should be scaled to the same order of magnitude as the particle speeds, as is accomplished by the inviscid preconditioning factor defined above. For low cell Reynolds numbers ($\text{Re} \ll 1$) and high acoustic cell Reynolds numbers ($\text{Re}/M \gg 1$) the diffusion rates should be scaled to the same order of magnitude as the acoustic speeds. For low cell Reynolds numbers and low acoustic cell Reynolds numbers the diffusion rates should be scaled to the particle speeds. The only way to satisfy these conditions simultaneously is to define a viscous preconditioning factor that is dependent on the Fourier wavenumber. Such a definition is not appropriate for implementation in a CFD code. To overcome the difficulties outlined above, a preconditioning factor based on local length scales which is tuned to damp the low wavenumber modes has been developed by the authors. This definition requires a priori assumption of the orientation of dominating convective and diffusion processes within a given grid configuration and the choice of $\varepsilon_{vis}$ is somewhat more involved. In three dimensions, there are three possible CFL numbers, and two possible VNN
numbers, and six possible values of $\varepsilon_{\text{vis}}$. The most restrictive of the CFL and VNN numbers are usually chosen for stability reasons and these values are the most likely candidates for determining $\varepsilon_{\text{vis}}$. Some freedom does exist, however, in how $\varepsilon_{\text{vis}}$ is evaluated.

In applications, most grid configurations are stretched near the wall, so that predominating diffusion processes, which is in a direction normal to the predominating convective processes, are resolved. Under these conditions, the rate limiting diffusion processes typically coincide with the maximum von Neumann number in a given cell. To retain the benefits of the time step given by Eq. 3.21, this quantity must be optimized with respect to the minimum CFL number. In three-dimensions, this is achieved by: 1) equating Eq. 3.21 with Eq. 3.22; 2) solving for respective values of $\varepsilon$; and 3) choosing the largest of the three values obtained. Performing this operation yields an expression of the form

$$
\varepsilon_{\text{vis}} = \max \left[ \frac{u^2 \delta_x (\delta_x - 1)}{u^2 \delta_x^2 + a_x^2}, \frac{v^2 \delta_y (\delta_y - 1)}{v^2 \delta_y^2 + a_y^2}, \frac{w^2 \delta_z (\delta_z - 1)}{w^2 \delta_z^2 + a_z^2} \right],
$$

(3.26)

where

$$
\delta_x = \max(\nu, \frac{\nu}{\Pr}, \frac{\nu}{Sc}, \frac{1}{\hat{u} VNN}),
$$

$$
\delta_y = \max(\nu, \frac{\nu}{\Pr}, \frac{\nu}{Sc}, \frac{1}{\hat{v} VNN}),
$$

$$
\delta_z = \max(\nu, \frac{\nu}{\Pr}, \frac{\nu}{Sc}, \frac{1}{\hat{w} VNN}).
$$

(3.27)

This equation takes into account the effects of momentum, energy, and mass diffusion processes on the overall convergence rate.
3.2 Spatial Discretization: Finite Volume Approach

3.2.1 Finite Volume Approach

The conservation laws of fluid motion presented in Chapter 2 can be expressed in differential or integral form. Finite differencing can be used to solve the differential equations. However, finite difference equations have inherent difficulties associated with irregular grid system (Hoffmann and Chiang, 1998). Integral methods, including finite volume and finite element methods, do not encounter such difficulties. In the current study finite volume approach is used to solve the governing equations.

To utilize the finite-volume approach, the governing equations are integrated over the control volume $V$ enclosed by the surface $S$ in the physical domain as

$$
\iiint_{V} \left( \frac{\partial Z}{\partial \tau} \frac{\partial Q}{\partial t} + \frac{\partial (E - E_v)}{\partial x} + \frac{\partial (F - F_v)}{\partial y} + \frac{\partial (G - G_v)}{\partial z} - H \right) dV = 0
$$

(3.28)

The generalized control volume in a structured grid system is a hexahedron formed by eight grid points as shown in figure 3.1. where $\vec{n}_\xi$, $\vec{n}_\eta$, and $\vec{n}_\zeta$ are area unit vectors normal to the surfaces in the $\xi$, $\eta$, and $\zeta$-directions, respectively.
Upon applying the Gauss’ divergence theorem over a hexahedral cell as shown in Fig. 3.1, Eq. 3.28 can be re-written as:

\[
\iiint_V \left( \mathbf{F} \frac{\partial \mathbf{Z}}{\partial \tau} + \frac{\partial \mathbf{Q}}{\partial t} \right) dV + \int_{S_1} \mathbf{W} \cdot \mathbf{n}_\zeta dS_\zeta + \int_{S_2} \mathbf{W} \cdot \mathbf{n}_\eta dS_\eta + \int_{S_3} \mathbf{W} \cdot \mathbf{n}_\xi dS_\xi \\
= \iiint_V \mathbf{H} dV , \quad (3.29)
\]

where

\[
\mathbf{W} = (\mathbf{E} - \mathbf{E}_0) \mathbf{i} + (\mathbf{F} - \mathbf{F}_0) \mathbf{j} + (\mathbf{G} - \mathbf{G}_0) \mathbf{k} . \quad (3.30)
\]
$S_{\xi}, S_{\eta}, S_{\zeta}$ are the surfaces that are perpendicular to the surface vectors $\vec{n}_{\xi}, \vec{n}_{\eta}$ and $\vec{n}_{\zeta}$, respectively. Surfaces $S_{\xi}, S_{\eta}, S_{\zeta}$ can be combined with the area unit vectors $\vec{n}_{\xi}, \vec{n}_{\eta}$ and $\vec{n}_{\zeta}$ to form the surface vectors $\vec{S}_{\xi}, \vec{S}_{\eta},$ and $\vec{S}_{\zeta}$ given by:

\[
\begin{align*}
\vec{S}_{\xi} &= S_{\xi} \vec{n}_{\xi} = S_{\xi,\xi} \vec{i} + S_{\xi,\eta} \vec{j} + S_{\xi,\zeta} \vec{k}, \\
\vec{S}_{\eta} &= S_{\eta} \vec{n}_{\eta} = S_{\eta,\xi} \vec{i} + S_{\eta,\eta} \vec{j} + S_{\eta,\zeta} \vec{k}, \\
\vec{S}_{\zeta} &= S_{\zeta} \vec{n}_{\zeta} = S_{\zeta,\xi} \vec{i} + S_{\zeta,\eta} \vec{j} + S_{\zeta,\zeta} \vec{k}.
\end{align*}
\]

(3.31)

And the unit area vectors are related to cell surface areas $S_{\xi}, S_{\eta},$ and $S_{\zeta}$ as

\[
\begin{align*}
\vec{n}_{\xi} &= \left( S_{\xi,\xi} \vec{i} + S_{\xi,\eta} \vec{j} + S_{\xi,\zeta} \vec{k} \right) / |\vec{S}_{\xi}|, \\
\vec{n}_{\eta} &= \left( S_{\eta,\xi} \vec{i} + S_{\eta,\eta} \vec{j} + S_{\eta,\zeta} \vec{k} \right) / |\vec{S}_{\eta}|, \\
\vec{n}_{\zeta} &= \left( S_{\zeta,\xi} \vec{i} + S_{\zeta,\eta} \vec{j} + S_{\zeta,\zeta} \vec{k} \right) / |\vec{S}_{\zeta}|.
\end{align*}
\]

(3.32)

The surface vectors and the cell volume can be calculated directly from the grid points (Kordulla and Vinokur, 1983):

\[
\begin{align*}
\vec{S}_{\xi} &= \frac{1}{2} (\vec{r}_{72} \times \vec{r}_{36}) = \frac{1}{2} \begin{vmatrix}
\vec{i} & \vec{j} & \vec{k} \\
x_{2} - x_{1} & y_{2} - y_{1} & z_{2} - z_{1} \\
x_{6} - x_{3} & y_{6} - y_{3} & z_{6} - z_{3}
\end{vmatrix}, \\
\vec{S}_{\eta} &= \frac{1}{2} (\vec{r}_{86} \times \vec{r}_{75}) = \frac{1}{2} \begin{vmatrix}
\vec{i} & \vec{j} & \vec{k} \\
x_{6} - x_{8} & y_{6} - y_{8} & z_{6} - z_{8} \\
x_{5} - x_{7} & y_{5} - y_{7} & z_{5} - z_{7}
\end{vmatrix},
\end{align*}
\]

(3.33)
\[
\bar{S}_\xi = \frac{1}{2} (\vec{x}_{74} \times \vec{x}_{83}) = \frac{1}{2} \begin{vmatrix}
\bar{i} & \bar{j} & \bar{k} \\
x_4 - x_7 & y_4 - y_7 & z_4 - z_7 \\
x_8 - x_7 & y_8 - y_7 & z_8 - z_7
\end{vmatrix},
\]

\[
\Delta V = \frac{1}{3} \vec{r}_{l7} \left( \bar{S}_\xi + \bar{S}_\eta + \bar{S}_\zeta \right).
\]

Assuming that the increments \( \Delta \xi = \Delta \eta = \Delta \zeta = 1 \) in the body-fitted coordinate system and substituting Eq. 3.30 and Eq. 3.32 into Eq. 3.29 yields the following governing equation in the general coordinates

\[
\left\{ \Gamma \frac{\partial \bf{Z}}{\partial \tau} + \frac{\partial \bf{Q}}{\partial t} \right\} + \left( \bf{E}_{\xi} - \bf{E}_{\eta} \right)_{i-1/2,j,k}^{i+1/2,j,k} + \left( \bf{F}_{\xi} - \bf{F}_{\eta} \right)_{i,j-1/2,k}^{i,j+1/2,k} + \left( \bf{G}_{\xi} - \bf{G}_{\eta} \right)_{i,j,k-1/2}^{i,j,k+1/2} = \bf{H},
\]

(3.34)

where the vectors \( \bf{E}_{\xi}, \bf{F}_{\eta}, \bf{G}_{\xi}, \bf{E}_{\eta}, \bf{F}_{\eta}, \) and \( \bf{G}_{\eta} \) are defined as

\[
\bf{E}_{\xi} = \left( \bar{S}_{\xi x} \bf{E} + \bar{S}_{\xi y} \bf{F} + \bar{S}_{\xi z} \bf{G} \right), \quad \bf{E}_{\eta} = \left( \bar{S}_{\eta x} \bf{E} + \bar{S}_{\eta y} \bf{F} + \bar{S}_{\eta z} \bf{G} \right),
\]

\[
\bf{F}_{\xi} = \left( \bar{S}_{\xi x} \bf{E} + \bar{S}_{\xi y} \bf{F} + \bar{S}_{\xi z} \bf{G} \right), \quad \bf{F}_{\eta} = \left( \bar{S}_{\eta x} \bf{E} + \bar{S}_{\eta y} \bf{F} + \bar{S}_{\eta z} \bf{G} \right),
\]

\[
\bf{G}_{\xi} = \left( \bar{S}_{\xi x} \bf{E} + \bar{S}_{\xi y} \bf{F} + \bar{S}_{\xi z} \bf{G} \right), \quad \bf{G}_{\eta} = \left( \bar{S}_{\eta x} \bf{E} + \bar{S}_{\eta y} \bf{F} + \bar{S}_{\eta z} \bf{G} \right).
\]

The quantities \( \bf{E}_{\xi,i\eta,j,k}, \bf{F}_{\xi,j\eta,i,k}, \bf{G}_{\xi,j,k,\zeta} \) and \( \bf{G}_{\eta,i,j,k,\zeta} \) represent the numerical fluxes associated with each cell interface. \( \tilde{S} \) represents cell surface areas per cell volume. In fact, the above analysis describes the transformation of a quadrilateral cell with a volume \( \Delta V \) in \( x-y-z \) coordinates to a cubic cell with unit volume in the general coordinate (i.e., \( \xi-\eta-\zeta \) coordinates).

To accelerate convergence, the pseudo-time integration is based on the local time step. The maximum pseudo-time increment \( \Delta \tau \) of each cell can be evaluated by
\[ \Delta \tau = \frac{\Delta \tau_{\xi} \Delta \tau_{\eta} \Delta \tau_{\zeta}}{\Delta \tau_{\xi} + \Delta \tau_{\eta} + \Delta \tau_{\zeta}} , \]  

(3.36)

where

\[ \Delta \tau_{\xi} = \frac{CFL \cdot \Delta V}{\rho(\lambda_{\xi})S_{\xi\xi} + \rho(\lambda_{\eta})S_{\xi\eta} + \rho(\lambda_{\zeta})S_{\xi\zeta} / |\tilde{S}_{\xi}|} , \]

\[ \Delta \tau_{\eta} = \frac{CFL \cdot \Delta V}{\rho(\lambda_{\xi})S_{\eta\eta} + \rho(\lambda_{\eta})S_{\eta\eta} + \rho(\lambda_{\zeta})S_{\eta\zeta} / |\tilde{S}_{\eta}|} , \]

\[ \Delta \tau_{\zeta} = \frac{CFL \cdot \Delta V}{\rho(\lambda_{\xi})S_{\zeta\zeta} + \rho(\lambda_{\eta})S_{\zeta\eta} + \rho(\lambda_{\zeta})S_{\zeta\zeta} / |\tilde{S}_{\zeta}|} . \]

### 3.2.2 Evaluation of Inviscid Fluxes

Different approaches used in evaluating the numerical fluxes lead to different schemes with disparate numerical characteristics. In the central difference scheme, the convective flux at any cell face in the \( \xi \)-direction can be written as

\[ \hat{E}_{\xi,i+1/2,j} = \frac{1}{2} \left[ E_{\xi}(Z^L) + E_{\xi}(Z^R) \right] , \]

(3.38)

where the left and right stencils are used to give the desired accuracy. The above equation corresponds to the stencil illustrated in Fig. 3.2. The superscripts \( L \) and \( R \) represent the left and right cells. Depending on the manner in which these terms are evaluated, a wide variety of central and upwind schemes can be obtained. According to Rai and Chakravarthy (1993), the numerical flux in Eq. 3.34 is computed as
\[ E_{\xi,i+1/2,j,k} = E_{\xi,i+1/2,j,k} - \phi^{(4)}_{i+1/2,j,k} \left( \frac{E_{\xi,i+3/2,j,k} - 2E_{\xi,i+1/2,j,k} + E_{\xi,i-1/2,j,k}}{24} \right), \]

(3.39)

where \( \phi^{(4)} \) is the flux limiter. This term switches the truncation error associated with the flux-difference from fourth-order accuracy when \( \phi^{(4)} = 1 \), to second-order accuracy when \( \phi^{(4)} = 0 \).

To evaluate Eq. 3.38 for the desired accuracy, the left and right state terms in Eq. 3.39 must be computed using the same or higher order accuracy. For uniform grid system, these terms are written as follows to facilitate easy switching and make the scheme TVD (total-variation-diminishing).

\[
Z_{i+1/2,j,k}^L = Z_{i,j,k} + \phi^{(2)}_{i+1/2,j,k} \left( \frac{3\nabla Z_{t+1,j,k} + \nabla Z_{t,i,j,k}}{8} \right) \\
+ \phi^{(4)}_{i+1/2,j,k} \left( \frac{-5\nabla Z_{t+2,j,k} + 7\nabla Z_{t+1,j,k} + \nabla Z_{t,i,j,k} - 3\nabla Z_{t-1,j,k}}{128} \right), 
\]

(3.40)

\[
Z_{i+1/2,j,k}^R = Z_{i,j,k} - \phi^{(2)}_{i+1/2,j,k} \left( \frac{\nabla Z_{t+2,j,k} + 3\nabla Z_{t+1,j,k}}{8} \right) \\
+ \phi^{(4)}_{i+1/2,j,k} \left( \frac{3\nabla Z_{t+3,j,k} - \nabla Z_{t+2,j,k} - 7\nabla Z_{t+1,j,k} + 5\nabla Z_{t,i,j,k}}{128} \right), 
\]

(3.41)

\[
\nabla Z_{i,j} = Z_{i,j} - Z_{i-1,j}. 
\]

(3.42)

These stencils can be used to get fifth-order accuracy (\( \phi^{(4)} = 1, \phi^{(2)} = 1 \)), third-order accuracy (\( \phi^{(4)} = 0, \phi^{(2)} = 1 \)), and first-order accuracy (\( \phi^{(4)} = 0, \phi^{(2)} = 0 \)), respectively. The present work utilizes second-order overall accuracy for spatial discretization with the exception of first order accuracy close to the physical boundaries. The third-order accurate evaluation of the left and
right states is thus employed. The fluxes in $\eta$, and $\zeta$-directions can be computed in a similar fashion as above.

However, non-uniform grids are generally used in practical applications. If the same procedure is used to evaluate the left and right state terms, Taylor series expansion shows that there will be a truncation error of first order. This will significantly reduce the overall order of accuracy of the numerical scheme. Previous experience shows that the numerical scheme is very dissipative. To achieve required order of accuracy, much more refined grids have to be used to resolve flow motions of interest.

![Figure 3.2. Schematic diagram of the stencil used in evaluating inviscid flux terms in the $x-y$ plane.](image)

Fosso et al. (2010) proposed higher-order accurate compact interpolation for curvilinear finite volume schemes to take into account the effect of grid non-uniformity. The values of interest at cell surfaces can be estimated from the cell average values in its neighborhood, by applying Taylor series expansion and solving the linear equations. Appropriate boundary treatment procedures have been developed for multi-block applications. However, this method is
more expensive due to extra calculations of the surface values in each iteration. The current study compromises by mimicking the so-called Cartesian-like scheme using curvilinear abscissa scheme in the cited work. Instead of implicit equations, explicit equations are obtained to improve the numerical accuracy of spatial differencing for convective flux evaluation.

3.2.3 Evaluation of Viscous and SGS Fluxes

A three-dimensional auxiliary cell is shown schematically by the dash-dotted lines in Fig. 3.3. The viscous fluxes need to be evaluated at the center of the cell faces, i.e., \( i + 1/2, j, k \) for the viscous flux in the axial direction. Using the Gauss’ divergence theorem and applying it to a small control volume \( \Delta V \), the viscous fluxes can be approximated as

Figure 3.3. Schematic diagram for a three-dimensional auxiliary cell.
\[ \nabla \cdot \vec{f} = \frac{1}{\Delta V} \oint_S \vec{f} \cdot \vec{n} dS. \] (3.43)

Applying the above formulation to the auxiliary cell at \((i+1/2, j, k)\) gives

\[
\left( \frac{\partial f}{\partial x} \right)_{i+1/2,j,k} = \frac{1}{\Delta V_{i+1/2,j,k}} \left[ f S_{\xi}^{x} \big|_{i+1/2,j,k} - f S_{\xi}^{x} \big|_{i,j,k} + f S_{\eta}^{x} \big|_{i+1/2,j+1/2,k} - f S_{\eta}^{x} \big|_{i+1/2,j-1/2,k} \right].
\] (3.44)

Similarly

\[
\left( \frac{\partial f}{\partial y} \right)_{i+1/2,j,k} = \frac{1}{\Delta V_{i+1/2,j,k}} \left[ f S_{\xi}^{y} \big|_{i+1/2,j,k} - f S_{\xi}^{y} \big|_{i,j,k} + f S_{\eta}^{y} \big|_{i+1/2,j+1/2,k} - f S_{\eta}^{y} \big|_{i+1/2,j-1/2,k} \right].
\] (3.45)

\[
\left( \frac{\partial f}{\partial z} \right)_{i+1/2,j,k} = \frac{1}{\Delta V_{i+1/2,j,k}} \left[ f S_{\xi}^{z} \big|_{i+1/2,j,k} - f S_{\xi}^{z} \big|_{i,j,k} + f S_{\eta}^{z} \big|_{i+1/2,j+1/2,k} - f S_{\eta}^{z} \big|_{i+1/2,j-1/2,k} \right].
\] (3.46)

Note that \(f\) in the above equations are elements of the viscous flux vectors \(E_{\xi}, F_{\eta}, \) or \(G_{\xi}.\)

Physical variables with one-half indices need to be interpolated from the quantities at the neighboring cell centers and are given by

\[
f_{i+1/2,j\pm1/2,k} = \frac{1}{4} \left( f_{i,j,k} + f_{i+1,j,k} + f_{i\pm1,j\pm1,k} + f_{i,j\pm1,k} \right),
\] (3.47)

\[
f_{i+1/2,j,k\pm1/2} = \frac{1}{4} \left( f_{i,j,k} + f_{i+1,j,k} + f_{i\pm1,j,k\pm1} + f_{i,j,k\pm1} \right).
\] (3.47)

The evaluation of SGS fluxes follows a similar procedure as for the viscous and diffusive fluxes.
The viscous term evaluation procedure outlined above results in lower order of accuracy for non-uniform grids for reasons similar to the convective flux terms. However, in large Reynolds number flows, convection is dominant, and the effect of grid uniformity is neglected in the current study. Further study is warranted to consistently improve the numerical accuracy.

### 3.2.4 Evaluation of Artificial Dissipation

Artificial dissipation plays a crucial role in the stability of a numerical scheme based on central differencing. The form of these artificial dissipation terms depends on the order of accuracy of the numerical scheme, and must be higher-order accurate to keep its magnitude minimal. For the present case, the numerical differentiation of the flux vectors is fourth-order accurate in the core region of the computational domain. Accordingly, the artificial dissipation is fourth-order accurate. The accuracy order of the numerical scheme decreases near the physical boundary, and the artificial dissipation also goes to a lower order. The form of numerical dissipation used in the present schemes is quite often a blending of second- and fourth-order dissipation terms. The second-order terms are used near shock waves and flame zones to prevent spurious oscillations within such thin regions, while the fourth-order terms are important for stability and convergence. The standard dissipation model can be written as

\[
AD = \text{artificial dissipation} = d_{i+1/2,j,k} - d_{i-1/2,j,k},
\]  

where
\[
d_{i+1/2,j,k} = \frac{\varepsilon_2}{8} \Delta t \frac{\partial Z}{\partial \xi}_{i+1/2,j,k} - \frac{\varepsilon_4}{8} \Delta t \frac{\partial^3 Z}{\partial \xi^3}_{i+1/2,j,k} + \frac{\varepsilon_6}{8} \Delta t \frac{\partial^5 Z}{\partial \xi^5}_{i+1/2,j,k} ,
\]

where \(\varepsilon_2, \varepsilon_4,\) and \(\varepsilon_6\) correspond to the coefficients of the second-, fourth- and sixth-order accurate artificial dissipation terms and in the present formulation, \(\Delta \xi = 1\).

Even though the standard dissipation model has been proven to be reasonably effective in many cases, there are strong motivations for reducing the numerical dissipation being produced. The standard model also has difficulties in hypersonic flows and in density stratified supercritical fluids with steep discontinuities as in the present case. A scalar dissipation model was constructed by Swanson and Turkel (1992) and by Jorgenson and Turkel (1993) to overcome the above difficulties. In their model

\[
d_{i+1/2,j,k} = \varepsilon_{i+1/2,j,k}^{(2)} \rho_{i+1/2,j,k}(\lambda) \frac{\partial Z}{\partial \xi}_{i+1/2,j,k} - \varepsilon_{i+1/2,j,k}^{(4)} \rho_{i+1/2,j,k}(\lambda) \frac{\partial^3 Z}{\partial \xi^3}_{i+1/2,j,k}.
\]

The modified eigenvalues are given by

\[
\tilde{\lambda}_1 = \tilde{\lambda}_2 = \tilde{\lambda}_3 = \tilde{\lambda}_4 = \tilde{\lambda}_5 = \tilde{\lambda}_6 = \rho(\lambda) ,
\]

where \(\rho(\lambda)\) is the spectral radius of the flux Jacobian matrix \(\Gamma^{-1}A\).

\[
\varepsilon_{i+1/2,j,k}^{(2)} = \kappa^{(2)} \max(\nu_{i-1,j,k}, \nu_{i,j,k}, \nu_{i+1,j,k}, \nu_{i+2,j,k}) ,
\]

\[
\nu_{i,j,k} = \frac{p_{i-1,j,k} - 2p_{i,j,k} + p_{i+2,j,k}}{p_{i-1,j,k} + 2p_{i,j,k} + p_{i+1,j,k}} .
\]
\[
\varepsilon_{i+1/2,j,k}^{(4)} = \max\left(0, \left(\kappa_{i+1/2,j,k}^{(4)} - \varepsilon_{i+1/2,j,k}^{(2)}\right)\right), \quad (3.54)
\]

\[
\kappa_{i+1/2,j,k}^{(2)} = \frac{1}{4} \sim \frac{1}{2}, \quad \kappa_{i+1/2,j,k}^{(4)} = \frac{1}{64} \sim \frac{1}{32}. \quad (3.55)
\]

The first term given in Eq. 3.50 is nonlinear. Its purpose is to introduce an entropy-like condition and to suppress oscillations in the neighborhood of shock discontinuities. This term is small in the smooth portion of the flow field. The switch \(\nu_{i,j,k}\) is important near discontinuities, since there are large pressure-gradients across them. For high-pressure fluid mixing and combustion, however, this switch is changed to include temperature- or density-gradients, as pressure may still be uniform across the boundary between different fluid layers. The fourth-order term is basically linear and is included to damp high-frequency modes and allow the scheme to approach a steady state. Only this term affects the linear stability of the scheme. It is reduced to zero near the discontinuity.

Although effective, the scalar dissipation model results in too much dissipation and contaminates the accuracy of the simulation. This effect is because the scalar dissipation model uses the same artificial dissipation coefficient for all the conservation equations regardless of the actual wave speeds, resulting in excessive smearing. This situation deteriorates in locations where the local preconditioning factor is not optimized such that the eigenvalues of the Jacobian matrix are in different orders of magnitude. Furthermore, the scalar dissipation is not conservative, and leads to mass conservation problem in practice.

To overcome the difficulties with the scalar dissipation model, matrix dissipation formulations are derived for real-fluid mixture systems following Swanson and Turkel (1992) and by Jorgenson and Turkel (1993). The formulations are implemented into the numerical scheme to remedy the deficiency of the scalar dissipation model. To demonstrate the procedure of adding
matrix artificial dissipation, backward time differencing is applied to the governing equations, giving:

\[
\left\{ \Gamma + a \frac{\Delta \tau}{\Delta t} \mathbf{T} \right\} \frac{\partial \mathbf{Z}}{\partial \tau} + \frac{\partial \mathbf{E}}{\partial x} + \frac{\partial \mathbf{F}}{\partial y} + \frac{\partial \mathbf{G}}{\partial z} = -\frac{1}{\Delta t} \left( a \mathbf{Q}^m - \phi \right),
\]

(3.56)

or equivalently:

\[
\frac{\partial \mathbf{Z}}{\partial \tau} + \left\{ \Gamma + a \frac{\Delta \tau}{\Delta t} \mathbf{T} \right\}^{-1} \left\{ \mathbf{A}_v \frac{\partial \mathbf{Z}}{\partial x} + \mathbf{B}_v \frac{\partial \mathbf{Z}}{\partial y} + \mathbf{C}_v \frac{\partial \mathbf{Z}}{\partial z} \right\} = -\frac{1}{\Delta t} \left\{ \Gamma + a \frac{\Delta \tau}{\Delta t} \mathbf{T} \right\}^{-1} \left( a \mathbf{Q}^m - \phi \right),
\]

(3.57)

where \( a = \frac{3}{2} \) and \( \phi = \frac{1}{2} (2 \mathbf{Q}^n - \mathbf{Q}^{n-1}) \). \( \mathbf{A}_v, \mathbf{B}_v, \) and \( \mathbf{C}_v \) are Jacobian matrices defined as

\[
\mathbf{A}_v = \frac{\partial \mathbf{E}}{\partial \mathbf{Z}}, \quad \mathbf{B}_v = \frac{\partial \mathbf{F}}{\partial \mathbf{Z}}, \quad \mathbf{C}_v = \frac{\partial \mathbf{G}}{\partial \mathbf{Z}}
\]

and are derived as following:

\[
\begin{bmatrix}
U \rho_p & \rho l_x & \rho l_y & \rho l_z & U \rho_T & U \rho_f \\
U l_x + uU \rho_p & \rho (U + ul_x) & \rho ul_y & \rho ul_z & uU \rho_T & uU \rho_f \\
U l_y + vU \rho_p & \rho vl_x & \rho (U + vl_y) & \rho vl_z & vU \rho_T & vU \rho_f \\
U l_z + wU \rho_p & \rho wl_x & \rho wl_y & \rho (U + wl_z) & wU \rho_T & wU \rho_f \\
(\rho h_{p} + \rho h_{p})U & \rho (h_{l_x} + uU) & \rho (h_{l_y} + vU) & \rho (h_{l_z} + wU) & (\rho h_{p} + \rho h_{p})U & (\rho h_{p} + \rho h_{p})U \\
fU \rho_p & \rho fl_x & \rho fl_y & \rho fl_z & fU \rho_T & (f \rho_f + \rho)U
\end{bmatrix}
\]

(3.58)

If we replace \( l \) with \( \xi, \eta, \) and \( \zeta \) we can get \( \mathbf{A}_v, \mathbf{B}_v, \) and \( \mathbf{C}_v \), respectively.

At this point, the eigenvalues and eigenvectors of the preconditioned system can be derived. Let
\[ S = \Gamma + d \frac{\Delta \tau}{\Delta t} T = \left(1 + \frac{3 \Delta \tau}{2 \Delta t}\right), \]

\[
\begin{pmatrix}
\rho_p^* & 0 & 0 & 0 & \rho_T & \rho_f \\
\rho_p^* u & \rho & 0 & 0 & u \rho_T & u \rho_f \\
\rho_p^* v & 0 & \rho & 0 & v \rho_T & v \rho_f \\
\rho_p^* w & 0 & 0 & \rho & w \rho_T & w \rho_f \\
\rho_p^* h_i + \frac{T}{\rho} \rho_T & \rho u & \rho v & \rho w & \rho c_p + h_i \rho_T & \rho_E + \rho E_f \\
\rho_p^* f & 0 & 0 & 0 & \rho_T f & \rho f \rho_f
\end{pmatrix}, \tag{3.59}
\]

where \( \rho_p^* = \frac{\gamma + \frac{3 \Delta \tau}{\beta} \frac{\partial}{\partial \rho} \left( \frac{\partial}{\partial p} \right)_{T,x} 1 + \frac{3 \Delta \tau}{2 \Delta t} \). Then \( S^{-1} \) can be derived as:

\[
S^{-1} = \frac{1}{1 + \frac{3 \Delta \tau}{2 \Delta t}} \begin{pmatrix}
g_{11} & \frac{u \rho_T}{d} & \frac{v \rho_T}{d} & \frac{w \rho_T}{d} & -\frac{\rho_T}{d} & g_{16} \\
-\frac{u}{\rho} & 1 & 0 & 0 & 0 & 0 \\
-\frac{v}{\rho} & 0 & \frac{1}{\rho} & 0 & 0 & 0 \\
-\frac{w}{\rho} & 0 & 0 & \frac{1}{\rho} & 0 & 0 \\
g_{51} & -\frac{u \rho_T^*}{d} & -\frac{u \rho_T^*}{d} & -\frac{u \rho_T^*}{d} & \frac{\rho_T^*}{d} & g_{56} \\
-\frac{f}{\rho} & 0 & 0 & 0 & 0 & \frac{1}{\rho}
\end{pmatrix}, \tag{3.60}
\]

where

\[
g_{11} = \frac{1}{d} \left\{ \rho c_p + \rho_T \left[ h - \frac{1}{2} (u^2 + v^2 + w^2) \right] + \left( \rho_f c_p - f \rho_T h_f \right) \right\}, \tag{3.61}
\]

\[
g_{16} = \frac{1}{d} \left( \rho_T h_f - c_p \rho_f \right),
\]
$$g_{51} = \frac{1}{d} \left\{ -\frac{T}{\rho} \rho_T + \rho_p^* \left[ h - \frac{1}{2} (u^2 + v^2 + w^2) \right] \right\} \left( \rho_f h_f - c_p \rho_f \right),$$

$$g_{16} = \frac{1}{d} \left( \frac{T}{\rho^2} \rho_f \rho_T - \rho_p^* h_f \right), \text{and } d = \rho c_p \left( \rho_p^* - \frac{\gamma - 1}{\epsilon} \right).$$

$$S^{-1}A_v = \frac{1}{1 + \frac{3 \Delta \tau}{2 \Delta t}} \begin{pmatrix}
U \epsilon' & \frac{\rho^2 c_p}{d} l_x & \frac{\rho^2 c_p}{d} l_y & \frac{\rho^2 c_p}{d} l_z & 0 & 0 \\
\frac{l_x}{\rho} & U & 0 & 0 & 0 & 0 \\
\frac{l_y}{\rho} & 0 & U & 0 & 0 & 0 \\
\frac{l_z}{\rho} & 0 & 0 & U & 0 & 0 \\
\frac{U}{d} \left( -\frac{T}{\rho} \rho_T \right) \left( \rho_p - \rho_p^* \right) & -\frac{T \rho_T}{d} l_x & -\frac{T \rho_T}{d} l_y & -\frac{T \rho_T}{d} l_z & U & 0 \\
0 & 0 & 0 & 0 & 0 & U
\end{pmatrix}.$$
where $B_1 = -\frac{T \rho_T}{\rho^2 c_p} \frac{\lambda_5 - \varepsilon' U b}{\lambda_5 - \lambda_4}$, and $B_2 = -\frac{T \rho_T}{\rho^2 c_p} \frac{\lambda_6 - \varepsilon' U b}{\lambda_4 - \lambda_5}$.

Following Swanson and Turkel (1992), the matrix dissipation term in $\xi$ direction is given by:

$$AD_\xi = d_{i+1/2} - d_{i-1/2},$$

(3.66)
\[
\mathbf{d}_{i+1/2} = \mathbf{\Gamma}_{i+1/2} |\mathbf{A}|_{i+1/2} \left( \varepsilon_{i+1/2}^{(2)} \frac{\partial \mathbf{Z}}{\partial \xi}_{i+1/2} - \varepsilon_{i+1/2}^{(4)} \frac{\partial^3 \mathbf{Z}}{\partial \xi^3}_{i+1/2} \right), \tag{3.67}
\]

\[
|\mathbf{A}|_{i+1/2} = \mathbf{M}_{i+1/2} |\mathbf{A}|_{i+1/2} \mathbf{M}^{-1}_{i+1/2}, \tag{3.68}
\]

where \( \mathbf{A} = \text{diag} \left( \lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5, \lambda_6 \right) \). The half point values are evaluated using Roe averaging technique. To avoid numerical difficulties caused by zero artificial viscosity at stagnation points or sonic regions, the eigenvalues are limited by:

\[
|\lambda_i| = \max \left( |\lambda_i|, V_n \rho(A) \right), \text{ with } \rho(A) = \max (\lambda_i), i = 1, 6. \tag{3.69}
\]

The higher-order term is not helpful to TVD or upwinding property, but is intended to eliminate high frequencies and accelerate numerical convergence.

The artificial dissipation coefficient \( \varepsilon^{(2)} \) is based on the following switch:

\[
\varepsilon_{i+1/2}^{(2)} = \kappa^{(2)} \max (\nu_i, \nu_{i+1}), \quad \nu_i = \max \left( \frac{(p_{i+1} - 2p_i + p_{i-1})}{\left[ (1 - \omega)(|p_{i+1} - p_i| + |p_i - p_{i-1}|) + \omega(p_{i+1} - 2p_i + p_{i-1}) \right]}, \frac{(T_{r+1} - 2T_i + T_{r-1})}{\left[ (1 - \omega)(|T_{r+1} - T_i| + |T_i - T_{r-1}|) + \omega(T_{r+1} - 2T_i + T_{r-1}) \right]}, \frac{(\rho_{r+1} - 2\rho_i + \rho_{r-1})}{\left[ (1 - \omega)(|\rho_{r+1} - \rho_i| + |\rho_i - \rho_{r-1}|) + \omega(\rho_{r+1} - 2\rho_i + \rho_{r-1}) \right]} \right), \quad (3.70)
\]

\[
\varepsilon_{i+1/2}^{(4)} = \max \left[ 0, (\kappa^{(4)} - \varepsilon_{i+1/2}^{(2)}) \right],
\]

where \( \frac{1}{4} \leq \kappa^{(2)} \leq \frac{1}{2}, \quad \frac{1}{64} \leq \kappa^{(4)} \leq \frac{1}{32}, \quad 0.05 \leq \omega \leq 0.5. \)

The resulting scheme is TVD if using the switches as given above.
3.3 Temporal Discretization

The physical time derivatives in Eq. 3.34 are evaluated by general backward differencing

\[
\frac{\partial Q}{\partial t} = \frac{1}{\Delta t} \left[ a_i Q^{m+1} - \phi(Q^n, Q^{n-1}, \cdots) \right]. \quad (3.71)
\]

The coefficient \( a_i \) and function \( \phi \) in Eq. 3.71 can be specified to any level of temporal accuracy desired. In the current work, a three-point backward difference with second-order accuracy is employed. For this situation

\[
a_i = \frac{3}{2}, \quad \phi = \frac{1}{2} (4Q^n - Q^{n-1}) . \quad (3.72)
\]

The superscripts \( m \) and \( n \) denote iterations within the pseudo-time domain (inner-loop) and physical time domain (outer-loop), respectively. The physical time term \( Q^{m+1} \) can be linearized as

\[
Q^{m+1} = Q^m + T \Delta Z^{m+1} . \quad (3.73)
\]

Substituting Eq. 3.71 and Eq. 3.73 into Eq. 3.34 yields the following discretized system

\[
\left\{ \Gamma + \frac{\Delta \tau}{\Delta t} \right\} \Delta Z + \left( E_{\xi} - E_{\xi}^{(i)} \right)_{(i-1/2,j,k)} + \left( F_{\eta}^{(i)} - F_{\eta}^{(j)} \right)_{(i,j-1/2,k)} + \left( G_{\zeta} - G_{\zeta}^{(i,j,k)} \right)_{(i,j,k-1/2)} = H^{m+1} - \frac{\Delta \tau}{\Delta t} (a_i Q^m - \phi) . \quad (3.74)
\]

A fourth-order Runge-Kutta (RK-4) scheme is used to solve the governing equation 3.74 in the pseudo-time space due to its higher temporal accuracy and relatively larger CFL number requirement (i.e., \( 2\sqrt{2} \) for an Euler calculation using RK-4). A thorough investigation of the stability characteristics of the RK-4 method, based on convection of the turbulence energy-
spectrum, has been performed by Apt and Yang (2001) to establish its creditability and accuracy. Using the four-stage Runge-Kutta scheme, each pseudo-time integration is completed through four consecutive intermediate steps, as given below

\[ Z_0 = Z^m, \]
\[ Z_1 = Z^m + \Delta Z_1, \quad (\Gamma + \frac{\Delta \tau}{\Delta t} T - \Delta \tau D)\Delta Z_1 = \alpha_1 \Delta \tau \cdot R(Z_0), \]
\[ Z_2 = Z^m + \Delta Z_2, \quad (\Gamma + \frac{\Delta \tau}{\Delta t} T - \Delta \tau D)\Delta Z_2 = \alpha_2 \Delta \tau \cdot R(Z_1), \] (3.75)
\[ Z_3 = Z^m + \Delta Z_3, \quad (\Gamma + \frac{\Delta \tau}{\Delta t} T - \Delta \tau D)\Delta Z_3 = \alpha_3 \Delta \tau \cdot R(Z_2), \]
\[ Z^{m+1} = Z^m + \Delta Z^{m+1}, \quad (\Gamma + \frac{\Delta \tau}{\Delta t} T - \Delta \tau D)\Delta Z^{m+1} = \Delta \tau \cdot R(Z_3), \]

where

\[ R(z) = H^m - \frac{1}{\Delta t} (a_1 Q^n - \phi) - I \left( E_z - E_{\phi} \right) \bigg|_{i-1/2,j,k}^{i+1/2,j,k} + \left( F_{\phi} - F_z \right) \bigg|_{i,j-1/2,k}^{i,j+1/2,k} + \left( G_{\phi} - G_z \right) \bigg|_{i,j,k-1/2}^{i,j,k+1/2}. \] (3.76)

Superscripts ‘m’ and ‘m+1’ stand for the solution at the ‘mth’ and ‘m+1 th’ pseudo-time steps, respectively. The coefficients \( \alpha_1, \alpha_2, \) and \( \alpha_3 \) can be varied to obtain a variety of schemes with different stability properties. The standard four-stage scheme has the following values (Jameson, 1983)

\[ \alpha_1 = \frac{1}{4}, \quad \alpha_2 = \frac{1}{3}, \quad \alpha_3 = \frac{1}{2}. \] (3.77)
The iterative solution of given governing equations begins from pseudo-time iteration (inner-loop). At convergence in pseudo-time, \( Q^m = Q^{m+1} = Q^{n+1} \), the solution is advanced one physical time step (outer-loop).

In order to enhance numerical efficiency and minimize the complexity arising from the irregular shape of the computational mesh, a curvilinear coordinate transformation of the governing equations is employed so that the grid spacing in the transformed domain is unity. This is equally important for the use of spatial filtering in the LES technique. Non-uniform filter sizes directly violate the assumptions behind the filtering approach. One has to apply the numerical methodology in the body-fitted coordinate system.

### 3.4 Boundary Conditions

In all cases considered, second-order accurate boundary conditions are implemented. The inlet and exit conditions are specified using the method-of-characteristics (MOC). Inviscid, adiabatic and non-analytic conditions are imposed at the solid wall. Elsewhere conditions are specified using second-order extrapolated values. These conditions produce zero normal gradients with respect to pressure, velocity, temperature, and species mass fraction.

#### 3.4.1 Characteristic Boundary Conditions

At the inlet and outlet boundary, care must be taken when specifying the numerical boundary conditions. One has to ensure that the unphysical spurious wave reflections are avoided at the boundary and the flow is capable of relaxing to ambient conditions in the prescribed ways, which can be satisfied using the MOC proposed by Poinset and Lele (1992). In the absence of a
significant diffusion processes, the MOC method provides correct number of conditions that must be specified, as well as conditioned information from the interior domain.

Implementation of the MOC procedure involves diagonalizing the governing system to a quasi one-dimensional characteristic form

\[
[S + LM^{-1} \Gamma^{-1} (\Gamma + \frac{\Delta \tau}{\Delta t} T - \Delta \tau D)] \Delta Z = -LM^{-1} \Gamma^{-1}
\]

\[
\left\{ \left( \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial G}{\partial z} \right) + \tilde{\Omega} + \frac{\Delta \tau}{\Delta t} \left( a_i Q^m - \phi \right) - H \right\}. \tag{3.78}
\]

All of the terms in Eq. 3.78 are evaluated at cell centroids using the finite difference methodology. The term \( \tilde{\Omega} \) is the vector of specified boundary conditions. The term \( L \) is a selection matrix that singles out the desired characteristics at respective boundaries. The Jacobian matrix \( S \) is defined as \( S = \frac{\partial \tilde{\Omega}}{\partial Z} \).

In the absence of significant diffusion processes, the MOC procedure dictates the correct number of conditions that must be specified at each boundary and provides well conditioned information from the interior domain. In this study, the conditions imposed at the inlet and exit planes are always subsonic. At the inlet, there is one outgoing characteristic and \( N+3 \) conditions must be specified. Here the temperature, velocity, and species concentrations are employed assuming fully-developed turbulent channel flow. These conditions are given by
\[
\begin{aligned}
\mathbf{L}_{\text{inlet}} &= \Delta V \\
&= \begin{pmatrix}
0 \\
\tilde{u} - \tilde{u}_{\text{ref}} \\
\tilde{v} - \tilde{v}_{\text{ref}} \\
\tilde{w} - \tilde{w}_{\text{ref}} \\
\tilde{T} - \tilde{T}_{\text{ref}} \\
\tilde{Y}_1 - \tilde{Y}_{1\text{ref}} \\
\vdots \\
\tilde{Y}_N - \tilde{Y}_{N-1\text{ref}}
\end{pmatrix},

\mathbf{L}_{\text{inlet}} &= \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0
\end{pmatrix}.
\end{aligned}
\] (3.79)

where \( \tilde{u}_{\text{ref}}, \tilde{v}_{\text{ref}}, \tilde{w}_{\text{ref}}, \tilde{T}_{\text{ref}}, \tilde{Y}_{1\text{ref}}, \ldots, \tilde{Y}_{N-1\text{ref}} \) represent the specified values of velocity, temperature, and species mass fraction, respectively. At the exit, there are \( N+3 \) outgoing characteristics and one condition must be specified. Here a far-field pressure condition is simulated using the methodologies proposed by Rudy and Strikwerda (1980), Poinsot and Lele (1992), and Baum et al. (1995).

To simulate the far-field boundary the incoming characteristic given by Eq. 3.78 is modified to provide a nonreflecting outflow condition. The equation of interest is given by the selection matrix

\[
\mathbf{L} = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0
\end{pmatrix}.
\] (3.80)

Associate with this equation is the term
\[ \Pi_2 = \lambda_2 \left[ \frac{1}{\varepsilon} \left( \frac{u}{a} \frac{\partial p}{\partial x} - \rho a \frac{\partial u}{\partial x} \right) \right] , \tag{3.81} \]

which characterizes the time variation of the normal component of acoustic waves which propagate from an infinitely distant downstream source into the computational domain. The term \( \lambda_2 \) is the acoustic eigenvalue given by Eq. 3.20. The terms \( p \) and \( u \) represent the pressure and axial velocity, respectively. Conceptually, a perfectly non-reflecting subsonic outflow condition can be obtained if this term is set equal to zero. Specifying such a condition, however, eliminates the information provided by the acoustic waves and leads to an ill-posed problem. To simulate this information Rudy and Strikwerda (1980), Poinsot and Lele (1992), and Baum et al. (1995) have proposed that Eq. 3.81 be replaced with the term

\[ \Pi_2^t = k(p - p_\infty) , \tag{3.82} \]

where \( k \) is a constant that determines the speed with which the average pressure in the computational domain relaxes towards the imposed pressure at infinity \( p_\infty \). This condition introduces small amplitude acoustic waves using scaling arguments that are based on known quantities at the exit. Rudy and Strikwerda (1980) propose that optimal values of \( k \) are given by

\[ k = 2 \frac{\sigma}{x_c} \frac{\varepsilon a^2 (1 - \overline{M}^2)}{\sqrt{u(1 - \varepsilon)^2 + 4\varepsilon a^2}} . \tag{3.83} \]

The factor presented here has been modified from that given by Rudy and Strikwerda (1980) to accommodate the dual-time preconditioned system. Here \( \overline{M}^2 \) represents the maximum Mach number in the computational domain, \( x_c \) is the characteristic axial length of the domain, \( \varepsilon \) is the local preconditioning factor, and \( a \) is the local speed of sound. The term \( \sigma \) is a scaling factor used for optimization. Poinsot and Lele (1992), and Baum et al. (1995) have shown that
values ranging from 0.25 to 0.5 provide the best results. When lower values are specified, solutions tend to drift away from the reference pressure. When larger values are specified, flow oscillations are introduced.

To implement the MOC methodology with the far field pressure condition described above, the $N + 3$ outgoing characteristics are selected and the incoming characteristic is modified by replacing the incoming wave amplitude given by Eq. 3.81. These conditions are given by

$$
\tilde{\Omega}_{outlet} = \Delta V \left( p - p_{ref} \right) = \begin{bmatrix}
0 \\
0 \\
0 \\
0 \\
0 \\
\vdots \\
0
\end{bmatrix} = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1
\end{bmatrix}.
$$

(3.84)

The far-field pressure condition has been shown to be effective in reducing reflections at the subsonic exit boundary and is relatively accurate and stable.

### 3.5 Parallel Implementation

Because the explicit time stepping numerical scheme (RK4) was applied in the current study, only the neighboring data instead of the data from the whole computational domain were required during the calculation of variables in each cell. Since the data dependence is weak, the domain decomposition technique is best suited for this kind of application. It is also commonly implemented in distributed-memory parallel computer systems. In the field of computational
fluid dynamics (CFD), it is generally referred to as mesh partitioning, based on the geometric substructure of the computational domain. In the domain-decomposition technique, the physical domain is divided into several sub-domains. Variables in each cell are updated to the next time step simultaneously. In order to calculate the spatial derivatives at the sub-domain boundaries, ghost cells or halo data around the computing cells are introduced. Figure 3.4 shows an example of a two-dimensional sub-domain with ghost cells. Because the variables in the ghost cell are updated in another sub-domain, message passing is required to synchronize data between different sub-domains. The communication overhead is directly proportional to the volume-to-surface ratio of the grid system in that sub-domain. Maximizing the computation-to-communication ratio leads to higher parallel execution efficiency.

Figure 3.4. Schematic of a two-dimensional sub-domain with ghost cells

Figure 3.5 shows the High Performance Computing (HPC) clusters used to conduct the large-scale computations required in the current studies. The system has two high-performance
servers and 59 Quad-socket hex-core compute nodes (with a total number of 1416 CPU’s), connecting through 32 Gbps high-speed Infiniband Fabric switches for high parallel efficiency. Each computing node contains 24 AMD 2.4 GHz processors and 64 GB RAM. The system can sustain 3.3 teraFLOPS peak speed, providing substantial number-crunching capabilities for large-scale calculations.

Parallel operation is accomplished through the implementation of MPI (Message Passing Interface) libraries. Representative parallel performance of CFD algorithms on 100 AMD 2.4 GHz processors with fast Infiniband interconnections is about 90% efficient.

Figure 3.5. Infiniband switch connected high performance computing clusters.
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Chapter 4

Validation of the Numerical Scheme

4.1 Problem Description

Sandia Flame D is a piloted methane-air jet flame stabilized on a burner developed at the University of Sydney (Masri et al., 1996). The Flame D has a small probability of local extinction and a moderate Reynolds number of 22400. The velocity field is measured with a Laser Doppler Velocimetry (LDV) technique by Schneider et al. (2003); and the temperature is obtained with Rayleigh measurements; the mass fractions of the chemical species and the mixture fraction are achieved with the Raman and LIF measurements, by Barlow and Frank (1998). It has been simulated by many researchers as a part of their code validation studies (for example, Pitsch and Steiner, 2000, Cutrone et al., 2010). Hence, it has also been selected for the validation case in the present study. The steady flamelet model is not applicable to this flame, as the fuel is partially premixed. Consequently, the Flamelet/Progress-Variable approach is used. As the two models are quite similar in implementation, this also validates the Flamelet model.

The methane fuel is diluted with air. The volume fraction of air is 75%. The fuel is injected through a nozzle (ID 7.2 mm, OD 7.7 mm) at a mean bulk velocity of 49.6 m/s, a temperature of 294 K, and a pressure of 0.1 MPa. The pilot nozzle has an inner diameter of 18.2 mm and an outer diameter of 18.9 mm. The pilot flame is a lean mixture of C\textsubscript{2}H\textsubscript{2}, H\textsubscript{2}, air, CO\textsubscript{2},
and N\textsubscript{2} with the same nominal enthalpy and chemical equilibrium composition as the main jet at an equivalence ratio of 0.77. The heat release of the pilot flame is about 6\% of the main jet flame. The mean bulk velocity of the pilot jet is 11.4 m/s. The entire jet flame is enclosed by an air flow at a velocity of 0.9 m/s and at 291 K.

Figure 4.1 shows a two-dimensional slice of the computational domain and the grid distribution with every 6th grid point in axial and radial directions. It has 310 points in the axial direction, 130 points in the radial direction, and 64 points in the azimuthal direction, respectively, and a center region that consist of a 16 × 16 × 310 grid distribution to avoid the singularity problem. The total number of grid points is 2.96 million. The grid is divided into 142 blocks for parallel computing. The grid is clustered at the wall, with 26 grid points for the resolution of the thickness of the nozzle rim. The computational domain covers 17 jet diameters at injector exit, and 43 jet diameters at the domain exit in the radial direction. The length of the computational domain is 83 jet diameters.

In the numerical simulation, the inlet velocity profile is given as a sum of the experimental mean velocity profile and broad-band white noise fluctuations that have the same turbulence intensity as in the experiment. The static Smagorinsky model, associated with the Flamelet/Progress-Variable turbulent combustion model is used in this simulation. FlameMaster code developed by Pitsch (1998) associated with the 72-step reduced kinetic mechanism developed by Peters and Rogg (1993) has been used to generate the flamelet library. The code is first run for more than three flows through times before time-averaged data are collected.
4.2 Results and Discussion

Figure 4.2 shows the instantaneous temperature distribution of the jet flame after the flow achieves stationery state. The color scale is cutoff at 400 K for a better illustration of the flow field. It is clearly observed that the jet flame features very dynamic flow and flame structures a few jet diameters away from the nozzle exit. A bright flame zone is showing around x/D = 40, where the mixing, and the combustion of the fuel and oxidizer is complete and thus a maximum flame temperature is achieved. The flame tip is located around x/D = 65, which is very close to the visible flame length of 67 jet diameters measured in the experiments. It is also noted that in the vicinity of the fuel nozzle exit, the flow structures resemble that of a laminar flow. This has also been found in many other experimental and numerical studies. In this laminar flow region, the effect of differential diffusion effect might be important and strongly affect the flame structures further downstream for fuels that have Lewis numbers different from unity. For the methane air flame, the Lewis number is close to unity, and thus this effect is not expected to be important.

Figure 4.3 shows the profiles of the mean axial velocity and its root mean square (RMS) value along the centerline of the jet flame. The prediction agrees fairly well with the experimental results. However, the velocities are over predicted near the injector exit, but are accurately predicted in the downstream (x > 40D). This is explained by the lower value of the RMS velocity near the injector exit. It indicates that the turbulent motions in the near injector exit are very weak in the simulation. This phenomenon persists when the coefficients of turbulent viscosity and artificial dissipation are minimized in this region. This is probably due to the treatment of the inlet boundary condition. Random noise is added to the mean velocity profile to mimic the turbulence fluctuations. However, this approach might not be the best way to
implement the turbulence conditions at the inlet (Sagaut, 2001). The predicted velocity profile can be significantly improved by giving better inlet boundary conditions.

Figure 4.3 also shows the mean temperature profiles along the jet centerline. The mean temperature agrees very well with the experiment result. The predicted RMS values are also very accurate. Even the local minimum of the RMS temperature is well captured. However, the temperature is under-predicted near the injector exit. This is due to two reasons: (1) low turbulent fluctuations at the center-line; (2) neglect of radiation heat transfer in the present analysis. Radiation heat transfer from the encompassing flames might increase the centerline temperature significantly (Modest, 2003). In the far downstream region, the predicted temperature is under predicted by about 300 K. It is also noticed that the mass fraction of oxygen is much larger than the experiment measurements in this region; and that the mass fraction of combustion products are significantly under-predicted in the same region. It seems that there is excessive mixing here to dilute the high temperature combustion products. The reasons for this prediction can be partially attributed to the coarse grid resolution in this region. The grid size at the exit is more than 30 times that at the injector exit; however, the flame width is only about 5 times larger than that at the injector exit. The coarse grid resolution may cause the under-prediction of the centerline temperature.

The centerline mixture fraction profile is very close to that of the experimental results in a very large region. However, more than 10% deviation is observed in the upstream region of the injector exit, that is, 10 to 20 jet diameters from the jet exit. This is consistent with the axial velocity profiles. The large-scale motions are not well predicted in this region, so that the resulting jet center region is not affected by the outer mixing layer in the upstream region, and a long fuel jet is obtained. The mass fractions of major combustion products show similar trend as that of the mixture fraction and temperature. In the upstream region, the combustion of the
centerline region is delayed and less combustion products are present at the jet centerline. Going downstream, as the large-scale turbulent motions develop, the jet breaks down, and the mixing of the fuel and oxidizer is more complete, associated with a better prediction of the mass fractions of the combustion products, and temperature.

The radial profiles of mean axial velocity, mean temperature, and the corresponding RMS values at different axial locations are shown in Figure 4.4. Overall speaking, the agreement with the experimental results is reasonably good. In the upstream region (x/D = 15), the centerline temperature is under-predicted by almost 200 K; however, the peak value of the temperature is over-predicted by about 200 K. The mean axial velocity at this location shows very good agreement with the experimental values, with a small deviation at the centerline. The centerline jet velocity is almost the same as the inlet velocity, indicating rare turbulent fluctuations are present near the jet centerline. It is noted that the RMS velocity is about 50% smaller than that of the experimental value, at regions that are far from the mixing layer. This indicates that the predicted turbulent fluctuations are too weak to affect the jet centerline, as well as the far outer region of the flame. If better turbulent motions are predicted at this location, the radial profile of the mean temperature is expected to be much better. In the further downstream region (x/D = 30), the temperature is systematically under-predicted by about 10%, especially in the outer region of the flame. The velocity profiles at the same location can partially explain this result. The centerline velocity is still 20% larger, but the RMS value at the centerline already becomes close to the experimental value. However, the outer region of the flame is still characterized with a much smaller RMS value, indicating a less dynamic outer region than that of the experiment. The effect of the turbulence under-prediction is that less fuel and oxidizer are mixed and burned, and less combustion products can be brought to the outer region. Thus, the temperature at this location is low. In the far downstream region (x/D= 45), all the radial profiles agree very well
with the experimental measurements, except for a 10% over-prediction of the centerline jet velocity. It means that the predictions become much better as turbulent motions develop along the axial direction.

From the above analysis, it is clear that the combustion of the partially premixed jet flame is mainly controlled by the turbulent motions, instead of the chemical reaction. Very good predictions can be achieved when turbulence is well predicted. Extreme caution is required for the treatment of turbulence modeling to achieve physically meaningful results.

To further evaluate the performance of the turbulent combustion model, the conditionally averaged quantities are presented in Figures 4.5 and 4.6. It is clear that the conditionally averaged predictions are in very good agreement with that of the experimental values. In the upstream region (x/D =15), although the mass fractions of CO$_2$ and CO are very good, the mass fractions of the fuel, oxidizer are under-predicted in the rich region, while H$_2$O and H$_2$ are over-predicted in the rich region. This indicates that the predicted combustion in the rich regions is more intensive than in the experimental case. This means an over-prediction of the reaction rate in the rich region. However, in further downstream regions, (x/D = 30, and x/D =35), all the profiles are in very good agreement with that of the experimental measurements. The experimental uncertainties are 3% for temperature, 4% for the mass fractions of water and CO$_2$, 10% for OH, and 10-20% for CO (Barlow and Frank, 1998). Considering these experimental uncertainties, and the above discussion, the present results agree quite well with the experimental results, and validate the numerical scheme.
Figure 4.1. Grid distribution on a two dimensional slice (every 6th grid point in axial and radial directions).

Figure 4.2. Instantaneous temperature distribution. a) the entire jet flame, b) the upstream region.
Figure 4.3. Profiles of mean axial velocity, mean temperature, mean mixture fraction, and mean mass fractions along flame centerline: symbols, the experimental data; lines, the current LES results.
Figure 4.4. Radial profiles of mean axial velocity, mean temperature, mean mixture fraction, and mean mass fractions along flame centerline: symbols, the experimental data; lines, the current LES results.
Figure 4.5. Conditionally-averaged temperature, and mass fractions of oxygen, methane, CO₂, and CO at different axial locations: symbols, the experimental data; lines, the current LES results.
Figure 4.6. Conditionally-averaged mass fractions of \( \text{H}_2\text{O} \), \( \text{H}_2 \), and \( \text{OH} \) at different axial locations: symbols, the experimental data; lines, the current LES results.
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Chapter 5

Cryogenic Fluid Dynamic Response of Swirl Injector to External Forcing at Supercritical Conditions

In liquid rocket engines, injection is a key process, through which all feedback couplings of the combustion chamber with other engine components are realized. In addition to its main function of providing a combustible mixture, an injector also acts as a sensitive element that may generate and modify the flow oscillations (Bazarov and Yang, 1998).

As discussed in Chapter 1, the dynamic characteristics of injectors are of great importance to the performance of the entire combustion system. To investigate the dynamic response of the cryogenic fluid dynamics of swirl injectors to external forcing at supercritical conditions, the previous study by Zong and Yang (2008) is extended to investigate the flow dynamics with external forcing. External forcing is imposed through periodic oscillations of the mass flow rate at the injector tangential inlets over a broad range of frequencies relevant to the intrinsic flow instabilities of the injector.

5.1 Injector Configuration and Flow Conditions

The geometry of the swirl injector remains identical to the baseline case of the previous study (Zong and Yang, 2008). Figure 5.1 shows a schematic diagram of a swirl coaxial injector. For simplicity, only the central LOX post of the coaxial injector is considered, which is referred
to as a simplex swirl injector. Although the effect of the coflow gas and/or the interactions between the liquid and gas streams cannot be included in simplex swirl injector studies, it is still very valuable to study the dynamic response of these injectors, as have been done by many other researchers (Bazarov and Yang, 1998, Inamura et al., 2001, 2003, Kim et al., 2007, Richardson et al., 2007, Fu et al., 2010). With the simplified geometry configuration, focus can be placed on the dynamic characteristics of the central element, without involving too many uncertainties associated with the flow interactions between the swirling liquid flow and the coaxial gaseous flow. The studies on simplex swirl injectors can also serve as a comparison basis to sharpen our knowledge in the dynamics of swirl coaxial injector flows. The geometrical parameters of the injector under consideration are listed in Table 5.1, where $R_s$, $R_n$, and $R_p$ denote the radii of the vortex chamber, discharge nozzle, and tangential inlet, respectively, and $L$ is the injector length (Zong and Yang, 2008). The geometrical characteristic constant $K$ is defined as $K \equiv A_n R_{in} / A_{in} R_n$, where $R_{in}$ is the radial location of the inlet passage center, $A_n$ is the nozzle area, and $A_{in}$ is the total area of tangential entries.

<table>
<thead>
<tr>
<th>$R_s$ (mm)</th>
<th>$R_n$ (mm)</th>
<th>$R_p$ (mm)</th>
<th>$L$ (mm)</th>
<th>$K$</th>
<th>$\dot{m}$ (kg/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>2.5</td>
<td>0.85</td>
<td>25</td>
<td>3.2</td>
<td>0.15</td>
</tr>
</tbody>
</table>

Table 5.1. Baseline injector dimensions and mass flow rate.

Liquid oxygen with a fixed temperature of 120 K is injected from the tangential passages into the injector tube and is then delivered downstream to the ambient gaseous oxygen, which is at 300 K and 10 MPa. For reference, the critical pressure and temperature of oxygen are 5.04 MPa and 154.6 K, respectively.
External forcing, imposed by pulsating the mass flow rate at selected frequencies at the tangential inlet of the injector, is given by

\[
\dot{m} = \dot{m}_0 \left[ 1 + \alpha \sin 2\pi f_p t \right],
\]

where \(\alpha\) is the oscillation magnitude. The forcing frequency covers a range of 0.55-14 kHz, considering the broad band nature of the injector flow dynamics. Turbulence with an intensity of 8% of the mean flow quantity is provided by super-imposing broadband noise onto the instantaneous mass flow rate.

As discussed in Chapter 1, no experimental data are available for supercritical flow dynamics in swirl injectors. Thus no direct comparison with experimental results is made in the current simulation. The validity of the numerical scheme can be justified by the previous studies on supercritical fluid mixing (Zong et al., 2004, Liu et al., 2006). In those studies, the same numerical procedure as in the current study was used and validations were made against experimental data.

5.2 Liquid Film Thickness and Spreading Angle

The liquid film thickness \(h\) and the spreading angle \(2\alpha\) at the injector exit are often employed to characterize the injector performance of a swirl injector (Bazarov et al., 2004). The former dictates the size of the fluid parcel after the film breaks up, and the latter affects the intra-element mixing efficiency. The key variables influencing the injector flow dynamics include the geometric constant \(K\), the injector length \(L\), the injector exit diameter \(D_n\), and the thermophysical properties of the injected fluid, such as the density \(\rho\) and viscosity \(\mu\). Two dimensionless
equations for the film thickness and spreading angle can be obtained in terms of those variables (Zong and Yang, 2008).

\[
\frac{h}{D_n} = f \left( \frac{\rho_{inj}}{\rho}, \frac{u_{inj}}{u_\infty}, \text{Re}_L, K \right), \tag{5.2}
\]

\[
\alpha = \tan^{-1} \left( \frac{u_{el}}{u_{ex}} \right) = f \left( \frac{\rho_{inj}}{\rho}, \frac{u_{inj}}{u_\infty}, \text{Re}_L, K \right). \tag{5.3}
\]

The Reynolds number of the liquid film is defined as \( \text{Re}_L = \rho_{inj} u_n L / \mu_{inj} \). Among these parameters, the density and viscosity ratio are fixed for a given flow condition. The geometric constant and injector length are fixed for a given injector configuration.

In a steady state flow, the film thickness \( h \) has been defined to match the inlet mass flow rate and the local mass flow rate of the liquid film. This is given by:

\[
\dot{m}_l = \int_{R_c-h}^{R_c} \rho r u r 2\pi r dr. \tag{5.4}
\]

However, in studies with pulsating inlet mass flow rate, the instantaneous local mass flow rate is an unknown. Film thickness based on the net mass flow rate is introduced so that the instantaneous net mass flow rate \( \dot{m}_{net} \) is given by:

\[
\dot{m}_{net} = \pi \left[ R_n^2 - R_n^2 - h^2 \right] \bar{\rho}_l \bar{V}_l. \tag{5.5}
\]

where the subscript \( l \) denotes liquid. To evaluate \( \bar{\rho}_l \) and \( \bar{V}_l \), we first need to clarify the definition of a *liquid* at supercritical conditions. At these conditions, due to the reduction in surface tension and the enthalpy of vaporization, the two-phase concepts may introduce confusion under supercritical conditions. Bellan (2000) recommended that the boundary of a droplet submerged
in a supercritical environment be the location of the maximum density gradient. Following this concept, liquid here refers to the fluid between the injector wall and the surface of the local maximum density gradient. Since the density change is not considerable inside the high density region, it takes the value of the injection counterpart. $\bar{V}_l$ assumes the axial velocity that is averaged over the liquid film.

Different definitions of the film thickness, such as those based on the critical temperature and the maximum density gradient, are also used to calculate the film thickness. These are given by Eq. 5.6 and Eq. 5.7.

$$h_r = R_n - r|_{r=R_r} \quad (5.6)$$

$$h_{\text{max}\rho|} = R_n - r|_{\text{max}\rho|} \quad (5.7)$$

However, as it is shown in Figure 5.2, no significant difference in the film thickness is observed among the three definitions. In the rest of this paper, the film thickness given by Eq. 5.5 is used.

In the steady-state flow, the spreading angle is calculated from the ratio of mean circumferential and axial velocities. However, in the forcing studies, this definition is not applicable for the instantaneous spreading angle. In the present study, the spreading half angle at the injector exit is calculated in the liquid (the fluid encompassed by maximum density gradient surfaces), and then a mass weighted average is taken over the liquid to get the instantaneous spreading half angle.
5.3 Results and Discussion

5.3.1 Free Oscillation Flow

A parametric study has been conducted by Zong and Yang (2008) to investigate the effects of injector geometry and operating conditions on the liquid spray behavior over a pressure range of 10-20 MPa while keeping the temperature of liquid oxygen at 120 K and the ambience at 300K, respectively. After the liquid oxygen is delivered tangentially into the injector, under the influence of the centrifugal force, a gaseous core is formed, which connects the injector with the downstream region acoustically. Thus, any disturbance downstream of the injector may propagate upstream into the injector and affect the LOX film behavior through its influence on the mass flow rate. Furthermore, the acoustic resonance rises if the natural frequencies of the injector and the chamber match each other. The Liquid Oxygen (LOX) film is convected downstream along the wall before it exits the injector as a nearly conical sheet. This process features three-dimensional hydrodynamic instability waves in both longitudinal and circumferential directions, of which the former propagates in a form similar to that of a shallow-water wave in an incompressible flow, and the latter is convected downstream by the mean flow. The Power Spectral Density (PSD) analysis of the pressure fluctuations inside and near the exit of the injector reveals that the intrinsic instability modes are 0.55, 1.04, 3.15, and 14 kHz. The 0.55 kHz mode is closely related to the longitudinal wave of hydrodynamic instability within the LOX film. The harmonic of 3.15 kHz is attributed to the acoustic oscillation in the injector, which acts as a quarter-wave resonator with the natural frequency estimated to be 3.2 kHz. A dominant frequency of 1.04 kHz is related to the precession of the Central Toroidal Recirculation Zone (CTRZ) immediately downstream of the injector exit. The 14 kHz frequency fluctuations result
from the recirculating flow between the tangential inlet and the injector head-end and. Due to the viscous dissipation, these high-frequency fluctuations decay rapidly and disappear as the LOX film moves downstream. A Proper-Orthogonal-Decomposition (POD) analysis is conducted to extract energetic coherent structures from the calculated flow fields. The instability mode shapes are visualized in the POD analysis. The effect of flow conditions and geometry on injector behavior is also investigated. The results are compared with predictions from classical hydrodynamic theories in terms of the film thickness, spreading angle and velocity distributions.

5.3.2 Flow Evolution under External Forcing Conditions

Figures 5.3-5.9 show the temporal evolution of the temperature fields at forcing frequencies from 0.55 kHz to 14 kHz. Time is set to zero after the flow reaches a stationary state (about 10 flow-through times after the forcing is added). For all cases, similar to the free oscillation flow, the wave structures share some common characteristics. Small disturbances upstream of the injector develop as they are convected downstream. These structures feature three-dimensional hydrodynamic instability and propagate in a form similar to the shallow-water wave for an incompressible flow.

Low-frequency forcings (0.55 kHz and 1.0 kHz) significantly affect the flow field. As shown in Figures 5.3 and 5.4, small-sized high frequency disturbances were suppressed or weakened in fluctuating magnitude when the liquid film is larger than its average value. Small disturbances reappear when the liquid film becomes thin. Thus, the film thickness at the injector exit varies greatly as the inlet mass flow rate fluctuates at the forcing frequencies. The spreading angle and the breakup length of the liquid conical sheet fluctuate in a similar manner. The film thickness is closely related to the resulting droplet size, and the spreading angle affects the spray
fan, consequently the mixing efficiency. Low frequency forcing potentially couples with the heat release process and may even lead to system failures due to local intensified heat transfer at the injector face or the chamber wall.

The intermediate-frequency forcings (1.9 kHz, 2.1 kHz, 3.2 kHz and 6.0 kHz) generate similar influence on the flow dynamics. The hydrodynamic waves are more obvious and appear more often than they do in the natural oscillation case. The wave structures on the LOX film develop and evolve into an array of coherent structures and merge into larger-scale structures as they are convected downstream. Particularly for the 3.2 kHz and 6.0 kHz cases, the structures break up shortly after their appearance and dissolve into the high temperature environment.

The highest-frequency forcing (14 kHz) does not show any significant influence on the flow dynamics. The high-frequency fluctuations decay rapidly and disappear as the LOX film moves downstream due to viscous dissipation; therefore, forcing at this frequency does not affect the flow field significantly.

The frequency spectra of the pressure fluctuation, as shown in Figures 5.10-5.16, provide a more quantitative insight into those instability waves in the injector flow. The results show that the fluctuation at the forcing frequency has a spike profile in the frequency space. In addition, the forcing makes the power of the fluctuations at other frequencies much smaller, a situation commonly known as the frequency-locking phenomenon.

### 5.3.3 Dynamic Response at the Injector Exit

Figures 5.17-5.23 show the variations of the mass flow rate at the injector tangential inlet and the injector exit, as well as the variations of the film thickness and the spreading angle for all the forcing cases considered. The corresponding power spectral densities are also presented.
Except for the case of 14 kHz, all the other external forcings cause the mass flow rate and film thickness to vary in a more periodic manner and the fluctuation magnitude of the spreading angle to become larger, compared with the free oscillation flow. The observations are also consistent with the aforementioned temporal flow evolution and the PSD profiles. The external forcing extracts energy from the fluctuations of a wide range of frequencies and energizes the fluctuation at its own frequency.

Figures 5.24-5.25 show the time-averaged film thickness and the spreading angle as a function of forcing frequency. The bars in the figures show the root mean square of the fluctuations. Although neither the mean values nor the RMS of the film thickness and spreading angle change much with the external forcing frequencies, due to conservation of mass and momentum, the spectral energy distributions are much different, which may cause totally different dynamics response of the injector.

5.3.3.1 Mass Transfer Function

The injection dynamics can be quantified globally in terms of the mass transfer function, defined as:

$$\Pi_m f = \frac{\hat{m}_a}{\bar{m}_m},$$

(5.8)

where $\hat{m}_a$ is the Fourier component of the mass flow-rate fluctuation at the forcing frequency. Figure 5.26 shows the magnitude of mass transfer function as a function of the forcing frequency. This quantity reaches its maximum around 1.9 kHz, corresponding to the dominant frequency of the intrinsic injector flow instability under the condition without external forcing. The mass transfer function at 1.0-2.1 kHz is substantially larger than unity. This shows that the external
forcing suppresses or weakens fluctuations at other frequencies and energizes the fluctuations at their own frequencies. This can substantially alter the dynamic characteristics of the combustion system.

Table 5.2 shows the effect of forcing magnitude on the resulting time-average film thickness, spreading angle, and mass transfer function. The forcing magnitude is varied from 7.5% to 22.5% of the mean mass flow rate, and the forcing frequency is fixed at 3.2 kHz. For the first two cases, the resulting spreading angle and film thickness do not show much difference, indicating that an even smaller forcing level exerts almost the same effect on the atomization and mixing processes. The decrease in the value of transfer function implies that higher efficiency of forcing is achieved at a lower forcing amplitude. However, the largest forcing magnitude leads to a significant increase of the spreading angle as well as a reduction of the film thickness. This may result from the enhanced mixing of the low temperature oxygen with the warm environment due to the large-scale coherent structures under the large forcing magnitude condition. Inamura et al. (2003) also indicated that an increase in the mass flow rate resulted in a larger spreading angle. In the present study, due to the nonlinear effect of external forcing, the averaged spreading angle is increased greatly when the forcing magnitude reaches 22.5% of the mean mass flow rate.

Table 5.2. Effect of forcing magnitude.

<table>
<thead>
<tr>
<th>Forcing amplitude, $a$</th>
<th>Spreading angle, $2\alpha$, (deg)</th>
<th>Film thickness, $h$, (mm)</th>
<th>Transfer function, $\Pi_m(f)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.075</td>
<td>75.2</td>
<td>4.1</td>
<td>0.87</td>
</tr>
<tr>
<td>0.150</td>
<td>76.2</td>
<td>4.2</td>
<td>0.81</td>
</tr>
<tr>
<td>0.225</td>
<td>81.3</td>
<td>3.5</td>
<td>0.72</td>
</tr>
</tbody>
</table>
5.3.4 Conclusions

The dynamic response of a pressure swirl injector to external excitations has been investigated under supercritical conditions. The results show that forced flow is dominated by flow motions of the forcing frequencies except for the high-frequency forcing case. Although the time-averaged film thickness and spreading angle do not show significant variations compared to the unforced flow, the instantaneous spreading angle and the film thickness fluctuate strongly at the forcing frequency. Thus, the external forcing may affect the atomization and mixing processes significantly. It is also found that the external forcing can weaken or suppress fluctuations that are of frequencies different from that of the forcing; meanwhile, it energizes the flow motions that are of the forcing frequency. The calculated mass transfer function at some forcing frequencies can be substantially larger than unity. The effect of forcing magnitude is also studied. When the forcing magnitude is relatively small, the time-averaged spreading angle and film thickness show small variance; however when the forcing magnitude is very large, the time-averaged spreading angle and film thickness show very strong responses.
Figure 5.1. A schematic diagram of a pressure swirl injector.

Figure 5.2. Temporal evolution of film thickness based on different definitions.
Figure 5.3. Temporal evolution of temperature field, external forcing at 0.55 kHz.

Figure 5.4. Temporal evolution of temperature field, external forcing at 1.0 kHz.
Figure 5.5. Temporal evolution of temperature field, external forcing at 1.9 kHz.

Figure 5.6. Temporal evolution of temperature field, external forcing at 2.1 kHz.
Figure 5.7. Temporal evolution of temperature field, external forcing at 3.2 kHz.

Figure 5.8. Temporal evolution of temperature field, external forcing at 6.0 kHz.
Figure 5.9. Temporal evolution of temperature field, external forcing at 14 kHz.

Figure 5.10. Power spectral densities of pressure fluctuations at different locations inside the injector, external forcing at 0.55 kHz.
Figure 5.11. Power spectral densities of pressure fluctuations at different locations inside the injector, external forcing at 1.0 kHz.

Figure 5.12. Power spectral densities of pressure fluctuations at different locations inside the injector, external forcing at 1.9 kHz.
Figure 5.13. Power spectral densities of pressure fluctuations at different locations inside the injector, external forcing at 2.1 kHz.

Figure 5.14. Power spectral densities of pressure fluctuations at different locations inside the injector, external forcing at 3.2 kHz.
Figure 5.15. Power spectral densities of pressure fluctuations at different locations inside the injector, external forcing at 6.0 kHz.

Figure 5.16. Power spectral densities of pressure fluctuations at different locations inside the injector, external forcing at 14 kHz.
Figure 5.17. Mass flow rates, film thickness and spreading angle time history and their power spectral densities; external forcing at 0.55 kHz.

Figure 5.18. Mass flow rates, film thickness and spreading angle time history and their power spectral densities; external forcing at 1.0 kHz.
Figure 5.19. Mass flow rates, film thickness and spreading angle time history and their power spectral densities; external forcing at 1.9 kHz.

Figure 5.20. Mass flow rates, film thickness and spreading angle time history and their power spectral densities; external forcing at 2.1 kHz.
Figure 5.21. Mass flow rates, film thickness and spreading angle time history and their power spectral densities; external forcing at 3.2 kHz.

Figure 5.22. Mass flow rates, film thickness and spreading angle time history and their power spectral densities; external forcing at 6.0 kHz.
Figure 5.23. Mass flow rates, film thickness and spreading angle time history and their power spectral densities; external forcing at 14 kHz.

Figure 5.24. Variation of spreading angle with forcing frequency.
Figure 5.25. Variation of average film thickness at injector exit with forcing frequency.

Figure 5.26. Frequency spectrum of magnitude of injector mass transfer function. Effect of Forcing Magnitude.
Chapter 6

Large-Eddy Simulation of GO₂/GH₂ Combustion of a Shear Coaxial Injector

Cryogenic oxygen and hydrogen propellants associated with shear coaxial injectors have been prevalingly used in liquid-propellant rocket engines, such as RL-10, SSME, RS-68, LE-7 and Vulcain2, due to the high specific impulse (Isp) and the historical experience with them in western society. However, the development of all of the existing liquid rocket engines have relied heavily on costly and time-consuming tests, with the guidance of rules of thumb and empiricism (Tucker et al., 2007). It has been common to copy from previous successful designs and apply small and incremental changes and validation tests to meet requirements for a new application. However, in the highly nonlinear combustion system, small changes might result in significant changes to the system, rendering no guarantee of success for the new designs. Thus, the tedious and costly iterative trial and error process cannot be avoided before a feasible design can be achieved. This situation exists only because the current understanding of a series of non-linear physicochemical processes occurring in the geometrically complicated combustion device under extreme operating conditions is not sufficient, as discussed in the introduction chapter.

CFD has become increasingly affordable and is potentially useful in revealing and understanding more physical phenomena associated with the extreme operating conditions and large-scale complicated geometry. However, CFD has not played an important role in the design process (Tucker et al., 2007), due to reasons that fall into two categories (1) lack of validation of CFD codes, and (2) the accuracy and numerical difficulties associated with the CFD applications.
For the first requirement, lack of detailed experimental data makes the validation of numerical schemes sparse for supercritical combustion studies. This insufficiency is mainly a result of the harsh operating conditions which make almost all of the measurement probes or tracers unable to survive or be detected in LRE environments. The existing flow visualization techniques are not sufficient to support the acquisition of detailed quantitative information regarding the complicated processes occurring in the combustion chambers. For the latter category, the current CFD tools have inherent accuracy and numerical difficulty problems for treating supercritical turbulent combustion. First, the simulations of turbulent combustion at atmospheric conditions are open research issues themselves. Uncertainties exist in modeling turbulence and turbulence/chemistry interactions associated with the multi-scale physical processes. Secondly, rapid thermodynamic property variations and transport abnormality arise as injection fluids transit from trans-critical to supercritical states. The turbulence SGS model and turbulent combustion models for these conditions are not yet well developed. Thus, faithful validation of those numerical schemes must be conducted against well designed experiments before meaningful CFD results can be used to provide guidance for the design optimization.

It would be valuable to evaluate the CFD predictability of gaseous propellant combustion in typical rocket engines against experimental results without the involvement of more complicated trans-critical processes. The recent work of Tucker et al. (2007, 2008) represents attempts of this kind to validate several CFD schemes against experimental wall heat flux of a single element rocket combustor.

As one of the joint efforts, the current study presents the results of Large-Eddy Simulation of the same model problem using an advanced flamelet turbulent combustion model to account for the turbulence/chemistry interactions. The results serve as a validation of the current numerical scheme. The validated numerical frame can be applied to more relevant
supercritical combustion in liquid rocket engines and provide insights into the flow and combustion dynamics, and ultimately help the development of liquid rocket engines.

6.1 Subgrid-Scale Turbulent Combustion Models

The modeling of turbulence/chemistry interaction in a physically meaningful manner represents a critical and challenging issue in the present study of high-pressure combustion. Zong and Yang (2007b) evaluated the applicability of the laminar flamelet method to supercritical LOX/CH₄ combustion. In that study, the Reynolds number, based on the fuel properties and the splitter thickness, is 76,000. It was found that the Kolmogorov time scale remains at least one order-of-magnitude greater than the chemical time scale throughout the entire flowfield. In the current study, the Reynolds number based on the fuel stream properties and injector dimension (60,000) is approximately of the same value. The fact that hydrogen flame is generally thinner compared with methane flame due to faster chemical reaction rates at the same pressure, justifies the use of the flamelet method for the current study.

The thermochemistry state relation is established through a steady-state flamelet approach featuring a detailed H₂/O₂ reaction mechanism that includes 8 species (i.e., H₂, O₂, H, O, OH, HO₂, H₂O, and H₂O₂) and 19 reversible reactions. (Conaire et al., 2004) This mechanism has been validated against experimental data over a pressure range of 0.05 to 87 atmosphere. Calculations were performed for counter-flow diffusion flames of oxygen and hydrogen at 11 different nominal strain rates between 10 and 680,000 s⁻¹ to build the flamelet library. For all the flame calculations, the pressure is fixed at 5.2 MPa and the inlet temperature of oxygen and hydrogen is set the same as the inlet conditions of the experiment (Pal et al., 2006). It has been noted by Ribert et al. (2008) that high-pressure oxygen/hydrogen flame is extremely resistant to
flow strain. Therefore, no flame solution at extinction state is considered for the establishment of the flame library.

### 6.2 Computational Domain and Boundary Conditions

The experiment selected to validate the current numerical scheme was conducted in the Cryogenic Combustion Laboratory at The Pennsylvania State University (Pal et al., 2006). The physical model used in the experiment is shown in Figure 6.2. In the numerical simulation, only 5 mm of the injector upstream of the injector exit is included in the computational domain, thus, all the inlet conditions given hereafter are for the computational domain used in the current study. The dimensions of the shear coaxial injector, the combustion chamber, and the nozzle are summarized in Table 6.1. The flow conditions for the two propellant streams are listed in Table 6.2. The oxidizer, which is a mixture of 94.5% oxygen and 5.5% water vapor by mass preconditioned at 711 K, is injected through the central tube at a bulk velocity of 150 m/s; the fuel, which is a mixture of 40.2% hydrogen and 59.8% water vapor by mass preconditioned at 800 K, is injected from the annulus at a bulk velocity of 750 m/s. The instrumented heat sink combustion chamber has coaxial thermocouples embedded in it to measure the wall temperature and heat flux along the chamber wall. The measured temperature profile is fed to the CFD code as an isothermal boundary condition; then the wall heat flux predicted with the CFD code is compared with the experimental data for validation purpose.

Figure 6.2 shows the computational domain and the grid distribution (showing every 5th grid in $x$ direction and every 8th in $y$ direction) on a 2D slice. The computation domain covers 5 mm upstream of the injector exit, the whole combustion chamber, and the converging-diverging nozzle. A total number of 6.8 million grid points are used to resolve large-scale motions. Special
attention is paid to the grid resolution close to the chamber wall in order to ensure an accurate prediction of wall heat flux. A minimum of 5 micron grid size for the first grid points along the wall is used, which corresponds to $y^+ < 1$. The stretching factor near the wall is less than 1.1. Grids are also clustered at the near field of the injector to resolve the flow dynamics. Finally, the computation domain is divided into 297 blocks, with each calculated on a 2.4 GHz Opteron processor of a distributed-memory High Performance Computing cluster.

The measured wall temperature is used to set the isothermal boundary condition of the combustion chamber, while adiabatic boundary conditions is assumed at the injector wall boundaries. A uniform temperature of 755 K is assumed at the oxidizer post and the head of the combustion chamber. At the inlet, the mean velocity profile of a fully developed pipe flow is assumed with the overall mass flow rates matching the mean experimental values. The temperatures of both streams are fixed and the pressure is obtained through a one-dimensional approximation to the axial momentum equation. A supersonic outlet boundary is employed at the downstream boundary. The non-slip conditions are enforced at the wall.

### 6.3 Results and Discussion

To assist the data analysis of the current results, the computational grid used in the current study and those used by Oefelein, Menon, Merckle, and Tucker (Tucker et al., 2008, Lian et al., 2010, Masquelet and Menon, 2010) in their numerical simulations are listed in Table 6.3. Compared to the current study, Oefelein’s grid is four times finer in the axial and azimuthal directions, and twice finer in the radial direction; Menon's grid has a similar number of grid points in axial and azimuthal directions, but is much coarser in the radial direction, with a near wall grid resolution that is 40 times coarser than that in the current work. Compared to Oefelein's
case, a relatively small number of grid points (60) are used in the azimuthal direction in the current study. It is not expected to affect the results significantly, because of the small swirl velocity in the problem.

Figure 6.3 shows the measured wall temperature and the heat flux profiles along the chamber wall for all the numerical studies as well as the experimental result. Note that the experimental heat flux is calculated from the measured temperature by coaxial thermocouples. Although the wall temperature has a local minimum near the combustor headend, the experimental heat flux does not reflect this feature but rather a rapid monotone increase to a single maximum located between 0.03 m and 0.09 m, and then a gradual decrease to the end of the cylindrical combustion chamber. Oefelein's 3D LES result agrees quite well with the experimental result throughout the range of the plot. All the other numerical studies either under-predict (the current study, Menon's LES, and Tucker's RANS) or over-predicts (Merkle's URANS) the heat flux by more than 50 percent in the upstream region (A-B-C, $0 \leq x \leq 0.06$ m). In the region further downstream, except for Tucker's RANS case, which agrees well with the experiment in a quite large region ($0.06$ m $\leq x \leq 0.11$ m) but over-predicts more than 50 percent in the downstream region, all the other numerical studies capture the trend of the heat flux very accurately. Surprisingly and interestingly, the two dimensional URANS case agrees quite well with both the Oefelein's 3D LES and the experimental results in the downstream region. Both Menon's and the current 3D LES results predict an almost identical heat flux in the same range with a under-prediction of about 15 percent. Based on these observations, it is convenient to divide the combustion chamber into two regions, the upstream region (A-B-C region), and the downstream region (C-D region), for further discussion.

Before further analysis, it is valuable to examine the experimental results to understand the experimental uncertainties. The heat flux measurement uncertainties were reported to be
about 0.2 MW/m2-s (Pal et al., 2006), which is less than two percent of the mean heat flux. In the experiment, coaxial thermocouples were press-fit into the chamber wall. The first sensor is located at the surface of the chamber wall (contoured to fit the chamber curvature), and measures the temperature exactly at the surface of the combustion chamber. The second sensor is recessed by a quarter inch. The two sensors of the coaxial thermocouple measure the temperature at two different radial locations. The heat flux is calculated from the temperature measurements of the two sensors. To get the heat flux at the wall, transient heat conduction equations are solved using the given temperature measurement as boundary conditions. However, only the heat conduction in radial direction is considered. Longitudinal heat conduction was neglected based on the argument that it is negligibly smaller than the radial heat conduction. Unfortunately, the axial temperature gradient is comparable to the radial temperature gradient, especially in the upstream region, where the axial temperature gradient is quite large as shown in Figure 6.3. To assess the importance of axial heat conduction, careful examination of the temperature gradient in both radial and axial directions are re-evaluated here. Tables 6.4 shows the mean temperature gradient in the axial and radial directions at different locations (as labeled on Figure 6.3). Here when evaluating the heat flux, a fixed value of 400 W/K-s for the thermal conductivity of copper has been used. The effect of temperature on the thermal conductivity of copper is neglected here for simplicity. From this rough estimation, the error in heat flux caused by axial heat conduction is very large (26%) at the local minimum location. Even the smallest error can be as large as 7% of the radial heat flux. So the measured heat flux is lower at peaks and higher at troughs compared to the true heat flux, which is still unknown.

In the upstream region (A-B-C), although Oefelein's result agrees best with the experiment result, it did not show a local minimum corresponding to the wall temperature profile. Based on the analysis of the experimental result, it seems to have overshot the heat flux near the
location B. Interestingly, the current study, Menon's LES, and Merkle's URANS all predicted the local minimum in heat flux profile and the spike profile in the very vicinity of the headend. At the corner of the combustion chamber, the flow is constrained by the chamber wall, and it is reasonable to have a vanishing heat flux there. As the flow becomes dynamic further away from the headend, the heat flux rapidly increases. This flow feature explains the spike profile in the very near region of the headend. In the upstream region, Menon's heat flux is too small, while Merkle's is too large. The current study is closest to the real heat flux in the upstream region.

In the region further downstream (C-D), it is also reasonable to raise the same question about the accuracy of the experiment results. If the axial heat conduction has a significant effect on the heat flux profile, the true heat flux may be between those predicted by Oefelein and that of the current study.

To understand the physics behind the prediction of heat fluxes, more detailed information regarding the flow field is necessary. The wall heat flux is calculated as:

$$\dot{q} = (k_{\text{lam}} + k_{\text{turb}}) \frac{dT}{dr}\Big|_w.$$  \hspace{1cm} (6.1)

Since the temperature at the wall is fixed, the heat flux is determined totally by the sum of molecular and turbulent conductivity, and the temperature of the gas near the wall. The laminar conductivity is a strong function of the gas composition near the wall, and the turbulent conductivity is calculated based on the local velocity profiles. Examining the mean species concentration, the mean streamline and mean temperature distribution, assists the interpretation of the results and sheds lights on methods for further improvement.

Figure 6.4 shows the time-averaged temperature distribution, and Figure 6.5 shows the mean streamlines overlapped on the mean temperature contour in the upstream region. In this region, the temperature distribution is significantly different from each other, which explains the
disagreement in heat flux predictions. The current study gives the highest temperature in the corner region, and comparable potential core length among the LES studies. The RANS result predicts a very large cold region associated with a much larger potential core. Due to the singularity problem, the 2D URANS result also shows a long tail in the potential core. If 3D grid has been used, the potential core should have been much smaller. However, in the downstream region, all the cases show uniform temperature distributions in radial directions except for Oefelein's case, which is characterized with a hot core region and a very thick thermal boundary layer with a much lower temperature. Although significant difference exists between those mean streamlines as shown in Figure 6.5, there are some common flow structures. Except for Oefelein's case, all other cases give two closed recirculation zones: a smaller one in the corner and a larger and stronger one next to it, with a resemblance of a backward-facing step flow, although the sizes of those recirculation zones are not exactly the same. Oefelein's case showed a very large recirculation zone next to the headend and a squeezed long recirculation zone along the wall. This result is qualitatively different from those of other studies. It is note-worthy that, in spite of the temperature difference, the current study and Menon's case share almost the same recirculation zones and very similar downstream temperature distribution except for the difference in thermal boundary layer thickness. This partially explains why the two studies predict very close agreement in the heat fluxes.

Figure 6.6 shows the radial temperature profiles at \( x = 0.0125m, 0.025m, 0.05m, \) and \( 0.15 \) \( m \). The first three locations are located in the upstream region, while the last location corresponds to the downstream region, where the flow becomes much more uniform in radial direction. At \( x = 0.0125m \), except for the URANS case, all cases show a rapid temperature increase from the oxygen inlet temperature to a peak value and then a decrease to about 1800 K. The current study, however, shows a much larger temperature as further away from the
centerline, corresponding to a temperature between the URANS and other studies. The peak corresponds to a flame region between the fuel and oxidizer streams. The fact that the URANS case does not show a peak profile might be because that the recirculation zone temperature is too high (almost 3000K). All the results have a rapid decrease to the wall temperature, but the boundary layer thicknesses are different. At $x = 0.025m$, and $0.05m$, the peaks gradually flatten, corresponding to the spreading of the flame and the temperature increase in the outer regions. The centerline temperature also increases as the jet breaks up. However, Menon's case increases the fastest, while the URANS and RANS cases increase much more slowly. In the current study, the centerline temperature first increases faster then more slowly than Oefelein's case. In the downstream region, ($x = 0.15m$), Oefelein's temperature profile is very different from that of all other studies. It has a flat core region and then a moderate temperature decrease from 8mm to 16 mm in radial direction. The current study and Menon's case show very close temperature profile in a very large region, except the difference in the thickness of the thermal boundary. This difference may be related to the fact that the grid resolution in the current study is more than 40 times finer than that of Menon's study at the chamber wall. Menon's grid resolution might result in a much larger effective conductivity and thus more rapid heat transfer from the bulk flow to the wall. The URANS and RANS cases show similar temperature profile in the core region, which is about 180 K higher than that of the current study in the center region. But the RANS case has a slight temperature decrease in radial direction. The temperature gradients at the wall for the RANS, URANS, and the current study are very steep and similar to each other; the temperature gradients of Oefelein and Menon's results are smaller and of different values. Although the URANS and Oefelein's cases have the most different temperature gradients at the wall, the corresponding heat fluxes show the closest agreement with that of the experimental result. The current study and Menon's case also have very different temperature gradients, but the
corresponding heat fluxes are very close, especially in the downstream region. From this observation, it is clear that although the temperature gradients at the wall are very different, the predicted heat fluxes are in close agreement. This agreement indicates that the effective conductivity at the wall also have very different values, but the products of the effective conductivities and the temperature gradients are of about the same value, which is heat flux.

The species composition strongly affects both the molecular conductivity and the mixing and combustion processes. Among all the species considered here, hydrogen has the most distinctly different diffusivity. Figures 6.7 and 6.8 show the spatial distribution and radial profiles of the hydrogen mass fraction, respectively. Once again, the hydrogen distributions by the current study and by Menon show the closest shape and magnitude, with a slight difference in the spreading angle of the hydrogen stream in the near region of the injector. The URANS result shows a similar trend in hydrogen distribution but has a much earlier breakup of the hydrogen jet. Oefelein's case features the most distinct hydrogen distribution among all the studies. In Oefelein's case, after being injected into the combustion chamber, the hydrogen jet is rapidly broken up and divided in three different paths. Part of the hydrogen reacts with the oxygen in the flame region. A significant portion of the hydrogen is trapped in the big recirculation bubble, from which a third part of the hydrogen is leaked along the wall all the way to the nozzle exit, with little burning. The RANS case shows similar trapping of hydrogen in the upstream region, but the hydrogen rich region is much larger in volume, and no hydrogen leakage along the wall is observed; instead, the downstream distribution is similar to that of other numerical studies.

Those observations are more clearly shown in the radial profiles. In the upstream region, the current study and those by Menon and Merkle have the most similar hydrogen profiles in general, with a difference in hydrogen stream width and magnitudes of the hydrogen mass fraction. Oefelein and Tucker's cases have similar values of hydrogen mass fraction but slightly
different shapes in the mass fraction profiles. Tucker's case does show a peak value of hydrogen mass fraction, with the peak profile corresponding to the hydrogen jet stream. In the downstream region \((x = 0.15m)\), all the numerical studies have similar values of hydrogen mass fraction except for Oefelein's case, which has a hydrogen rich layer occupying a significant region of the combustion chamber. The huge difference in hydrogen mass fraction at the wall results in very different molecular conductivities, and thus dramatically different effect on the heat flux, because (1) the molecular diffusivity of hydrogen is significantly larger than that of other species, and (2) turbulence insensitivity become much weaker in the downstream of the combustion chamber, where the axial bulk velocity is about \(50m/s\), indicating a small turbulent conductivity value.

From numerical simulation point of view, when the grid resolution is so fine that \(y^+\) has a value of close to unit, such as in both the current study and Oefelein's case, the first grid point next to the wall is located in the buffer region of turbulent boundary layer, resulting in a negligibly small turbulent viscosity compared to the molecular viscosity at the first grid point. Although the temperature gradient in Oefelein's study is much smaller than that of the current result, the calculated heat flux is even larger because of the higher hydrogen concentration in the wall boundary layer. The current study and Menon's case have similar hydrogen profiles near the wall, but the temperature gradient is very different, a phenomenon caused mostly by the different grid resolution. Menon's grid is 40 times coarser compared to that of the current study, and thus the turbulent thermal diffusivity is dominant in determining the heat flux. The RANS case has a hydrogen mass fraction profile very close to that of Oefelein’s, and the URANS case shows a hydrogen mass fraction similar to that of the current study. But their effects on the heat fluxes are small, because the grids used are very coarse compared to both Oefelein’s and the current studies, turbulent thermal diffusivity is the dominating factor that affects the heat fluxes.
Energy balance can be calculated by taking the computational domain as a control volume. Energy enters the combustion chamber in the form of chemical energy; in the combustion chamber, it is converted to internal energy through chemical reactions, and is subjected to energy loss at the non-adiabatic wall; finally, it exits the combustion chamber in the form of both thermal and kinetic energy. If we take the upstream region of the combustion chamber as a control volume, that is, from the headend to $x = 0.15\, m$, the energy conservation can be expressed as Eq. 6.2. The rate of energy flow into the combustion chamber can be calculated from the mass flow rates of the two propellant streams and their specific enthalpies. The energy loss can be obtained from the experimental heat flux profiles. Then, the mean temperature at $x = 0.15\, m$ should be around 3200 K, which is very close to that predicted by the current study and Menon. The URANS and RANS cases over-predict the mean temperature by approximately 150 K, while Oefelein’s case shows a smaller mean temperature because a significant portion of hydrogen leaves the combustion chamber without burning. The energy conservation analysis indicates that the mean temperature prediction by the current study and by Menon are more reasonable compared to that of others.

$$\dot{E}_{\text{in}} = \dot{E}_{\text{loss}} + \dot{E}_{\text{out}}.$$  \hspace{1cm} (6.2)

The flame structure can dramatically affect the flow field and, in turn, the heat flux. The spatial distributions of OH mass fraction are shown in Figure 6.9, and their radial profiles at different axial locations are shown in Figure 6.10. Again, as expected, the OH mass fractions show very different characteristics in spatial distributions and in radial profiles. The current study and Menon’s case share very much similar spatial distributions except for in the recirculation zones. In the upstream recirculation zones, the OH mass fraction achieves its maximum in the flame region between the oxygen and hydrogen streams, but has very low values in the fuel-rich recirculation bubbles. The high OH mass fraction region rapidly spreads to the
entire combustion chamber further downstream, with a near uniform profile in radial direction, indicating the flame spreading from the mixing layers to the entire combustion chamber. Generally, the OH mass fraction in the current study is larger than that of all other studies, and it is non-zero in the vicinity of the chamber wall. This result is because that the current study adopts a steady flamelet combustion model, which gives an OH distribution based on the local mixture fraction and scalar dissipation, regardless of the local temperature because of the model deficiency. Because of the same reason, the OH mass fractions of the current study and Menon’s case have similar profiles in the mixing layers, but very different values in other regions. Oefelein’s case has an OH distribution strongly correlated to the temperature distribution, with a broader flame region in the upstream, a strong flame region in the core region in the downstream associated with very weak combustion in the encompassing outer region. The URANS case features an OH spatial distribution similar to that of Oefelein’s case in the upstream, but the radial profiles are closer to that of the current stream in the same region. In the downstream, the URANS case shows an almost flat profile of OH, resembling that of the current study, with a different magnitude and lower values at the centerline and the wall region. The difference at the centerline is caused by the 2D singularity problem; the deviation near the wall is due to model deficiency of the current study. The RANS study is mostly different from all other studies in terms of the flame shape. It has a very long flame length and almost no combustion outside the fuel oxidizer mixing layer before the jet breaks up at the flame tip. The most intensive combustion is located in the thin flame region between fuel and oxidizer, and at the flame tip at around 0.15m; a uniform OH profile in radial direction is present in the downstream.

At $x = 0.0125m, 0.025m,$ and $0.05m$, the OH profiles of the current study follow the same trend as those by Oefelein and Menon, except for the difference in larger radial locations, which is due to the model effect. The URANS case does not show any peaks, indicating no
distinct flame region. But its magnitude away from the centerline region shows a comparable values compared with the current study. The RANS case consistently shows a very steep profile of OH in the upstream regions, corresponding to the long flame length. In the downstream region \((x = 0.15m)\), the current study has the largest OH mass fraction and is uniform in the combustion chamber, with a value more than twice of other studies. This is again attributed to the flamelet model effect. Menon and Merkle's OH profiles share almost the same profile, except in the centerline region due to the 2D characteristic of the RANS case. Oefelein's result is consistent with the temperature profiles, indicating negligible combustion from radius of 0.01m to the chamber wall, which occupies 75% of the combustion volume. The RANS case shows similar trend compared with Oefelein's case, but with a much larger amplitude. From these observations, it seems that the current study and Menon's case have the most comparable combustion zones, with a difference in flame strength in the downstream. The URANS case is also closer to the current study in the downstream region. While Oefelein's flame structure has similar trends as the current study in the upstream region, but it has a huge discrepancy in the downstream. Although the similarity in flame structure in the upstream region, Oefelein's case gives a very different heat flux prediction there. But Menon's flame structure as well as the heat flux have similar trend compared to the current study. Although there are significant deviations of OH distributions in the downstream, all the LES and URANS cases show comparable heat flux. It seems that the effect of the flame shape on the heat flux prediction is also limited.

Based on the above discussions of the heat flux profiles, the stream line distribution, the spatial distribution of mean temperature, OH and hydrogen mass fractions, we can see there are huge discrepancies among almost all of the cases. Even though, we can still draw some conclusions concerning these simulations. In general, the current study shows very consistent agreement with Menon's study. The heat flux profiles capture the same trend in the upstream
region and are almost identical in the downstream region. The flame shapes in the upstream region are very close to each other. The two recirculation zones have almost the same structure and size. The radial profiles of the mean temperature in the downstream and species concentration profiles in both upstream and downstream regions show the closest agreement among all the numerical studies. Oefelein's case, although it has the best grid resolution and shows the best agreement with the experiment in terms of heat flux, missed the heat flux trough in the upstream region, and predicts recirculation zones, and species profiles dramatically different from almost all other numerical studies. It features the smallest temperature gradient and the largest molecular thermal diffusivity near the wall. The URANS case, which has the same agreement of heat flux in the downstream, has very much different recirculation bubbles and flame structures as well as very much different profiles in temperature and mass fraction at all the considered axial locations compared with other studies. Compared to Oefelein’s case, there must be different mechanisms contributing to the same heat flux profiles. Merkle’s case is characterized by a much larger temperature gradient and smaller effective thermal diffusivity. The standard CFD simulation by Tucker's RANS case has the longest flame length and potential core, associated with very different temperature and species distributions. It dramatically under-predicts the heat flux in the upstream and over-predicts the heat flux in the downstream region.

If the near-field heat flux analysis is corrected by including axial heat conduction, and a tolerance of 15% in heat flux is considered, it seems that the heat flux predictions show a weak convergence as model fidelity and grid resolution improves (A-B-C). The RANS case has the least model fidelity and the largest deviation in heat flux prediction. The URANS case includes the effect of large-scale coherent motions and thus, it is able to capture the trend as well as the value of the heat flux pretty well, but the deviation is much larger in the upstream. With the inclusion of more complicated combustion model and better grid resolution, improvement in heat
flux prediction is achieved in the upstream region for Menon’s case. The current study uses an even finer grid resolution in the upstream region and the near wall region, and it gives a better prediction of heat flux in the upstream region. With the best grid resolution and dynamic turbulence SGS model, Oefelein’s case shows the best prediction of heat flux. Unfortunately, data is missing for the near headed region, and thus it is not sure if it captures the heat flux profile in the upstream region. But detailed analysis as given above shows that very much different mechanisms are underlying these similar heat flux profiles.

A plot of mean axial velocity shows that the mean velocity magnitude correlates strongly with the heat flux profile. Another proof that the flow determines the heat flux is that, when changing the Van Driest damping function, the heat flux first increases due to larger conductivity but then decreases due to smaller temperature gradient. Initially, when the grid is coarse in the corner region, no small recirculation zone is observed; a dead corner is predicted instead. The heat flux calculated is much smaller compared to that with a refined grid in the corner. This result confirms that the velocity solution determines the heat flux to a very large extent.

As discussed before, the numerical studies presented here predict a reasonable heat flux profile due to very different mechanisms. The heat flux is at the end of a series of processes occurring in the combustion chamber. After the propellants are delivered into the combustion chamber, mixing is achieved through the mixing layers between the fuel and the oxidizer streams. Flame is anchored in the near field of the injector and rapidly spreads to the whole combustion chamber as propellant jet breaks up and mixing completes. Heat is released at flame regions, and combustion products are convected with large scale turbulent motions to the combustion wall, where heat transfer from the hot gases to the chamber wall occurs. Temperature non-uniformity in the axial directions causes axial heat conduction within the copper heat sink, from which the temperature is measured for calculation of heat flux at the wall chamber. In modeling these
physical processes, various uncertainties rise up. The grid resolution, modeling of turbulence and turbulence/chemistry interactions, and the wall boundary layer resolving/modeling all pose significant effects on the final prediction of heat flux. From the validation of a numerical study point of view, no firm conclusions can be made about the accuracy of the numerical schemes based on the comparison of the heat flux predictions and the experimental results. More information in the combustion chamber might be helpful in assessing the credibility of the numerical schemes. Specifically, if the flow field images, such as shadowgraph and OH emission images, can be obtained along with the heat flux measurement, it will be much easier to assess the accuracy of the numerical schemes. If both heat flux profiles and flow/flame structures can be simulated correctly, the credibility of CFD codes can be dramatically improved and the validated numerical schemes can be very helpful in future design optimization in a cost effective manner.

Figure 6.11 shows the instantaneous snapshots of temperature, mass fractions of hydrogen, oxygen, water vapor, and OH radicals. After propellants are introduced into the combustion chamber, the strong shear layer between oxygen and hydrogen streams results in very rapid development of shear layers, which promote the jet breakup in a shorter range of the combustion chamber. Large structures of oxygen and hydrogen are shed off after the breakup of the propellant jets. Further mixing is completed shortly after the jet breakup, resulting in a relatively uniform distribution of temperature and species concentrations. From the instantaneous snapshots, it is clear that the flow and combustion in the combustion chamber is very dynamic and characterizes very strong fluctuations of mixing and combustion, especially in the upstream region, where the flame anchoring and spreading have a significant effect on the subsequent heat release and flow motions.
6.4 Conclusions

The high-pressure combustion of gaseous hydrogen/gaseous oxygen for shear coaxial injector has been conducted using the large-eddy simulation technique. The predicted heat flux is compared with the experiment study by CCL at Penn State University and the numerical studies by Oefelein, Menon, Merkle and Tucker. Detailed analysis and comparisons are made to understand the heat flux predictions. The current study predicts a heat flux profile that agrees well with the experimental results. Although a variety of differences exist among the numerical studies, such as the grid resolution, the turbulent combustion model, and the differences between the spatial distribution of temperature, species, and velocities, all the numerical simulations predict very similar heat flux profiles. If Shadowgraph and/or chemical emission images can be taken in the near field of the injector exit, the results can be used to confirm the flame structures in the near field of the injector exit and thus, to assess the accuracy of the numerical studies.
Figure 6.1. Grid distribution (every 5th grid in x and every 8th in y) on a 2D slice.

Table 6.1. Dimension of the shear coaxial injector and the combustor chamber.

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxygen post inner diameter (mm)</td>
<td>5.26</td>
</tr>
<tr>
<td>Fuel annulus inner diameter (mm)</td>
<td>6.3</td>
</tr>
<tr>
<td>Fuel annulus outer diameter (mm)</td>
<td>7.49</td>
</tr>
<tr>
<td>Oxygen post recess length (mm)</td>
<td>0.43</td>
</tr>
<tr>
<td>Combustion chamber length (mm)</td>
<td>337 mm</td>
</tr>
<tr>
<td>Combustion chamber diameter (mm)</td>
<td>38.1</td>
</tr>
<tr>
<td>Nozzle throat diameter (mm)</td>
<td>8.17</td>
</tr>
</tbody>
</table>
Table 6.2. Flow Conditions and thermodynamic properties of the two propellant streams.

<table>
<thead>
<tr>
<th></th>
<th>Oxidizer stream</th>
<th>Fuel stream</th>
</tr>
</thead>
<tbody>
<tr>
<td>( p ) (MPa)</td>
<td>5.2</td>
<td>5.2</td>
</tr>
<tr>
<td>Stream composition</td>
<td>0.945 ((\text{O}_2)/)</td>
<td>0.402 ((\text{H}_2)/)</td>
</tr>
<tr>
<td>by mass</td>
<td>0.055 ((\text{H}_2\text{O}))</td>
<td>0.598 ((\text{H}_2\text{O}))</td>
</tr>
<tr>
<td>( T ) (K)</td>
<td>711</td>
<td>800</td>
</tr>
<tr>
<td>( u ) (m/s)</td>
<td>150</td>
<td>750</td>
</tr>
<tr>
<td>( \rho ) (kg/m(^3))</td>
<td>26.8</td>
<td>3.3</td>
</tr>
<tr>
<td>( \dot{m} ) (kg/s)</td>
<td>0.09</td>
<td>0.032</td>
</tr>
<tr>
<td>( C_p ) (J/kg·K)</td>
<td>1110</td>
<td>7240</td>
</tr>
<tr>
<td>( \nu ) (m(^2)/s)</td>
<td>1.35×10(^{-6})</td>
<td>5.44×10(^{-6})</td>
</tr>
<tr>
<td>( k ) (W/m·K)</td>
<td>0.06</td>
<td>0.26</td>
</tr>
<tr>
<td>( \alpha ) (m(^2)/s)</td>
<td>2.03×10(^{-6})</td>
<td>1.08×10(^{-7})</td>
</tr>
<tr>
<td>( a ) (m/s)</td>
<td>513</td>
<td>1470</td>
</tr>
<tr>
<td>( O/F ) ratio</td>
<td>6.61</td>
<td>6.61</td>
</tr>
<tr>
<td>( (\rho u^2)_F/(\rho u^2)_O )</td>
<td>2.92</td>
<td>2.92</td>
</tr>
<tr>
<td>( M )</td>
<td>0.31</td>
<td>0.51</td>
</tr>
<tr>
<td>( \text{Re} )</td>
<td>6.0×10(^5)</td>
<td>1.6×10(^5)</td>
</tr>
</tbody>
</table>
Table 6.3. Grid distribution in the combustion chamber for the three studies.

<table>
<thead>
<tr>
<th>Studies</th>
<th>Axial direction</th>
<th>Radial direction</th>
<th>Azimuthal direction</th>
<th>Total grid number (million)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Current study</td>
<td>440</td>
<td>188</td>
<td>60</td>
<td>225</td>
</tr>
<tr>
<td>Menon</td>
<td>611</td>
<td>87</td>
<td>65</td>
<td>3.5</td>
</tr>
<tr>
<td>Oefelein</td>
<td>1536</td>
<td>368</td>
<td>256</td>
<td>6.7</td>
</tr>
<tr>
<td>Merckle</td>
<td>160</td>
<td>120</td>
<td>--</td>
<td>0.02</td>
</tr>
<tr>
<td>Tucker</td>
<td>98</td>
<td>98</td>
<td>--</td>
<td>0.01</td>
</tr>
</tbody>
</table>

Table 6.4. Mean Temperature gradient at different locations.

<table>
<thead>
<tr>
<th>ranges considered</th>
<th>A-B</th>
<th>B-C</th>
<th>C-D</th>
<th>B-D</th>
</tr>
</thead>
<tbody>
<tr>
<td>axial direction $</td>
<td>\nabla T</td>
<td>_x$</td>
<td>5730</td>
<td>2650</td>
</tr>
<tr>
<td>point locations</td>
<td>A</td>
<td>B</td>
<td>C</td>
<td>D</td>
</tr>
<tr>
<td>radial direction $</td>
<td>\nabla T</td>
<td>_r$</td>
<td>18,600</td>
<td>33,000</td>
</tr>
<tr>
<td>$</td>
<td>\nabla T</td>
<td>_x/</td>
<td>\nabla T</td>
<td>_r$</td>
</tr>
</tbody>
</table>

Figure 6.2. Grid distribution (every 5th grid in x and every 8th in y) on a 2D slice.
Figure 6.3. Wall heat flux profiles along the combustion chamber wall compared with experimental and other numerical studies. a) heat flux profiles of the experimental and numerical studies; b) The measured wall temperature profile.
Figure 6.4. Mean temperature distribution for all the numerical cases. a) the current study, b) Menon's 3-D LES, c) Oefelein's 3-D LES, d) Merkle's 2-D URANS, e) Tucker's 2D RANS.
Figure 6.5. Mean streamlines overlapped on temperature distribution plots. a) the current study, b) Menon’s 3-D LES, c) Oefelein’s 3-D LES, d) Merkle’s 2-D URANS, e) Tucker’s 2D RANS.
Figure 6.6. Radial temperature profiles at various axial locations.
Figure 6.7. Mean distributions of H$_2$ mass fraction. a) the current study, b) Menon's 3-D LES, c) Oefelein's 3-D LES, d) Merkle's 2-D URANS, e) Tucker's 2D RANS.
Figure 6.8. Radial profiles of time-averaged temperature at various axial locations.
Figure 6.9. Mean OH mass fraction distributions.  a) the current study, b) Menon's 3-D LES, c) Oefelein's 3-D LES, d) Merkle's 2-D URANS, e) Tucker's 2D RANS.
Figure 6.10. Radial profiles of time-averaged OH mass fractions at various axial location.
Figure 6.11. Instantaneous snapshots of Temperature, and mass fractions of hydrogen, oxygen, water vapor, and OH radicals.
Chapter 7

Flamelet and Flamlet/Progress-Variable Methods Applied to LES of LOX/Methane Flames at Supercritical Conditions

Liquid rocket engines using liquid oxygen (LOX) and methane as propellants have recently attracted considerable interest for the future development of high-performance liquid rocket engines (Neill et al., 2009). Methane as a liquid rocket propellant has several advantages over other propellants due to its thermodynamic and chemical characteristics (Klepikov et al., 1997, Pempie et al., 2001, Burkhardt et al., 2003, Haeseler et al., 2004). Firstly, methane has lower viscosity and a higher specific heat capacity compared with kerosene, which results in super cooling properties. Secondly, methane has much larger density than hydrogen. Furthermore, methane is a ‘soft’ cryogenic propellant compared with hydrogen, and it requires less insulation. Methane has a storage temperature similar to that of liquid oxygen and allows a simpler design in tank architecture. All these properties allow for less tank mass and a potential improvement in efficiency. Thirdly, compared to kerosene, methane has better metal compatibility, due to its sooting, coking and corrosion characteristics. Fourthly, it has highest specific impulse (Isp) among hydrocarbon fuels. Finally, methane is a ‘green’ propellant and is less expensive than hydrogen and kerosene. The long range availability for methane is considerable better than kerosene, and methane can possibly be harvested from other planets,
including Mars (Ash et al., 1978, Landis and Linne, 2001). These advantages make LOX/Methane a very good candidate for liquid rocket propellants.

A thorough understanding of the propellant injection, mixing, and the combustion process is essential for an efficient engine design. Although a series of tests have been conducted (Neill et al., 2009), no flight experience exists for LOX/CH₄ rockets. Limited effort has been made to investigate the flow and combustion dynamics of LOX/methane in liquid-propellant rocket engine environments, as discussed in Chapter 1.

To improve the fidelity of CFD codes in studying supercritical mixing and combustion at typical liquid rocket operational conditions and ultimately provide guidance in initial rocket design as well as to reduce cost and turnaround time, an appropriate turbulent combustion model is crucial in the establishment of a comprehensive theoretical/numerical framework to systematically treat supercritical turbulent combustion. Although very important, a turbulent combustion model appropriate for supercritical combustion has not yet been well developed. The current efforts try to assess the validity of flamelet/flamelet-progress-variable models applied to LES simulations of non-premixed combustion at supercritical conditions.

### 7.1 Model Justification

To justify the use of the turbulent combustion models, systematic discussions have been made regarding the basic assumptions of the steady laminar flamelet models.

The intrinsic assumptions behind the combustion model, here the flamelet approach, have to be addressed carefully before any faithful results can be obtained with the selected turbulent combustion model. It requires comparison of length and time scales in turbulent combustion flows to justify the validity of the model. However, the flame thickness is not the characteristic
length scale of for a non-premixed flame (Peters, 2000, Poinsot and Veynante, 2005). It varies with time and local stretching. To avoid the ambiguity, the characteristic time scales of the smallest turbulent eddies and the flame characteristic time are used to characterize the interactions of the two processes. If the smallest mixing time scale (Kolmogorov time scale) is always much larger than the flame time scale, turbulent eddies are unable to affect the inner structure of the flame and thus justify the assumption that laminar flamelets are embedded in the smallest turbulent eddies.

In turbulent flame studies using the flamelet model, the smallest turbulent scales and flame thickness are sub-grid scales and cannot be resolved. The only way to compare the scales of turbulent eddies and flame scales is to use other estimate methods. However, those time scales are dependent on flow conditions. A posteriori DNS provides all information about the smallest turbulent eddies and flame structures; however, if DNS is available, there is no need to conduct LES studies any more. Furthermore, DNS is also impractical for industrial interested applications.

Following Peters (2000), the characteristic time scale of the flamelets can be calculated as

\[ t_f = \frac{f_{st}^2 (1 - f_{st})^2}{\chi_q}, \tag{7.1} \]

where \( f_{st} \) is the value of the mixture fraction at the stoichiometric condition and is 0.2 for LOX/methane propellants. The extinction scalar dissipation \( \chi_q \) is calculated from a counter-flow diffusion flame at a near-extinction state, which takes the value of \( 0.36 \times 10^6 \text{ s}^{-1} \) at stoichiometric condition, giving a flame time of \( 7.1 \times 10^8 \text{ s} \).

The Kolmogorov time scale is given by
Kinematic viscosity is readily available in LES studies. It takes a value of $1.1 \times 10^{-5} \text{ m}^2/\text{s}$ at flame regions in the present work. The turbulent dissipation rate can be estimated from the resolved flow fields given by

$$
\varepsilon = \frac{u'^3}{l},
$$

where the turbulent velocity can be estimated from the root mean square velocity. If we take the splitter plate thickness as the integral length scale and maximum root mean square velocity in the domain, 20 m/s, we can get

$$
t_\eta = 7.0 \times 10^{-7} \text{ s}.
$$

Here the turbulent velocity is one third of the methane inlet velocity. This is because combustion induces very strong volume dilatation and thus the local combustion-induced velocity fluctuations can lead to an RMS velocity of much higher values. One can see, even with the strictest criteria, the turbulent time scale is still one order of magnitude larger than that of the flame time scale. As shear layers develop downstream, the integral length scale increases as a function of axial distance. Thus the slow moving Kolmogorov scale eddies are not able to interact with the flame chemistry significantly because of the disparity in time scales. The estimation justifies the flamelet model assumption.

In the present work, for the flamelet model, the thermo-chemistry state relation is established through a steady-state flamelet approach featuring a detailed oxygen/methane chemistry with 16 species and 16 chemical reactions (Sung et al., 1998). This mechanism has been validated against experimental data over a pressure range of 1-20 atm for different flame configurations. Calculations for counter-flow diffusion flames of LOX and methane are
performed for strain rates in the range 20 to $1.76 \times 10^6$ $s^{-1}$, covering near-equilibrium and near-extinction limit strain rates. For all the calculations, the pressure is fixed at 10.0 MPa, and the inlet temperatures of oxygen and methane are taken as 120 K and 300 K, respectively. Consistent with the flamelet assumption, the corresponding scalar dissipation rate, $\chi$, for each solution is evaluated as a function of filtered mixture fraction. The effect of strain rate on the thickness of a counter-flow diffusion flame of gaseous methane and liquid oxygen under supercritical pressure has been systematically investigated by Pons et al. (2009). At a constant ambient pressure, the flame thickness is inversely proportional to the square root of the strain rate. To facilitate the establishment of the flamelet library, each flamelet solution obtained has been expressed as a function of the mixture fraction. The solutions are then integrated based on Eq. 2.129 and tabulated as functions of $\tilde{\chi}$, $\tilde{f}$, and $f^{\prime 2}$. The currently formulated table has 20 support points in $\tilde{\chi}$ direction and is resolved by 201×15 nodes in $f \times f^{\prime 2}$ space. The calculated filtered mixture fraction, mixture fraction variance, and the scalar dissipation rate from LES simulation are used to determine the appropriate entry in the table.

For the Flamelet-Progress-Variable model, the flamelet library is generated using the FlameMaster code developed by Pitsch (1998). Since this computer code can only accommodate ideal gas thermodynamic properties, the inlet temperature for the oxygen stream is changed to 300 K. The reduced kinetic mechanism by Peters and Rogg (1998) is used. 40 grid points in the progress-variable space are used.
7.2 Computational Domain and Boundary Conditions

As shown in Figure 7.1, the computational domain measures 1 mm upstream of the splitter plate tip, 20 mm downstream, and 10 mm in transverse direction. No-slip boundary conditions are applied to the solid surface, and slipping boundary conditions are enforced at the side boundaries. At the inlet, a turbulence fluctuation is added with an intensity of 10%, with a 1/7 law velocity profile to account for the upstream development of the boundary layer along the flat plate splitter.

To study the effect of ideal gas and real gas flamelet libraries, the effect of turbulent SGS model, and momentum flux ratio, six cases are studied, as listed in Table 7.1. The baseline case uses the steady flamelet method (case B). Variations are made to study the effect of the corresponding changes on the modeling of turbulent combustion. A flamelet-progress-variable case (case F) is compared to the ideal gas flamelet case (case D) because they share the ideal gas flamelet library and can be compared in order to study the difference between the flamelet and the flamelet-progress-variable approach.

7.3 Results and Discussion

A total number of 250,000 grid points are used in the two-dimensional study to resolve the large-scale eddies. Grids are clustered in the vicinity of the splitter plate wall to fully resolve the upstream boundary layers, which might be important in determining the downstream flow dynamics. 151 grid points are used in the vertical direction of the splitter plate, with a minimum grid size of 2 micron in the near field of the splitter plate. The spectrum of kinetic energy in Figure 7.2 shows a -5/3 slope in the log-log scale, indicating that the grid scale is in the range of
the inertial sub-range and is fine enough to resolve associated flow motions. The extremely fine grid resolution assures that the model is grid independent, thus excluding the grid resolution effect on the results.

The instantaneous temperature distributions for all cases are presented in Figure 7.3. The mixing layers start from the edge of the splitter plate and fluctuate strongly as they are convected downstream. Fresh oxidizer and fuel are brought into the mixing layer by the large-scale motions. As the parings of vortices involve larger scales of mixing, the flame rapidly spreads outward and forms intensive burning regions. A closer examination of the flame structure in the exact vicinity of the splitter plate shows that two counter-rotating vortex layers are formed at the fuel and oxidizer streams, respectively. However, the oxidizer recirculation zone is dominant only in the region very near the splitter plate, and rapidly merges into the methane vortices. On the other side, small vortices are formed in the methane mixing layer, which is initially less intensive than the oxygen vortex, but rapidly grows and becomes dominant in the downstream.

In pure mixing of LOX and methane (case A), as surface tension and the enthalpy of vaporization vanish, the high-speed methane is able to perturb the liquid oxygen significantly and form large-scale mixing layers. Stringy finger-like structures form at the surface of the liquid oxygen, a phenomenon which is also observed in experimental studies (Chehroudi et al., 2002b). The finger-like structures are rolled up and penetrate further into the methane stream. While mixing with the hotter methane stream, liquid oxygen is heated up and damped out, leaving a long tail of low temperature oxygen-rich structures in the mixing layers. In combustion cases, the introduction of flame dramatically changes the mixing layer structures. Heat release from the flame region introduces much larger temperature and species gradient adjacent to the liquid oxygen, which strongly enhance the thermal diffusion, promoting the evaporation of liquid oxygen. In all combustion cases, those finger-like structures along the liquid oxygen jet surface
are penetrating more into the liquid oxygen. The flames bear similar structures: (1) the location and temperature of intensive recirculation zone are comparable; (2) the flame follows the liquid oxygen surface; and (3) folding and wrinkling finer flame structures are formed in all cases. However, there are still differences. First, cases D and F, which use the ideal gas flamelet library, bear a flame temperature much higher than other cases. Second, the flamelet-progress variable case is mostly different from other cases, as will be elaborated later.

To further compare the flame spreading and its mean structure, time-averaged temperature distributions are shown in Figure 7.4. Consistent with the snapshot contours, the mean flame structures share very much the same structures for all cases. A bright spot is observed right after the splitter plate, which represents the high temperature recirculation zone observed in the snapshots of Figure 7.3, which is also observed in the experiment of LOX/H₂ combustion at the same pressure (Mayer and Tamura, 1996a). This confirms that the flame starts in the vicinity of the splitter plate and spreads towards the two propellant streams. By visual inspection, it can be seen that the mean flames share similar flame structures. However the ideal gas flamelet library cases (cases D and F) are characterized with higher temperature in both the recirculation zone and the downstream flame regions. This is consistent with the instantaneous temperature distribution and can be attributed to the difference in the flamelet libraries. The higher momentum ratio case (case E) shows a much smaller spreading angle at the fuel side but a similar spreading angle in the oxygen side. The mean temperature is also higher than in the other flamelet cases. At a higher momentum flux ratio, the stronger inertia force in the methane stream contracts the flame toward the liquid oxygen side; however, liquid oxygen is almost incompressible and does not allow the flame to further penetrate into the liquid oxygen. Thus, the flame region becomes smaller and more intense.
It can be seen that the hot recirculation zones in combustion cases are larger in size than in the cold flow case, while the fuel side recirculation zone becomes much smaller. The reason for this is that combustion heats up this region and volume dilatation is stronger than in the cold flow case, resulting in a stronger recirculation zone in the combustion case. From the mean streamlines as shown in Figure 7.11, it is also observed that the volume expansion in the combustion regions makes the two propellant stream flow sideward, accelerating the speed of each stream. As will be shown later, the combustion case has higher RMS velocities compared to the cold flow case due to the fact that combustion induces more kinetic energy into the shear layer and may introduce turbulence because of chemical reaction.

The mean density distributions, shown in Figure 7.5, confirm the afore-mentioned observations. The density gradient in combustion cases is steeper than in the cold flow case due to a higher temperature gradient introduced by combustion heat release. From the mean mixture fraction contours in Figure 7.6, it can be seen that the mixture fraction is transported to a much larger region, compared to the combustion cases. Again, this comes from the fact that the heat release introduced volume dilatation pushes the combustion products outward and hinders further mixing of fuel and oxidizer.

To quantitatively compare the flame structures discussed above, the flame boundary is defined at the isothermal line of 1000 K. The resulting flame structures are plotted in Figure 7.7. As observed in the contour plots, the flame spreading angle is small at first and rapidly increases as shear layers develop downstream and experiences another inflection further downstream. The ideal gas library case (case D) has the largest flame expansion at both sides. The higher momentum ratio case (case E) has a contracted flame in the fuel side due to higher momentum flux of the methane stream and a small expansion of flame in the downstream region. Other combustion cases share almost the same flame boundaries at the fuel side and slightly different
flame boundaries at the oxygen side. Figure 7.8 compares the flame width based on the flame shapes in Figure 7.7. The ideal gas library case has the largest flame width at all axial locations. The dynamic SGS model case has a flame shape closest to the flamelet baseline case among all the combustion cases, indicating a negligible effect of the turbulent SGS model. The FPV case has the second thickest flame, which is due to the combined effect of the higher flame temperature and more realistic flamelet structures compared to the ideal gas library case. The higher momentum ratio case has the thinnest flame; specifically, it shows a rapid decrease further downstream, where the flame is constricted by both the high density liquid oxygen and the high-inertia methane stream.

Figure 7.9 shows the mean profiles of the same variables along the centerline of the splitter plate. The temperature achieves peak values in the vicinity of the splitter plate. Although an adiabatic wall is assumed at the face of the splitter plate, it does not produce a maximum temperature at the wall, because fresh propellants (CH₄) continue to come into this region and then mixes, reacts with the high temperature mixtures. However, since little oxygen can penetrate the flames to react with the fresh methane, the temperature is much lower than the adiabatic flame temperature. As can be seen, the mixture next to the wall is richer than the location where the mean temperature achieves its maximum value. In practice, heat transfer occurs between the injector post and neighboring fluids. If a non-adiabatic boundary condition is assumed at the splitter plate, it is reasonable to expect a rapid increase of the mean temperature from the wall to the center of the mean recirculation zone. The near wall temperature might be smaller, but it is not likely to cool the recirculation zone significantly because the splitter plate is not cooler than 120 K, while the recirculation zone survives over the bottom LOX stream. Although it seems that the flame is always attached to the wall, it is the small recirculation zone which sustains a very high temperature that provides the heat source and chemical radicals to
anchor the flame and ensures a stable combustion. A bright spot right next to the injector LOX post is also observed in Mayer et al.'s LOX/H₂ experiment study, and it probably is the bright spot that stabilizes the flame.

Consistent with the above observations, the ideal gas library cases (D and F) has the largest temperature in the recirculation zone. The higher momentum ratio case also has a larger flame temperature. The RMS velocities rapidly increase with distance from the splitter plate and then decrease slightly and come to almost constant. The higher momentum ratio case has larger RMS velocities, but all the flamelet cases have similar temperature fluctuations.

Figure 7.10 shows the mean profiles of temperature, velocity, mixture fraction and RMS velocities along vertical directions at different axial locations. In the upstream region (at x/δ = 1), the flame is trapped in the recirculation zone and the methane mixing layer. Aside from the higher momentum ratio case, all combustion cases show very similar profiles at different axial locations. The cold flow case shows better mixing, as discussed before.

Figure 7.11 shows the streamlines overlapped on the mean temperature contours. It clearly shows the anticlockwise strong recirculation zoned in the oxidizer side and the clockwise rotating methane mixing layer. These vortices compete and the oxygen vortex dominates in the vicinity of the splitter plate. The shear layer rapidly expands as warmed up by the neighboring hot gaseous stream. However, further downstream the fuel side vortex dominates the flow and enhances the large-scale mixing of fuel and oxidizer. The anticlockwise recirculation zone featuring high temperature is dominant in the near field of the splitter plate in all flows. The methane mixing layer does not show closed streamlines because the mean vorticities are convected downstream on average at higher velocity. Compared to the cold flow case, the recirculation zone is generally larger in combustion cases. This is because heat release from combustion increases the kinetic energy and further enhances the LOX evaporation, thus creating a stronger
recirculation flow. However, the ideal gas library cases, which have the highest flame temperature, give a recirculation zone slightly larger than the cold flow case. The higher momentum ratio case (E) has a recirculation zone 40 percent larger than the baseline case. This indicates that as momentum ratio increases, the flame becomes more stable.

A close-up view of the near field of the splitter plate is helpful in understanding the flame anchoring mechanism. Figure 7.12 shows a time evolution of temperature contours in the near field of the splitter plate for the flamelet baseline case. The time interval is 0.02 ms. Vortices rotating clockwise are continually shedding off from the tip of the splitter plate at the methane stream, which is initially much smaller than the anti-clockwise rotating vortex at the oxygen side. However, they rapidly grow up in a short distance (generally 1.5 non-dimensional lengths) after shedding off and overshadow the vortices originating from the oxygen mixing layer. The counter-rotating mixing shear layers bring fresh reactants into the recirculation zone, where they are burned and convected downstream. As the combustion products are convected downstream, the flame continues to burn the fuel and oxidizer that are brought to the flame by turbulent mixing. Going downstream, the flame also becomes thicker and stronger due to more propellants being mixed and burned. The flame anchoring mechanism shown here is different from the subcritical counterpart observed in the subcritical LOX/methane combustion experiment conducted by Singla et al. (2007b) In that experiment, OH PLIF images showed flames were lifted from the LOX post and are susceptible to the turbulent flows. The difference in the flame anchoring mechanism can be attributed to the distinct difference of subcritical and supercritical LOX injection, and subsequent evaporation and mixing. At subcritical pressures, vaporization is the slowest process (Yang, 2000) and is combustion rate controlling. The effect of surface tension gives rise to a round jet at the exit of the injector, and the round jet is subjected to aerodynamic force from the high-speed gaseous fuel stream and forms a classical spray and
vaporization process. At the LOX post tip, LOX does not have enough time to evaporate into the gaseous phase. The flow behaves like a backward-facing step flow, in which the flow separation of the methane stream gives rise to a clockwise recirculating flow, the size of which can be 6-7 times of the LOX post size, covering a long region behind the splitter plate. Within that recirculation region, there is longer time for atomization and vaporization to occur and produce combustible mixtures; thus, a lifted flame can be stabilized in the low speed region of the backward-facing step flow. At supercritical pressures, due to the vanishing of surface tension and the enthalpy of vaporization, a variable density fluid-fluid mixing process occurs in a much shorter time scale (Snyder et al., 1997). Turbulent mixing of the oxidizer and fuel occur immediately after the splitter plate, forming a combustible mixture immediately after the splitter plate. This is supported by Delplanque and Sirignano’s study (1994), in which they found that the LOX jet gasification rate under supercritical conditions is at least one order or magnitude greater than that of droplet vaporization at atmospheric pressure. In summary, at supercritical conditions, it takes much less time to form a combustible mixture than at subcritical conditions. If the heat loss to the splitter plate is not significant enough to quench the flame and the local strain is not strong enough to stretch the flame to extinction, a burning recirculation zone remains burning and stabilizes the flame since the flame hides itself in the recirculation zone and is not likely to be blown off. The difference of the LOX/GCH₄ injection, (vaporization), mixing and combustion at sub- and supercritical conditions might be the reason that different flame stabilization was observed.

Note that the current flamelet and the flamelet-progress variable method are unable to consider the temperature effect on combustion. This can be remedied by using reduced temperature as progress-variable instead of using main combustion product mass fractions. The effect of wall temperature on the flame stabilization will be addressed in future studies.
Although the flame is stabilized in the recirculation zone in all cases, it is still valuable to study the limiting cases, where, for unknown reasons, local flame extinction occurs near the splitter. The dynamic response of the flame re-stabilization or blow-off is of interest. When the flame base is quenched, sufficient premixing occur upstream of the flame. The flamelet method is unable to resolve such a flame. The flamelet-progress-variable approach is used for this purpose. Figure 7.13 shows the dynamic response of the flame after being artificially quenched 6 mm and 10 mm away from the splitter plate, respectively. The left column corresponds to the 6mm case. A short time after the flame quenching, when there is a negative velocity occurring near the flame associated with a vortex shedding process, the flame base is transported rapidly upstream and re-stabilized behind the splitter plate. However, when the quenching distance is increased to 10 mm (the right column, compared to the mean recirculation length of 6.6 mm), although the flame can be brought back to some extent, the negative velocity is not strong enough to re-stabilize it. Finally, the flame is blown out of the computation domain. This indicates that the flame stabilization is strongly correlated to the dynamic processes of the vortex shedding and the strong recirculation zone. Although the upstream region is partially premixed, the flame propagation does not play an important role in re-establishing the flame stabilization. The reasons are two-fold: (1) the laminar flame speed continues to decrease with pressure, due to the reduction of diffusivity and increase of density, although the reaction rate increases with pressure, and (2) turbulent mixing at small scales might be important in enhancing the local mixing and increasing the flame speed though the current study does not show a flame speed large enough to withstand the upcoming flow. Therefore, it is the large scale flow structures that make the local flow speed smaller or even negative to re-establish the flame stabilization.
7.3.1 Pure Mixing of LOX and CH₄

As summarized by Yang (2000) and Bellan (2000) and observed by Chehroudi et al. (2002b), trans-critical LOX exhibits totally different mixing characteristics compared to the subcritical mixing, because of the vanishing of surface tension and the enthalpy of vaporization at critical temperatures. A variable density fluid-fluid mixing is present. Thermal diffusivity becomes very small when the temperature approaches 154 K, and dilatation instead of heat conduction plays a more important role.

From the instantaneous distribution of temperature, vorticity, and species composition as shown in Figure 7.14, it is clear that the temperature and species contours share exactly the same structure. The reason for this similarity is the distinct temperature difference of the two mixing streams. As high temperature methane is convected/diffused to low temperature oxygen, energy is transferred along with mixing of the two flow streams. The temperature distribution is determined totally by the mixing process and thus the resemblance of the distribution of these two variables. One can also observe that due to the lack of surface tension, the liquid oxygen and methane mixing process behaves like a variable density fluid-fluid mixing. High density oxygen rolls up under the effect of shear layers and continues to mix with warmer fuels as vortex pairing develops downstream.

From the mean temperature distributions as shown earlier in Figure 7.3, a broad range of flow is brought to a higher temperature and lower density. The mean density in the oxygen side seems smaller than that expected from a mass conservation point of view because of the way of taking time-average is algebraic time-averaging. At low temperatures, density is much larger than the high temperature fluid. Thus, the averaged density seems smaller compared to the instantaneous snapshots.
Figure 7.15 presents the Power Spectrum Density (PSD) of the axial velocity at different locations in the LOX/CH\textsubscript{4} mixing layers. In the exact vicinity of the splitter plate, turbulence is weak and no dominant frequencies are observed there. Instead, the flow is featured with multi-mode flow dynamics. In the methane shear layer and LOX shear layer, although the fluctuation magnitude is small, the dominant frequencies are different. The shear layers have different characteristic length scales and velocity scales. However, a frequency of 4 kHz is totally dominant in the downstream region, indicating that the mixing layer is characterized by a dominant scale of motions.

### 7.3.2 Flamelet Baseline

Figure 7.16 shows the instantaneous distributions of temperature, density, vorticity in z direction, and mass fractions of CH\textsubscript{4}, O\textsubscript{2}, OH, and H\textsubscript{2}O. The flame anchors at the recirculation zone right after the splitter plate and spreads as the vortices roll up and develop downstream. The predicted scalar dissipation rate in the near field of the splitter plate is too small to quench the flamelets; thus, the flame is always anchored at the LOX post. Since the flame is diffusion- and mixing-controlled, the flame structure correlates strongly with the mixing layers. The combustion process introduces very large temperature gradients, and thus very rapid thermodynamics variations are observed in the direction of steep density gradients. The snapshots of the species mass fractions as well as the density distributions show that there is unburned liquid oxygen shedding off from the liquid oxygen due to the shear stress from the fast and hot combustion products, resulting in a larger expansion of the flame. The unburned oxygen structures continue to mix with methane in the outer region, forming secondary flames. The secondary flames can be sustained for a while before the oxygen particle is completely depleted.
through reactions with the rich mixtures, resulting in either an emergence with larger flame structures due to vortex rollings/pairings, or a disappearance by dilution into the low temperature fuel stream. Secondary flames were also observed in Singla et al.’s (2005) experiment study. However, the secondary flames here are formed from large-scale mixing and insufficient small-scale mixing of fuel and oxidizer, which is different from those observed in Singla’s experiments, where droplets penetration through the flame accounts for the secondary flame.

As the flames are convected downstream, multiple pairings of vortices make the flame a multi-fold big plume. The flame may form a ring, and shed off from the main flame structure, when mixing with cold reactants, losing energy to them due to heat transfer. The flame generally continues to follow the shape of the oxygen jet and is very close to the high density oxygen. This tendency occurs because the stoichiometric mixture fraction is 0.2 for O₂/CH₄. A small mass fraction of CH₄ and a much larger mass fraction of O₂ are required to form a stoichiometric mixture. So the flame is closer to O₂, instead of CH₄. Furthermore, LOX has a much higher density. When a small fraction of LOX is heated to low density gaseous O₂, it is enough to burn out the coming CH₄ brought up by turbulence mixing. These two factors contribute to the small distance between the flame and the LOX stream. Between the LOX stream and the hot flame region, there must be a thin layer of oxygen that has a temperature close to critical temperature of oxygen. In that oxygen layer, the thermal diffusivity is very small, resulting in a weak heat conduction from the flame to the liquid oxygen. The overall effect is to have the flame close to the high density liquid oxygen.

Scalar dissipation reflects the fact that the unresolved laminar flamelets are subjected to external turbulence stretching, the effect of which is on the structures of the unresolved laminar flamelets. At sufficiently large scalar dissipation, the chemical time scale becomes smaller than the mixing time scales. In other words, Da number is less than unity, thus, flame extinction
occurs. No scalar dissipation rate larger than the quenching value is observed in the current study. Poinset and Veynante (2005) pointed out that, even if the instantaneous scalar dissipation rate is several times larger than the quenching limit value, the flame can still survive. This means that a turbulent flame is stronger than predicted by laminar counter-flow flames. Thus, it is safer to say that there is no flame extinction due to flame stretching in the current simulations. At intermediate scalar dissipation rate values, the laminar flamelets have different species profiles in the mixture fraction space and, thus, the filtered species difference. This translates to the local combustion status of resolved flame structures. The variance of the mixture fraction simply means that the cell averaged mixture fraction features a fluctuation of the standard deviation $f^2$. The larger this value, the broader the PDF shapes of the mixture fraction and consequently the product profiles. However, as the flames flow downstream, the scalar dissipation rate and the variance of mixture fraction decrease and, combustion can continue to proceed to equilibrium products; thus, total heat released is about the same but at a different time and locations.

The vorticity contour compared with the cold flow case shows that the fine structure for the combustion case is much more abundant. The heat release from combustion induces extra energy into the flame regions and perturbs the flow and thus the mixing and combustion processes significantly.

It is also noted that the mean temperature is much lower than the instantaneous maximum temperature. If one looks at the temperature profile in mixture fraction space, it is clear that the temperature is much lower than that of a laminar counter flow flame that is close to equilibrium while, on the other hand, the rich methane stream is heated to a higher temperature. Since the reactants are not fully consumed in the computational domain, chemical energy is not fully released. The heat released by the flame is re-distributed among the two propellant streams such that the mean temperature is much lower than that of the theoretical adiabatic flame temperature.
Although not shown here, the time-averaged energy flow rate at the inlet and exit are compared, and the energy conservation is confirmed. Energy is redistributed among the products and the two reactants. In general flamelet studies at low pressures, it is common to look up all volumetric, thermodynamic, and transport properties through the flamelet library, no transport equations for energy is necessary (Peters, 2000). However, the energy equation is un-avoidable in the current studies to account for energy transfer among the products and the reactants.

In Figure 7.10, the mean temperature in the axial direction along the center line of the splitter plate shows a peak value in the recirculation zone and first decreases and then increases downstream. This profile is consistent with the observation that the flame is anchored in the recirculation zone after the splitter plate. The shear layers are thin and not fully developed in the upstream, and only a small fraction of fuel and oxidizer can be involved into the shear layers and get burned. Moving downstream from the recirculation zone, the flame floats up and down under the effect of the two competing vortices, losing energy to the fuel and oxygen streams and resulting in a mean temperature smaller than the recirculation zone. However, moving further downstream, the large scale mixing caused by vortex rolling up and pairing enhances the mixing of the two streams, and more fuel and oxidizer can burn and release more heat, giving rises to an increase in temperature along the axial direction.

Although not shown here, the axial mean pressure profile for the cold flow shows low pressures in the shear layer and decreases as a function of axial distance. This corresponds to the high velocity shear layer with larger dynamic pressure and smaller static pressure. However, no obvious pressure distribution is observed in the combustion cases. This is explained partially by the fact that the combustion induced-heat release changes the pressure distribution there. However, numerical errors could also play an important role, because any small error in continuity equation can lead to large pressure uncertainties.
7.3.3 Effect of Turbulent SGS Models

To assess the effect of the turbulent viscosity model on the combustion modeling, the dynamic SGS model is applied to compare with the baseline case. The calculated turbulent viscosity does not show a significant difference from the static model case (case B). Similar flow and flame structures are observed in the dynamic SGS model case. The mean flame shape also agrees well with that of the baseline case, indicating a negligible effect of the dynamic SGS model. Thus, for simplicity and computation speed, the static Smagorinsky model has been used in all other cases.

7.3.4 Effect of Momentum Flux Ratio

From the instantaneous and mean temperature distribution of the higher momentum flux ratio case, shown in Figure 7.18, one can observe that the mean temperature shape tends to bend toward the oxidizer stream. This can be attributed to the fact that it is more difficult for the rolled vortices to penetrate into the higher-momentum methane stream, as they are trapped in the low speed oxidizer stream. The high mass flow rate and smaller residence time of the methane stream also makes that the rich zone is only heated to a smaller temperature before it leaves the computational domain. Thus, as the momentum flux ratio increases, the liquid oxygen stream tends to be shorter. In a real shear coaxial injector, this may correspond to a shorter LOX potential core and faster burnout of the propellants.
7.3.5 Effect of Flamelet Library

The flamelet library for the baseline case is generated from counter-flow diffusion flames under the same operation conditions, that is, the same inflow temperatures and pressure. To assess the importance of the real-gas effect on the flamelet library, a flamelet case using ideal gas library is conducted to compare with the real-gas library baseline case. The ideal gas library is generated using the same procedure, but using 300 K for both oxygen and methane for the inlet temperature and the ideal gas equation of state for the volume properties. The laminar counter-flow flames are different in both the physical and the mixture fraction space, due to the higher temperature of the oxygen and the accuracy of the equation of state. More products are produced for the same mixture fraction, resulting in a higher temperature.

Figure 7.19 shows the instantaneous distribution of the flamelet case using the ideal gas flamelet library. It is obvious that the flame temperature is much larger than that of the baseline case. Several reasons cause the difference between ideal-gas and real-fluid flamelet library cases: First, the inlet temperature of oxygen is higher, which increases the initial enthalpy of the oxidizer. Second, the thermodynamic and transport properties are different from the liquid oxygen case, which can change the flame shape significantly. The combined effect is to obtain different species profiles at given flow conditions and mixture fractions, resulting in a different heat release and flow structures. Even with this difference, the results are similar in terms of flame structure and flame anchoring location. However, a higher temperature is achieved with the ideal gas flamelet library.
7.3.6 Flamelet -Progress Variable Approach

In practical combustion devices, a lifted flame might be more realistic (Poinsot and Veynante, 2005). However, flamelet method is not capable of resolving a lifted flame when the flame lifting mechanism is not a result of the quenching of non-premixed flames. The flamelet/progress variable method is used here in an attempt to account for the possibility of a lifted flame.

Due to the intrinsic limitations with the steady flamelet model, it is not possible to model local extinction in non-premixed combustion if the flame stabilization mechanism is the premixed flame propagation, instead of being the quenching of the diffusion flame. An anchored flame predicted by the laminar flamelet model means only that the predicted local scalar dissipation is not large enough to quench the flame at the LOX post. It does not imply that a lifted flame is not possible. To remedy this deficiency of the flamelet model, the extended flamelet/progress-variable approach is used to investigate the flame stabilization mechanism at supercritical conditions.

Figure 7.20 shows the instantaneous and time-averaged temperature distribution of the flamelet-progress-variable case. From the results, one can see that no lifted flame has been resolved in the current study. The flame structures are different from the flamelet baseline case and the ideal gas library flamelet case. The FPV case uses the ideal gas library, which gives rise to a larger mean temperature than the flamelet baseline case. However, the flame structure is also different from the ideal gas library case. If one looks at the flames in the rich regions, more oxygen is observed than in the ideal gas library case. This can be attributed to the fact that the chemical reaction in the rich zone is slower (CO oxidization) and it takes a much longer time to translate the reactants to combustion products than in the near stoichiometric regions.
To evaluate the effect of the initial conditions on the flame anchoring point, a simulation is re-initialized with a stationary state flow while artificially quenching the flame in the downstream of the splitter plate. It was shown that as the artificial quenching distance is small, the flame is always able to propagate upstream and re-attach itself to the splitter plate. However, if the flame is quenched very far away from the splitter plate, the flame can be totally blown out. The current results indicate that it is possible to resolve a lifted flame with the flamelet/progress variable model, given appropriate operating conditions. The FPV results, combined with the flamelet baseline cases and the experiments studies discussed in the introduction section, confirm that the flame is most likely anchored in the recirculation zone of the splitter plate. No lifted flame is expected for the supercritical combustion of LOX and methane, at least for operating conditions studied in the current work.

The species concentration and temperature scattering plots in mixture fraction space for the flamelet and FPV cases are shown in Figures 7.21 and 7.22, respectively. Turbulence fluctuations in the flames regions act as an external stretching effect on the unresolved laminar flamelets since the flame inner layer thickness is at least one order of magnitude smaller than the Kolmogorov scale. The smallest eddies can at most affect the outer region of the flames, enhancing the thermal and species diffusion, thus changing the flame shape and structures. The global effect of turbulence on flame structures is quantified as the scalar dissipation rate and the variance of the mixture fraction. In the mean sense (a computational cell), the combustion products at fixed mean mixture fraction fluctuate due to the effect of the scalar dissipation and the mixture fraction variance. If one looks at the temperature scattering plot, it appears that the temperature fluctuation is even stronger than that of species. This is not only because of the species fluctuation, but also because heat transfer contributes to the temperature variation, resulting in a broader distribution of temperature. By comparing Figure 7.21 and Figure 7.22, it
is clear the species profiles are totally different from each other. This is expected because the flamelet libraries used are different, which results in totally different species profiles, and thus different temperatures. For example, the CO mass fraction is much smaller than that in the real-gas case. CO$_2$ profiles show contrary profiles. This is because ideal-gas flamelet library gives a more complete combustion of reactants. More CO$_2$ and less CO are formed, correspondingly, it results in a higher flame temperature. In this sense, the effect of the real-gas flamelet library plays a very important role in determining the flamelet inner structures.

Another difference between the two cases is the range of values of the species mass fractions for a given mixture fraction value. In the FPV case, near-pure mixing realizations of species profiles are observable, but are not observed in the flamelet baseline case. This is a direct result of the model difference. In the flamelet baseline case, since the calculated scalar dissipation rate is always smaller than the quenching limit of flame at that pressure conditions the flame structures fluctuates only slightly around the equilibrium state. As discussed in the introduction, this cannot account for a pure mixing when the scalar dissipation rate is small. This is an intrinsic defect of the flamelet method. However, in the FPV case, the progress variable is used to account for the unsteady effect of combustion, as discussed previously. At some locations (for example, near the wall), no chemical reaction is possible, and the progress variable is always close to zero. This corresponds to the pure mixing realizations in the mixture fraction space. The intermediate states between combustion and pure mixing represent the transient process to combustion state. The number of those points is much smaller than that of the reacting states, therefore, they are not a major focus in the current case. Another observation is that at fuel rich regions, there is more oxygen leakage into the fuel-rich region. This is because the reaction rates of the rich mixtures are much smaller. The combustion is not complete even before the particles escape the computational domain.
7.4 Conclusions

The flamelet model and flamelet/progress-variable model have been successfully applied to the large-eddy simulations of LOX/methane flames at supercritical pressures. The basic assumptions associated with the flamelet model are discussed systematically in the context of the supercritical combustion of LOX and methane. The results show that the flame is always anchored in the recirculation zone immediately after the splitter plate. Turbulence is not strong enough to extinguish the non-premixed flame. The flame stabilization is found to be achieved through the recirculation zone formed in the near region of the splitter plate. The flame anchoring mechanism is compared to that of the sub-critical flame experiments and the difference is attributed to the difference in the gasification time scales at sub- and supercritical conditions. The flamelet-progress variable case further confirms that the artificially quenched flame can be re-established as far as the quenching distance is within the recirculation zone.

At higher momentum flux ratio, the size of the recirculation is increased, indicating a better stabilized flame. This provides an explanation for the effect of momentum flux ratio on the combustion stability.

The effect of turbulence models is also investigated. The results do not show significant difference. For numerical efficiency, the static model is appropriate for future studies.

Considering the complexity and computation load associated with the FPV model, it is more practical to use the flamelet model if the wall temperature effect is not of interest.

The turbulent combustion models developed here can be used in the investigations of supercritical combustion of swirl- and shear coaxial injectors and provide more insight into the flow and combustion dynamics of those injectors.
Table 7.1. Computational Cases.

<table>
<thead>
<tr>
<th>Case</th>
<th>combustion model</th>
<th>SGS model</th>
<th>flamelet library</th>
<th>momentum flux ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>2 species cold flow</td>
<td>Static</td>
<td>--</td>
<td>2.65</td>
</tr>
<tr>
<td>B (baseline)</td>
<td>Flamelet</td>
<td>Static</td>
<td>Real gas</td>
<td>2.65</td>
</tr>
<tr>
<td>C</td>
<td>Flamelet</td>
<td>dynamic</td>
<td>Real gas</td>
<td>2.65</td>
</tr>
<tr>
<td>D</td>
<td>Flamelet</td>
<td>Static</td>
<td>Ideal gas</td>
<td>2.65</td>
</tr>
<tr>
<td>E</td>
<td>Flamelet</td>
<td>Static</td>
<td>Real gas</td>
<td>6.0</td>
</tr>
<tr>
<td>F (FPV)</td>
<td>FPV</td>
<td>Static</td>
<td>Ideal gas</td>
<td>2.65</td>
</tr>
</tbody>
</table>

Figure 7.1. Computational domain and boundary conditions.
Figure 7.2. Kinetic energy spectra in the near field of the splitter plate.

Figure 7.3. Instantaneous Temperature Comparison of all cases.
Figure 7.4. Mean temperature distribution for all cases.
Figure 7.5. Mean density distribution for all cases.
Figure 7.6. Mean mixture fraction distribution for all cases.
Figure 7.7. Mean flame shape for all cases, T=1000K.

Figure 7.8. Mean Flame width as a function axial direction.
Figure 7.9. Axial profiles of mean and RMS of Temperature, as well as of mean vertical velocity, and mean mixture fraction along the centerline of the splitter plate.
Figure 7.10. y profiles at 1, 5 and 15 non-dimensional axial locations.
Figure 7.11. Streamlines overlapped on mean temperature contours.
Figure 7.12. Flame stabilization mechanism for case B, $\Delta t = 10$ ms (left to right, top to bottom).
Figure 7.13. Flame evolution after artificially quenching.
Figure 7.14. Instantaneous snapshots of temperature, vorticity, and mass fractions of oxygen and methane, for cold flow.
Figure 7.15. Velocity spectra at different probe locations in pure mixing of LOX and methane.
Figure 7.16. Instantaneous snapshots of flamelet baseline case.
Figure 7.17. Instantaneous snapshots for dynamic SGS case.
Figure 7.18. Instantaneous snapshots for ideal gas library case.
Figure 7.19. Instantaneous snapshots for higher momentum ratio case.
Figure 7.20. Instantaneous snapshots for flamelet-progress-variable case.
Figure 7.21. Scattering profiles of species and temperature in mixture fraction space, baseline case.
Figure 7.22. Scattering profiles of species and temperature in mixture fraction space, FPV case.
Chapter 8

Conclusions and Recommendations

8.1 Conclusions

A unified theoretical and numerical framework has been established to investigate real fluid turbulent combustion. It includes real-fluid thermodynamics and transport phenomena over the entire temperature and pressure regimes of concern, and incorporates the steady flamelet and the flamelet/progress-variable models to account for turbulent/chemistry interactions. The resulting equations are solved numerically using a preconditioned, density-based finite volume method along with a dual-time stepping technique. The numerical accuracy of the framework is significantly improved by means of a higher-order accuracy compact interpolation scheme, combined with the matrix dissipation method to ensure numerical stability in flows with extremely large gradients of density and thermodynamic properties, with minimized numerical dissipation on the flow field. The resulting numerical scheme is validated against the Sandia Flame D, and then applied to study propellant mixing and combustion dynamics under conditions that are of typical contemporary liquid rocket engines.

The computer program has been validated against the Sandia Flame D. Reasonably good agreement with the experimental results is achieved in terms of axial and radial profiles of velocity, temperature, and mass fractions of major species. The conditionally averaged mass
fraction profiles at different axial locations show very good agreement with that of the experimental results. Since the numerical scheme has been validated against supercritical mixing of nitrogen jet by Zong et al. (2004) and Liu et al. (2006), and the current effort validates the turbulent combustion model, the resulting numerical procedure can be applied to study the supercritical flow and combustion dynamics in liquid rocket environment.

The dynamic response of a pressure swirl injector to external excitations has been investigated under supercritical conditions. The results show that the forced flow is dominated by coherent flow motions of the forcing frequency except the cases in which very high frequency forcing is imposed. The time-averaged film thickness and spreading angle do not show significant variations compared to that of the unforced flow; however, the instantaneous spreading angle and film thickness fluctuate at the forcing frequency. Thus, the external forcing may affect the atomization and mixing processes significantly. When external forcing is added, the responses of the turbulent fluctuations are related to the frequencies of the coherent structures. The external forcing energizes the flow motions that are of the forcing frequency; and it suppresses or weakens fluctuations that are of frequencies different from the forcing frequency. The resulting mass transfer function at some forcing frequencies can be substantially larger than unity. The effect of forcing magnitude shows strong non-linear characteristics when high-amplitude forcing is imposed. The effect of external forcing on the rate of mixing, evaporation and subsequent combustion is tremendous. Extreme caution has to be exercised to avoid any of these instabilities, especially those instabilities characterized with large transfer functions, when designing the configuration and operating conditions of a new swirl injector.

The combustion of gaseous oxygen/gaseous hydrogen in a high-pressure combustion chamber for a shear coaxial injector is studied to assess the accuracy and the credibility of the computer program when applied to a laboratory-scale combustor. The predicted heat flux profile
is compared with the experimental study by the Cryogenic Combustion Laboratory (CCL) at Penn State University and the numerical studies by Oefelein, Menon, Merkle and Tucker. The current study predicts a heat flux profile that agrees well with the experimental results. Although all the numerical simulations predict the heat flux profile fairly accurately, especially in the downstream region, a variety of differences exist among the numerical studies, due to the inherent difference in model fidelity and uncertainties. To further evaluate the accuracy of the numerical methods, it is suggested to obtain emission images in the near field of the injector exit, so that the simulated flame structures can be compared with those images to assess the accuracy of the numerical schemes.

The flamelet and the flamelet/progress-variable models have been used to investigate the supercritical combustion of LOX/methane in the near field of a splitter plate. The basic assumptions associated with the flamelet model are discussed systematically in the context of supercritical combustion. The results show that the flame is always anchored in the recirculation zone right after the splitter plate. Turbulence fluctuations are not strong enough to extinguish the non-premixed flame. The flame anchoring mechanism at supercritical conditions is compared to that of the sub-critical flames. As it is already known, the LOX gasification rate at supercritical conditions is at least one order of magnitude faster than that at low pressure subcritical conditions. Thus, the flow patterns after the splitter plate are different at sub- and supercritical conditions, and this causes the difference in the flame stabilization mechanism. The flamelet-progress-variable case further confirms that artificially quenched flame can be re-established as far as the quenching distance is within the recirculation zone. Considering the flame stabilization mechanism at supercritical conditions, and the extra computation load associated with the FPV model, it is more practical to use the flamelet model if the wall temperature effect is not of interest. The effect of momentum flux ratio on the flame stabilization is related to its effect on
the size of the recirculation zone. This indicates a higher momentum flux ratio will improve the flame anchoring and thus the combustion stability.

8.2 Recommendations for Future work

The theoretical and numerical framework established in the present study is proved to be robust, efficient and accurate. Significant improvement has been achieved by using the less dissipative matrix artificial dissipation method, as well as the adoption of higher-order accuracy spatial differencing scheme. However, further improvement can be made by utilizing the higher-order compact interpolation schemes. However, unfortunately, the higher order compact scheme is more expensive due to the calculations of extra equations. Further investigation is necessary to achieve a cost-effective higher-order accurate numerical scheme.

The all-Mach number preconditioning scheme is used in the current numerical scheme to speed up convergence, however, the explicit treatment of temporal differencing makes the CFL number limited to less than unity, resulting in a slow convergence rate. An implicit scheme for the internal region and explicit treatment at the internal boundaries are proposed for future studies. Multi-grid algorithms are also proposed to further expedite the numerical convergence.

The evaluation of thermodynamic properties is also very expensive for real-fluid mixtures, especially when the number of species is large. In the present study, a significant portion of the computation time has been spent on the evaluation of the thermodynamic and transport properties. This characteristic makes it prohibitively costive to apply the numerical simulations to industry interested studies. An In Situ Adaptive Tabulation (ISAT) method might be helpful in reducing the cost of evaluating thermodynamic properties for real-fluid mixture.
The treatment of turbulent inlet boundary conditions in the current study is very simple. However, the fluctuations generated with this method are not real turbulence, and they are not compatible with the Navier-Stokes equations, so that the fluctuations will be destroyed very soon after they are introduced at the inlet boundary. This type of fluctuations can only serve as a excitation for the flow to develop real turbulence structures. Generally a long developing section is required for turbulent structures to develop, thus it makes the method computationally expensive. If the developing section is too short that the upstream turbulence statistics is incorrect, the dynamics of the downstream mixing layers might be significantly different from the real physics. To overcome this shortcoming, more sophisticated inlet boundary condition treatments, such as the recycling method, are recommended to be included in the current numerical methods.

Finally, the current numerical scheme can only accommodate static grid system. In this situation, extreme care must be exercised to the grid stretching, grid configuration, and the total number of grid points to assure the grid is fine enough to meet the requirement of the large-eddy simulation technique. The grid distribution is generally not optimized, and there are regions where grids are redundant. This situation increases the computation cost. In addition, the grid generation process is case specific, and very much dependent on users' preference and experiences. Grid independence study becomes necessary, resulting in extra computation cost and longer turnaround time for the entire projects. The adaptive mesh refinement (AMR) algorithm seems very attractive to high-fidelity large-scale calculations. With AMR, the grid resolution requirement could be achieved dynamically based on the local flow solutions. The computational effort could be focused on the regions where are of most interest.
Appendix A

Properties of the Favre Average (Based on Reynolds Average)

The Favre average is defined as

\[ \bar{f} = \frac{\rho f}{\bar{\rho}}. \] \hspace{1cm} (A.1)

Based on the definition, we have

\[ \bar{\rho f} = \rho (\bar{f} + f') = \bar{\rho f} + \rho f' = \bar{\rho} \bar{\rho} f / \bar{\rho} + \rho f' = \bar{\rho} f / \bar{\rho} + \rho f' = \bar{\rho} f + \rho f'. \] \hspace{1cm} (A.2)

so,

\[ \bar{\rho f}' = 0. \] \hspace{1cm} (A.3)

The relation between Favre averaged and Reynolds averaged variables is given by:

\[ \bar{f} = \frac{\rho f}{\bar{\rho}} = \frac{(\bar{\rho} + \rho')(\bar{f} + f')}{\bar{\rho}} = \frac{\bar{\rho} \bar{f} + \rho f' + \rho' \bar{f} + \rho' f'}{\bar{\rho}} = \bar{f} + \rho f'. \] \hspace{1cm} (A.4)

We also have \( \bar{\rho f} = \bar{\rho} f + \rho f' = \bar{\rho} f \), then

\[ \bar{\rho f} = \bar{\rho} \bar{f}. \] \hspace{1cm} (A.5)

By definition, we have \( \bar{\rho f} = \bar{\bar{f}} = \bar{\bar{f}} \), so

\[ \bar{\bar{f}} = \bar{f}. \] \hspace{1cm} (A.6)
Another important relation is given by:

\[
\overline{\rho fg} = \rho (\overline{\tilde{f} + f'}) (\overline{\tilde{g} + g'}) = \rho \overline{\tilde{f}g} + \rho \overline{\tilde{f}g'} + \rho f' \overline{\tilde{g}} + \rho f' \overline{\tilde{g}'} = \overline{\rho \tilde{f}g} + \overline{\rho f'g'}.
\]  

(A.7)
Appendix B

Thermodynamics Relationships

The thermodynamics relations, such as those for evaluations of specific internal energy, specific enthalpy, and specific heat capacities, and those for evaluations of preconditioning and Jacobian matrices, are presented in this Appendix.

The partial density internal energy \( (\bar{e}_i) \) of species \( i \) will be derived. We first need to find the expression for the internal energy \( (e) \). From the fundamental thermodynamic theory, we have

\[
e(T, \rho) = e_0(T) + \int_0^\rho \left[ \frac{P}{\rho^2} - \frac{T}{\rho^2} \left( \frac{\partial p}{\partial T} \right)_\rho \right] d\rho ,
\]

where the subscript 0 indicates a reference ideal state at a low pressure.

Utilizing the modified SRK equation of state and the partial derivative relation Eq. 2.38-2.40, Eq. B.1 is integrated, which leads to the following relationship

\[
e(T, \rho) = e_0(T) + \frac{T^2}{bM_w} \left( \frac{\partial a \alpha/\rho \chi}{\partial T} \right)_{\rho \chi} \ln \left( 1 + \frac{b\rho}{M_w} \right) ,
\]

where the partial derivative \( \frac{\partial a \alpha/\rho \chi}{\partial T} \) is presented in Appendix C.

According to the definition for the partial density property, the partial density internal energy \( (\bar{e}_i) \) can be expressed as
\[ \tilde{e}_i = e_{i,0} + \frac{2}{bM_{wi}} \left[ \sum_j x_j \left( T \frac{\partial}{\partial T} (a_{ij} \alpha_{ij}) - a_{ij} \alpha_{ij} \right) \right] \ln \left( 1 + \frac{b \rho}{M_w} \right) \]

\[ + \frac{b_i}{bM_{wi}} \left[ T \frac{\partial}{\partial T} (a \alpha) - a \alpha \right] \left[ \frac{\rho}{M_w + b \rho} - \frac{1}{b} \ln \left( 1 + \frac{b \rho}{M_w} \right) \right]. \] (B.3)

In addition, utilizing Eq. B.3, the internal energy of a mixture can be related to the partial density internal energy as

\[ e = \sum_i Y_i \tilde{e}_i - \frac{1}{M_w} \left[ T \frac{\partial}{\partial T} (a \alpha) - a \alpha \right] \frac{\rho}{M_w + b \rho}. \] (B.4)

Based on thermodynamics,

\[ \rho h = \rho e + p. \] (B.5)

Following the definition for the partial density property, the following expression can be found by taking derivative of the partial density of the species \( i \) to both sides of the Eq. B.5, and keeping temperature and all the other partial densities constant

\[ \left( \frac{\partial \rho h}{\partial \rho_i} \right)_{T,P,p_i} = \left( \frac{\partial \rho e}{\partial \rho_i} \right)_{T,P,p_i} + \left( \frac{\partial p}{\partial \rho_i} \right)_{T,P,p_i}. \] (B.6)

It is equivalent to Eq. B.7

\[ \tilde{h}_i = \tilde{e}_i + \left( \frac{\partial p}{\partial \rho_i} \right)_{T,P,p_i}. \] (B.7)
Substituting Eq. B.7 into Eq. 2.46, and taking use of the fundamental enthalpy expression, which can be found in any thermodynamics textbook, the following relation concerning the partial mass enthalpy \( \overline{h_i} \) can be established

\[
\overline{h_i} = \bar{e}_i + \frac{T}{\rho} \left( \frac{\partial p}{\partial T} \right)_{\rho_i} \left( \frac{\partial p}{\partial \rho} \right)_{T,\rho_i}.
\]  

(B.8)

Next, we begin to find the expressions for the constant volume and the constant pressure heat capacities based on the SRK equation of state.

The definition of constant volume heat capacity is

\[
C_v = \left( \frac{\partial e}{\partial T} \right)_{\rho_i, v_i}.
\]  

(B.9)

Utilizing Eq. B.2, it is straightforward to find

\[
C_v = C_v^0 + \frac{T}{b M_w} \frac{\partial^2}{\partial T^2} (a \alpha) \ln \left( 1 + \frac{b \rho}{M_w} \right).
\]  

(B.10)

Following fundamental thermodynamic relationships, the constant-pressure heat capacity can be expressed as

\[
C_p = C_v + \frac{T}{\rho^2} \left( \frac{\partial p}{\partial T} \right)_{\rho_i}^2 \left( \frac{\partial p}{\partial \rho} \right)_{T,\rho_i}.
\]  

(B.11)

In order to find the thermodynamic relationships regarding chemical potential, the partial density and partial mass entropy have to be derived first
Based on the definition of partial density entropy, it is found

\[ s(T, \rho) = s_0(T, \rho_0) - \int_{\rho_0}^{\rho} \left( \frac{1}{\rho^2} \left( \frac{\partial \rho}{\partial T} \right)_p \right) \ d\rho. \]  

(B.12)

The partial mass entropy can be further related to the partial density entropy as

\[
\tilde{S}_i = \int_{T_{ref}}^{T} C_{p,i} \frac{dT}{T} - \frac{R_u}{M_{wi}} 1 + \ln x_i - \frac{R_u}{M_{wi}} \ln \frac{\rho}{\rho_{ref}} \frac{R_u T}{M_w} \left[ 1 - b \rho \right] - \frac{R_u}{M_{wi}} \frac{b_{w}}{b_{w} - b \rho} + \frac{b_{w}}{b_{w}} \frac{1}{b^2} \frac{\partial a \alpha}{\partial T} \left[ \frac{b \rho}{M_{w}} + b \rho \right] \\
- \ln \left[ 1 + \frac{b \rho}{M_{w}} \right] + \frac{2}{b M_{wi}} \left[ \sum_{j} x_j \frac{\partial}{\partial T} a_j \alpha_{ij} \right] \ln \left[ 1 + \frac{b \rho}{M_{w}} \right],
\]

(B.13)

The partial mass entropy can be further related to the partial density entropy as

\[ \bar{S}_i = \tilde{S}_i + \left( \frac{\partial p}{\partial T} \right)_{p,T} \bar{V}_i, \]

(B.14)

where the partial mass volume is

\[ \bar{V}_i = \frac{1}{\rho} \left( \frac{\partial p}{\partial \rho} \right)_{T,p} \left( \frac{\partial p}{\partial \rho} \right)_{T,Y_i}. \]

(B.15)

The chemical potential of species \( i \) can be calculated as

\[ \mu_i = \tilde{f}_i = \tilde{e}_i - T \tilde{s}_i. \]

(B.16)

The partial derivatives regarding chemical potential can be expressed as
When the mixture fraction equation instead of the species equations is solved for chemistry closure, the derivative of any scalar $\phi$ with respect to the mixture fraction is evaluated based on the chain rule, shown as following.

\[
\left( \frac{\partial \mu_i}{\partial p} \right)_{T,Y_j} = \bar{V}_i, \\
\left( \frac{\partial \mu_i}{\partial T} \right)_{T,Y_j} = -\bar{S}_i,
\]

(B.17) (B.18)

When the mixture fraction equation instead of the species equations is solved for chemistry closure, the derivative of any scalar $\phi$ with respect to the mixture fraction is evaluated based on the chain rule, shown as following.

\[
\left( \frac{\partial \phi}{\partial f} \right)_{T,p} = \sum_{i=1}^{N+1} \left( \frac{\partial \phi}{\partial Y_i} \right)_{T,p,Y_{\text{ref}}_i} \left( \frac{\partial Y_i}{\partial f} \right)_{T,p},
\]

where $\left( \frac{\partial Y_i}{\partial f} \right)_{T,p}$ is obtained from the flamelet library, that is, it is dependent on the local flame structures.

Next, we want to derive the partial derivatives needed in the calculation of the precondition and Jacobian matrices.

First, a thermodynamic relationship correlating pressure as a function of temperature, density, and mass fractions is derived. According to thermodynamics, each intensive property will depend on $N+1$ other intensive variables in a mixture. We begin with the following relation

\[
p = p(T, \rho_i),
\]

(B.20)

where $i = 1, \ldots, N$.

Only the differential form is interested, then it can be expressed as
\[ dp = \left( \frac{\partial p}{\partial T} \right)_{\rho_i} dT + \sum_{i=1}^{N} \left( \frac{\partial p}{\partial \rho_i} \right)_{T,\rho_{pi}} d\rho_i. \]  

(B.21)

Rearrange it, we have

\[ dp = \left( \frac{\partial p}{\partial T} \right)_{\rho_i} dT + \sum_{i=1}^{N-1} \left[ \left( \frac{\partial p}{\partial \rho_i} \right)_{T,\rho_{pi}} - \left( \frac{\partial p}{\partial \rho_N} \right)_{T,\rho_{pN}} \right] d\rho_i + \left( \frac{\partial p}{\partial \rho_N} \right)_{T,\rho_{pN}} d\rho. \]  

(B.22)

Since \( \rho_i = \rho Y_i \)

\[ d\rho_i = Y_i d\rho + \rho dY_i. \]  

(B.23)

Substituting Eq. B. 23 into Eq. B. 22 leads to following expression

\[ dp = A_T dT + A_i dY_i + A_{\rho} d\rho, \]  

(B.24)

where

\[ A_T = \left( \frac{\partial p}{\partial T} \right)_{\rho_i}, \]  

(B.25)

\[ A_i = \rho \left[ \left( \frac{\partial p}{\partial \rho_i} \right)_{T,\rho_{pi}} - \left( \frac{\partial p}{\partial \rho_N} \right)_{T,\rho_{pN}} \right], \]  

(B.26)

\[ A_{\rho} = \left( \frac{\partial p}{\partial \rho} \right)_{T,Y}. \]  

(B.27)

A very useful formulation can be derived from Eq. B. 24, which is
Next, a thermodynamic relationship correlating internal energy as a function of pressure, density, and mass fractions is derived. We begin with the following one

\[ \rho e = \rho e(T, \rho_i). \] (B.29)

where \( i = 1, \cdots, N \), and \( e \) is the internal energy per unit mass. Its differential form can be written as

\[ d\rho e = \rho \left( \frac{\partial e}{\partial T} \right)_{\rho_i} \ dT + \sum_{j=1}^{N} \left( \frac{\partial \rho e}{\partial \rho_i} \right)_{T, \rho_{j \neq i}} \ d\rho_i. \] (B.30)

Based on the definition of partial density properties, it is recognized

\[ \tilde{e}_i = \left( \frac{\partial \rho e}{\partial \rho_i} \right)_{T, \rho_{j \neq i}}, \] (B.31)

which is the partial density internal energy of species \( i \) in the mixture. The first derivative in Eq. B. 30 is the constant volume heat capacity \( C_v \). Substituting the partial density internal energy of each species into Eq. B. 30 leads to the following expression

\[ d\rho e = \rho C_v dT + \sum_{i=1}^{N} \tilde{e}_i d\rho_i. \] (B.32)

Inserting Eq. B. 23 into Eq. B. 32,
\[ d\rho e = \rho C_v dT + \sum_{i=1}^{N} \tilde{e}_i \rho dY_i + \sum_{i=1}^{N} \tilde{\varepsilon}_i Y_i d\rho. \] (B.33)

Since \( d\rho e = \rho de + ed\rho \), the following expression is easily derived

\[ de = C_v dT + \sum_{i=1}^{N-1} (\tilde{e}_i - \tilde{\varepsilon}_N) dY_i + \frac{1}{\rho} \left( \sum_{i=1}^{N} \tilde{\varepsilon}_i - e \right) d\rho. \] (B.34)

Substituting Eq. B.33 into Eq. B.34, we can establish

\[ de = B_T dT + B_p dp + \sum_{i=1}^{N-1} B_{i} dY_i, \] (B.35)

where

\[ B_T = C_v - \frac{1}{\rho} \left( \sum_{i=1}^{N} Y_i \tilde{e}_i - e \right) \left( \frac{\partial \rho}{\partial p} \right)_{T,Y} \left( \frac{\partial p}{\partial T} \right)_{\rho}, \] (B.36)

\[ B_p = \frac{1}{\rho} \left( \sum_{i=1}^{N} Y_i \tilde{\varepsilon}_i - e \right) \left( \frac{\partial \rho}{\partial p} \right)_{T,Y}, \] (B.37)

\[ B_i = \left\{ (\tilde{e}_i - \tilde{\varepsilon}_N) - \left( \sum_{i=1}^{N} Y_i \tilde{\varepsilon}_i - e \right) \cdot \left( \frac{\partial \rho}{\partial p} \right)_{T,Y} \cdot \left[ \left( \frac{\partial p}{\partial \rho} \right)_{T,p_{r_m}} - \left( \frac{\partial p}{\partial \rho} \right)_{T,p_{r_N}} \right] \right\}. \] (B.38)

Based on fundamental thermodynamic theories, the following relation can be obtained

\[ dh = de + \frac{1}{\rho} dp - \frac{p}{\rho^2} d\rho. \] (B.39)

Substituting Eq. B.35 into Eq. B.39, the following expression is derived after some straightforward manipulations
\[ dh = D_T dT + D_p dp + \sum_{i=1}^{N-1} D_{i} dY_i, \]  

where

\[ D_T = C_v - \frac{1}{\rho} \left( \frac{\partial p}{\partial T} \right)_{\rho_i} \left( \frac{\partial \rho}{\partial T} \right)_{T,\rho_i} \left( \sum_{i=1}^{N} Y_i \tilde{e}_i - e \right) - \frac{p}{\rho}, \]  

\[ D_p = 1 + \frac{1}{\rho} \left( \frac{\partial p}{\partial p} \right)_{T, \rho_i} \left( \sum_{i=1}^{N} Y_i \tilde{e}_i - e \right) - \frac{p}{\rho}, \]  

\[ D_{Y_i} = \tilde{e}_i - \tilde{e}_N - \left( \frac{\partial p}{\partial \rho} \right)_{T, \rho_i} \left( \sum_{i=1}^{N} Y_i \tilde{e}_i - e \right) - \frac{p}{\rho} \left[ \left( \frac{\partial p}{\partial \rho} \right)_{T, \rho_i} - \left( \frac{\partial p}{\partial \rho} \right)_{T, \rho_i, \rho_i} \right]. \]

According to the definition in thermodynamics, we recognize that the coefficient \( D_T \) equals to the constant pressure heat capacity \( C_p \) of a fluid mixture,

\[ C_p = D_T = C_v - \frac{1}{\rho} \left( \frac{\partial p}{\partial T} \right)_{\rho_i} \left( \frac{\partial \rho}{\partial T} \right)_{T, \rho_i} \left( \sum_{i=1}^{N} Y_i \tilde{e}_i - e \right) - \frac{p}{\rho}. \]  

Finally a relationship regarding the speed of sound in the mixture is derived. According to the definition of the speed of sound

\[ a^2 = \left( \frac{\partial p}{\partial \rho} \right)_{s,Y_i}. \]  

Based on the Eq. B.24, the following expression is obtained in a straightforward manner.

\[ \left( \frac{\partial p}{\partial \rho} \right)_{s,Y_i} = \left( \frac{\partial p}{\partial T} \right)_{\rho_i} \left( \frac{\partial T}{\partial \rho} \right)_{s,Y_i} + \left( \frac{\partial p}{\partial \rho} \right)_{T, \rho_i}. \]
In thermodynamics, the following relationship exists

\[ s = s(T, \rho, Y_i), \]  \hspace{1cm} (B.47)

where \( i = 1, \ldots, N - 1 \).

After utilizing some fundamental thermodynamic relationships, the following differential form of Eq. B.47 can be obtained

\[ ds = \frac{C_v}{T} dT - \frac{1}{\rho} \left( \frac{\partial p}{\partial T} \right)_{\rho_i} d\rho + \sum_{i=1}^{N-1} \left( \frac{\partial s}{\partial Y_i} \right)_{T,\rho,Y_{jm}} dY_i. \]  \hspace{1cm} (B.48)

Based on Eq. B.48, the following expression is further derived

\[ \left( \frac{\partial T}{\partial \rho} \right)_{s,Y_i} = \frac{T}{\rho^2} \left( \frac{\partial p}{\partial T} \right)_{\rho_i} \left/ C_v \right. \]  \hspace{1cm} (B.49)

Substituting Eq. B.49 into Eq. B.46, an expression of the speed of sound in the general fluid mixture is established as

\[ a^2 = \left( \frac{\partial p}{\partial \rho} \right)_{s,Y_i} = \frac{C_p}{C_v} \left( \frac{\partial p}{\partial \rho} \right)_{T,Y_i}. \]  \hspace{1cm} (B.50)

Equations B.24, B.35, B.40, and B.50 are the important thermodynamic relationships required in evaluating the preconditioning and Jacobian matrices.
Appendix C

Derivative Expressions in Soave-Redlich-Kwong Equation of State

In the Soave-Redlich-Kwong (SRK) equation of state, the terms $a\alpha$ and $\alpha_j a_j$ are functions of temperature. The derivative of $a\alpha$ to temperature is given as

$$\frac{\partial (a\alpha)}{\partial T} = \sum_{i=1}^{N} \sum_{j=1}^{N} x_i x_j \sqrt{a_i a_j} \frac{\partial \sqrt{\alpha_i \alpha_j}}{\partial T} ,$$

(C.1a)

where

$$\frac{\partial \sqrt{\alpha_i \alpha_j}}{\partial T} = \frac{1}{2} \left( \frac{\alpha_i}{\alpha_j} \right)^{\frac{1}{2}} \frac{\partial \alpha_j}{\partial T} + \frac{1}{2} \left( \frac{\alpha_j}{\alpha_i} \right)^{\frac{1}{2}} \frac{\partial \alpha_i}{\partial T} ,$$

(C.1b)

$$\frac{\partial \alpha_i}{\partial T} = -\frac{S_i}{\sqrt{T_{c,i}}} \left[ 1 + S_i \left( 1 - \frac{T}{T_{c,i}} \right) \right] ,$$

(C.1c)

$$\frac{\partial a_j \alpha_j}{\partial T} = \sqrt{a_j a_j} \frac{\partial \sqrt{\alpha_i \alpha_j}}{\partial T} .$$

(C.2)

The second derivative of parameter $a\alpha$ to temperature is

$$\frac{\partial^2 (a\alpha)}{\partial T^2} = \sum_{i=1}^{N} \sum_{j=1}^{N} x_i x_j \sqrt{a_i a_j} \frac{\partial^2 \sqrt{\alpha_i \alpha_j}}{\partial T^2} ,$$

(C.3a)

where
\[
\frac{\partial^2 \sqrt{\alpha_i \alpha_j}}{\partial T^2} = \frac{1}{2} \left( \frac{1}{\alpha_i \alpha_j} \right) \left( \frac{\partial \alpha_i}{\partial T} \right)^2 \left( \frac{\partial \alpha_j}{\partial T} \right)^2 - \frac{1}{4} \left( \frac{\alpha_i}{\alpha_j^3} \right) \left( \frac{\partial \alpha_i}{\partial T} \right)^2
\]

(C.3b)

\[
- \frac{1}{4} \left( \frac{\alpha_i}{\alpha_j^3} \right) \left( \frac{\partial \alpha_i}{\partial T} \right)^2 + \frac{1}{2} \left( \frac{\alpha_i}{\alpha_j} \right) \left( \frac{\partial^2 \alpha_i}{\partial T^2} \right) + \frac{1}{2} \left( \alpha_i \right) \left( \frac{\partial^2 \alpha_j}{\partial T^2} \right),
\]

\[
\frac{\partial^2 \alpha_i}{\partial T^2} = \frac{1}{2} \frac{S_i^2}{T_{c,i} T_{c,j}} + \frac{1}{2} \frac{S_i}{\sqrt{T_{c,j}}} \left[ 1 + S_i \left( 1 - \frac{T}{T_{c,i}} \right) \right].
\]

(C.3c)

The variable \( \alpha_i \) for species \( \text{H}_2 (\alpha_{\text{H}_2}) \), is treated differently since hydrogen is a quantum gas. The derivative of this variable is

\[
\frac{\partial \alpha_{\text{H}_2}}{\partial T} = -\alpha_{\text{H}_2} \left[ 0.30228 \frac{1}{T_{c,i}} \right],
\]

(C.4)

\[
\frac{\partial^2 \alpha_{\text{H}_2}}{\partial T^2} = \alpha_{\text{H}_2} \left[ 0.30228 \frac{1}{T_{c,i}} \right]^2.
\]

(C.5)
Appendix D

Jacobian Matrices

The Jacobian matrices employed in Chapter 3 are defined as follows.

D.1 Jacobian of Primitive Variables

The Jacobian of primitive variables $T = \partial Q / \partial Z$ is given by

$$T = \begin{bmatrix}
\frac{\partial p}{\partial \rho} & 0 & 0 & \rho_T & \rho_f \\
\tilde{u} \frac{\partial \rho}{\partial \rho} & \tilde{\rho} & 0 & \tilde{u} \rho_T & \tilde{u} \rho_f \\
\tilde{v} \frac{\partial \rho}{\partial \rho} & 0 & \tilde{\rho} & \tilde{v} \rho_T & \tilde{v} \rho_f \\
\tilde{w} \frac{\partial \rho}{\partial \rho} & 0 & \tilde{\rho} & \tilde{w} \rho_T & \tilde{w} \rho_f \\
\hat{h}_i + \left( \sum_{i=1}^{N} \tilde{y}_i \tilde{e}_i - \frac{p}{\rho} \right) \left( \frac{\partial \rho}{\partial \rho} \right)_{T,Y} & \tilde{p} \tilde{u} & \tilde{p} \tilde{v} & \tilde{p} \tilde{w} & \tilde{p} c_p + h_i \rho_T & \rho_f E + \tilde{p} E_f \\
\tilde{f} \left( \frac{\partial \rho}{\partial \rho} \right)_{T,Y} & 0 & 0 & \rho_T \tilde{f} & \tilde{p} + \tilde{f} \rho_f & \end{bmatrix}, \quad (D.1)
$$

$$\rho_T = \left. \frac{\partial \rho}{\partial T} \right|_{p,Y} = -\frac{A_T}{A_p}, \quad (D.2)$$
\[ \rho_f = \left( \frac{\partial \rho}{\partial f} \right)_{T,p} = \sum_{i=1}^{N-1} \left( \frac{\partial Y_i}{\partial f} \right)_{T,p,Y_{ji}} = \sum_{i=1}^{N-1} \left( \frac{A_i}{A_p} \right) \left( \frac{\partial Y_i}{\partial f} \right)_{T,p}, \]  

(D.3)

\[ E_f = \left( \frac{\partial E}{\partial f} \right)_{T,p} = \sum_{i=1}^{N-1} \left( \frac{\partial E}{\partial Y_i} \right)_{T,p,Y_{ji}} \left( \frac{\partial Y_i}{\partial f} \right)_{T,p}, \]  

(D.4)

\[ \rho_f E + \rho E_f = \sum_{i=1}^{N-1} \left( \frac{\partial Y_i}{\partial f} \right)_{T,p} \left( \frac{\partial \rho}{\partial Y_i} E + \rho B_i \right) = \sum_{i=1}^{N-1} \left( \frac{\partial Y_i}{\partial f} \right)_{T,p} \left[ \rho_i \tilde{h}_i + \rho \left( \tilde{h}_i - \tilde{h}_N \right) \right], \]  

(D.5)

where the coefficients \( A_p, A_r, A_v, B_p, B_r, \) and \( B_v \) are defined in the Appendix B. The terms \( e_i \) and \( h_i \) denote total energy and total enthalpy, respectively.

\[ e_i = e + \frac{1}{2} (\tilde{u}_i^2 + \tilde{v}_i^2 + \tilde{w}_i^2), \]  

(D.6)

\[ h_i = e_i + \frac{p}{\rho}. \]  

(D.7)

**D.2 Convective Flux Jacobians**

The Jacobian matrix \( A = \frac{\partial E}{\partial Z} \) is given by
where $l_x$, $l_y$, and $l_z$ represent the three scalars in the direction vector $\mathbf{l} = l_x \mathbf{i} + l_y \mathbf{j} + l_z \mathbf{k}$. If we replace $\mathbf{l}$ with any of the following vectors, we can get the Jacobian matrices $A = \partial E / \partial \mathbf{Z}$, $B = \partial F / \partial \mathbf{Z}$, and $C = \partial G / \partial \mathbf{Z}$, respectively.

\[
A = \begin{pmatrix}
U \rho_p & \tilde{\rho} l_x & \tilde{\rho} l_y \\
\rho_p (U + \tilde{\rho} l) & \rho v l_x & \rho v l_y \\
\rho p v l_z & \rho w l_x & \rho w l_y \\
\rho (U + \tilde{\rho} v l_z) & (\rho p \tilde{\rho} h_i + \rho v h_j) U & (\rho p \tilde{\rho} h_i + \rho v h_j) U \\
\tilde{\rho} f l_x & \tilde{\rho} f l_y & \tilde{\rho} f l_z \\
\end{pmatrix}
\]

(D.8)

where $l_x$, $l_y$, and $l_z$ represent the three scalars in the direction vector $\mathbf{l} = l_x \mathbf{i} + l_y \mathbf{j} + l_z \mathbf{k}$. If we replace $\mathbf{l}$ with any of the following vectors, we can get the Jacobian matrices $A = \partial E / \partial \mathbf{Z}$, $B = \partial F / \partial \mathbf{Z}$, and $C = \partial G / \partial \mathbf{Z}$, respectively.

\[
\begin{align*}
\xi &= \xi_x \mathbf{i} + \xi_y \mathbf{j} + \xi_z \mathbf{k}, \\
\eta &= \eta_x \mathbf{i} + \eta_y \mathbf{j} + \eta_z \mathbf{k}, \\
\zeta &= \zeta_x \mathbf{i} + \zeta_y \mathbf{j} + \zeta_z \mathbf{k}.
\end{align*}
\]
Bibliography


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