MODELING AND SIMULATION OF CRYOGENIC FLUID INJECTION AND MIXING DYNAMICS UNDER SUPERCritical CONDITIONS

A Thesis in
Mechanical Engineering

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

Doctor of Philosophy

May 2005
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ABSTRACT

This research focuses on the modeling and simulation of cryogenic fluid injection and mixing processes under supercritical conditions. The objectives are: 1) to establish a unified theoretical framework that could accommodate full conservation laws, turbulence closure, and real-fluid thermodynamics and transport phenomena; 2) to systematically investigate the underlying physiochemical mechanism at near and supercritical conditions, and 3) to construct 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.

The theoretical formulation is based on 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. Transport properties, such as viscosity and thermal conductivity, are estimated with an extended corresponding-state principle. Mass diffusivity is obtained by the Takahashi method calibrated for high-pressure conditions. Turbulence closure is achieved using a large-eddy-simulation (LES) technique, in which large energy-carrying structures are computed explicitly and effects of unresolved motions on the resolved scales are modeled. Modified Smagorinsky models extended to compressible flows is used to treat interaction with subfilter-scale. The resultant governing equations are calculated numerically using a preconditioned, density-based finite volume method along with a dual-time-stepping integration algorithm. All of the numerical relations, including the Jacobian matrices and eigenvalues, are derived from fundamental thermodynamics theories that can accommodate any equation of state. The resultant algorithm has been proven to be robust and efficient. Further numerical efficiency is achieved by
utilizing a parallel computation scheme that involves the message-passing interface (MPI) library and multi-block treatment.

The theoretical model and numerical scheme were first validated against experimental data of cryogenic nitrogen fluid injection under supercritical conditions. Both two- and three-dimensional simulations were conducted. Reasonably good agreement was obtained in terms of the mean density distribution and the jet spreading angle, with a maximum deviation of 8%. The jet dynamics were largely dictated by the local thermodynamic state through its influence on the fluid thermophysical properties. When the fluid temperature transited across the inflection point on an isobaric density-temperature curve, the resultant rapid property variations might qualitatively modify the jet behavior compared with its counterpart at 1 atm. Increasing ambient pressure produced an earlier transition of the jet to the self-similar region in the simulations.

We also examined the flow and flame dynamics of a shear coaxial injector using liquid oxygen and methane. Emphasis was placed on the effects of momentum flux ratio on the near-field flow evolution. An increase in momentum flux ratio enhanced the turbulent mixing between two streams, and gave rise to a shorter liquid oxygen jet core. The dynamics of liquid oxygen injection through a swirl injector was investigated systematically. The flow development inside the swirl injector could be divided into developing, steady, and acceleration regimes. The influences of various injector geometric parameters and flow conditions on the swirl injector performance were investigated through a parametric study. Results indicated that both the liquid film thickness and the spray cone angle, representing the most important design parameters of a swirl injector, were strongly influenced by the swirling strength of the injected fluid. Those parameters, however, did not depend strongly on the mass flowrate. Therefore, a larger oxidizer swirl element with greater mass flowrate than that of the shear coaxial injector still could obtain the required intraelement mixing efficiency.
# TABLE OF CONTENTS

LIST OF FIGURES .................................................................................................................viii

LIST OF TABLES...................................................................................................................xiii

ACKNOWLEDGEMENTS........................................................................................................xiv

Chapter 1  Introduction ............................................................................................................1

1.1 Motivation and Objectives.............................................................................................1

1.2 Review of Relevant Literature .....................................................................................5

1.2.1 Supercritical Fluid..................................................................................................5

1.2.2 Experimental Study on High-Pressure Cryogenic Fluid Injection and Mixing .......5

1.2.3 Experimental Study on High-Pressure Cryogenic Propellants Combustion ..........6

1.2.4 Theoretical and Experimental Study on Swirl Coaxial Injector Design ...............10

1.2.5 Numerical Works on High-Pressure Fluid Mixing and Combustion ..................17

1.3 Work Scope and Method of Approach...........................................................................21

Chapter 2  Theoretical Formulation and Property Evaluation ............................................26

2.1 Governing Equations....................................................................................................26

2.2 Turbulence Closure: Large-Eddy-Simulation ................................................................28

2.2.1 Filtering................................................................................................................33

2.2.2 Filtered Governing Equations ..............................................................................35

2.2.3 Subgrid-Scale Models ..........................................................................................37

2.2.3.1 Algebraic Smagorinsky Type Model ...............................................................38

2.2.3.2 Dynamic Smagorinsky Model .........................................................................40

2.3 Equation of State .........................................................................................................41

2.3.1 Modified Soave-Redlich-Kwong (SRK) Equation of State ..................................42

2.3.2 Benedict-Webb-Rubin (BWR) Equation of State ..................................................44

2.4 Thermodynamic Properties .........................................................................................46

2.4.1 Partial Molar and Partial Density Properties ......................................................47

2.4.2 Critical Point of Fluid Mixture ............................................................................51

2.5 Transport Properties ....................................................................................................53

2.5.1 Corresponding States Theories ............................................................................53

2.5.2 Mixing Rules for Mixtures ...................................................................................55

2.5.3 Viscosity of Mixtures ...........................................................................................57

2.5.4 Thermal Conductivity of Mixtures .......................................................................58

2.5.5 Binary Mass Diffusivity .......................................................................................59

Chapter 3  Numerical Methodology .....................................................................................62

3.1 Basic Approach ............................................................................................................62

3.2 Three-Dimensional Cartesian System ........................................................................63

3.3 A Unified Preconditioning Scheme for General Fluid Mixtures ..............................64

3.3.1 Important Thermodynamic Relationships .........................................................66
# LIST OF FIGURES

Figure 1.1: Schematic diagram illustrating the basic phenomena associated with injection and combustion of LOX and GH$_2$ at low heating value (subcritical chamber pressures) and high heating value (supercritical chamber pressures). ..............................................2

Figure 1.2: P-T phase diagram of a pure propellant and the operating conditions of different combustion devices. ........................................................................................................5

Figure 1.3: Transition of jet boundary from liquid-jet like to gas-jet-like appearance. .................8

Figure 1.4: Near Injector region of a liquid-oxygen-gaseous-hydrogen shear-coaxial injector, a) flame; and b) corresponding flowfield. Oxygen and hydrogen velocities are 30 and 300 m/s, respectively. The injection temperatures are 100 and 300 K for oxygen and hydrogen streams, respectively, and the chamber pressure is 4.5 MPa (Adopted from Mayer and Tamura, 1996). ..............................................................................15

Figure 1.5: Schematic of flame-holding mechanism. ..................................................................16

Figure 1.6: Schematic of swirl coaxial injector. ..........................................................................17

Figure 2.1: Concepts of DNS, LES and RANS. ........................................................................29

Figure 2.2: Molar volume of a mixture as function of composition at fixed pressure and temperature........................................................................................................................................48

Figure 2.3: T-V phase diagram of multi-component mixture with different compositions ($x_1$=0.4, 0.6). ..........................................................................................................................................52

Figure 3.1: Contours of the condition number as a function of the Mach number squared and the preconditioning factor. ..................................................................................................................75

Figure 3.2: Schematic of three-dimensional adjacent cells..................................................................80

Figure 3.3: Schematic diagram of the stencil used in evaluating inviscid flux terms in the $x-y$ plane. ................................................................................................................................................83

Figure 3.4: Schematic diagram for a three-dimensional auxiliary cell. ..............................................85

Figure 3.5: Multiple instruction multiple data (MIMD) architecture. .............................................96

Figure 3.6: Schematic of a two-dimensional sub-domain with ghost cells (adopted from Wang, 2002). .........................................................................................................................................99

Figure 4.1: Schematic of fluid jet. ..................................................................................................105

Figure 4.2: Grid system employed in the computation (at one-fourth of the original grid density). ..........................................................................................................................................106
Figure 4.3: Effect of grid resolution on radial distributions of mean axial velocity, turbulent kinetic energy, compressibility factor, and viscosity at different axial locations ($p_\infty = 4.3$ MPa, $T_\infty = 300$ K, $u_{\text{inj}} = 15$ m/s, $T_{\text{inj}} = 120$ K, $D_{\text{inj}} = 254$ µm). ..................107

Figure 4.4: Density and constant-pressure specific heat of nitrogen as the functions of temperature and pressure. ......................................................................................................................122

Figure 4.5: Effect of pressure on density, density gradient, temperature and vorticity fields ($T_\infty = 300$ K, $u_{\text{inj}} = 15$ m/s, $T_{\text{inj}} = 120$ K, $D_{\text{inj}} = 254$ µm, $t = 1.55$ ms). .......................123

Figure 4.6: Time evolution of jet surface structures ($p_\infty = 9.3$ MPa, $T_\infty = 300$ K, $u_{\text{inj}} = 15$ m/s, $T_{\text{inj}} = 120$ K, $D_{\text{inj}} = 254$ µm). .................................................................124

Figure 4.7: Power spectral densities of velocity fluctuations at different radial locations with $x/D_{\text{inj}} = 16$ ($p_\infty = 9.3$ MPa, $T_\infty = 300$ K, $u_{\text{inj}} = 15$ m/s, $T_{\text{inj}} = 120$ K, $D_{\text{inj}} = 254$ µm). .................................................................................................................125

Figure 4.8: Effect of pressure on power spectral densities of radial velocity fluctuations at two different axial locations with $r/D_{\text{inj}} = 0.5$. .................................................................126

Figure 4.9: Spatial growth rate as function of Strouhal number at different pressures. .............127

Figure 4.10: Vorticity budgets at different ambient pressures ($T_\infty = 300$ K, $u_{\text{inj}} = 15$ m/s, $T_{\text{inj}} = 120$ K, $D_{\text{inj}} = 254$ µm, $t = 1.55$ ms). .................................................................128

Figure 4.11: Effect of pressure on normalized density distribution in radial direction. ..........129

Figure 4.12: Effect of pressure on normalized velocity distribution in radial direction. ...........130

Figure 4.13: Effect of pressure on normalized density, normalized temperature, and compressibility factor along jet centerline. .................................................................................131

Figure 4.14: Radial distributions of mean thermophysical properties at $x/D_{\text{inj}} = 10$. ...........132

Figure 5.1: Effect of pressure on vorticity magnitude, $|\omega|$, temperature, $T$, and density gradient, $|\nabla \rho|$, fields ($T_\infty = 300$ K, $u_{\text{inj}} = 15$ m/s, $T_{\text{inj}} = 120$ K, $D_{\text{inj}} = 254$ µm, $t^* = 80$). .................................................................................................................................151

Figure 5.2: Thermo-physical properties of nitrogen as functions of pressure and temperature..........................................................152

Figure 5.3: Effect of pressure on specific heat, $C_p$, thermal diffusivity, $\alpha$, kinematic viscosity, $\nu$, and compressibility factor, $Z$, fields ($T_\infty = 300$ K, $u_{\text{inj}} = 15$ m/s, $T_{\text{inj}} = 120$ K, $D_{\text{inj}} = 254$ µm, $t^* = 88$). .................................................................................................................................153
Figure 5.4: Large coherent structures visualized by iso-surfaces of dilatation magnitude, \[ \nabla \cdot \mathbf{u} \], at 1.2 x 10^4, corresponding to 15% of the maxima, a) Case 1: \( p_{\infty} = 6.9 \) MPa, \( T_{\infty} = 300 \) K, \( u_{\text{inj}} = 15 \) m/s, \( T_{\text{inj}} = 120 \) K, \( D_{\text{inj}} = 254 \) µm; b) Case 2: \( p_{\infty} = 9.3 \) MPa, \( T_{\infty} = 300 \) K, \( u_{\text{inj}} = 15 \) m/s, \( T_{\text{inj}} = 120 \) K, \( D_{\text{inj}} = 254 \) µm..........................154

Figure 5.5: Time averaged pressure field and the time evolution of the density field showing the dense fluid jet disintegration process, Case 1: \( p_{\infty} = 6.9 \) MPa, \( T_{\infty} = 300 \) K, \( u_{\text{inj}} = 15 \) m/s, \( T_{\text{inj}} = 120 \) K, \( D_{\text{inj}} = 254 \) µm..............................................................155

Figure 5.6: Effect of pressure on the spatial averaged vorticity magnitude budgets at different axial locations (\( T_{\infty} = 300 \) K, \( u_{\text{inj}} = 15 \) m/s, \( T_{\text{inj}} = 120 \) K, \( D_{\text{inj}} = 254 \) µm, \( t^* = 88 \)). .........................................................................................156

Figure 5.7: Power spectral densities of pressure fluctuations at different axial locations with \( r / D_{\text{inj}} = 0.5 \), Case 1: \( p_{\infty} = 6.9 \) MPa, \( T_{\infty} = 300 \) K, \( u_{\text{inj}} = 15 \) m/s, \( T_{\text{inj}} = 120 \) K, \( D_{\text{inj}} = 254 \) µm........................................................157

Figure 5.8: Power spectral densities of pressure fluctuations at different axial locations with \( r / D_{\text{inj}} = 0.5 \), Case 2: \( p_{\infty} = 9.3 \) MPa, \( T_{\infty} = 300 \) K, \( u_{\text{inj}} = 15 \) m/s, \( T_{\text{inj}} = 120 \) K, \( D_{\text{inj}} = 254 \) µm..........................................................158

Figure 5.9: Effect of pressure on the normalized temperature, velocity, density along jet centerline, and the FWHM distributions (\( T_{\infty} = 300 \) K, \( u_{\text{inj}} = 15 \) m/s, \( T_{\text{inj}} = 120 \) K, \( D_{\text{inj}} = 254 \) µm)........................................................................159

Figure 5.10: The normalized density distributions in radial direction at different axial locations (\( T_{\infty} = 300 \) K, \( u_{\text{inj}} = 15 \) m/s, \( T_{\text{inj}} = 120 \) K, \( D_{\text{inj}} = 254 \) µm)...................................................159

Figure 5.11: Tangent of the jet visual spreading angle versus the ambience to injectant density ratio...........................................................................................................160

Figure 5.12: Effect of initial density ratio on velocity decay, a) velocity decay, b) velocity decay normalized using the pseudo-similarity laws suggested by Chen and Rodi (1980)..................................................................................................................161

Figure 5.13: The normalized turbulence intensity distributions along jet centerline (\( T_{\infty} = 300 \) K, \( u_{\text{inj}} = 15 \) m/s, \( T_{\text{inj}} = 120 \) K, \( D_{\text{inj}} = 254 \) µm). ..........................................................162

Figure 5.14: The normalized velocity distributions in radial direction averaged among the region \( 30 < x / D_{\text{inj}} < 35 \) (\( T_{\infty} = 300 \) K, \( u_{\text{inj}} = 15 \) m/s, \( T_{\text{inj}} = 120 \) K, \( D_{\text{inj}} = 254 \) µm)...........162

Figure 5.15: The normalized Reynolds stress components distributions in radial direction averaged among the region \( 30 < x / D_{\text{inj}} < 35 \) (\( T_{\infty} = 300 \) K, \( u_{\text{inj}} = 15 \) m/s, \( T_{\text{inj}} = 120 \) K, \( D_{\text{inj}} = 254 \) µm). .................................................................................................163
Figure 6.1: Schematic of shear co-axial injector employed in the simulation. ........................165

Figure 6.2: Thermo-physical properties of methane as functions of pressure and temperature. .................................................................................................................................................... 166

Figure 6.3: Thermo-physical properties of oxygen as functions of pressure and temperature. .................................................................................................................................................... 166

Figure 6.4: Grid system employed in the simulation (at one-fourth original grid density). ....169

Figure 6.5: Snapshots of oxygen mass fraction and vorticity fields of shear coaxial injection of LOX and methane for Cases 1 and 2. ...........................................................177

Figure 6.6: Mass fraction, density, vorticity, and velocity vector fields in the region near the LOX post for Cases 1 and 2 in Table 6.2. .................................................................... 178

Figure 6.7: Time evolution of vorticity field over one cycle of vortex pairing of Case 1 in Table 6.2 ...................................................................................................................... 179

Figure 6.8: Frequency spectra of the radial velocity oscillations along the inner and outer shear-layers, Case 1 in Table 6.2 .....................................................................................180

Figure 6.9: Frequency spectra of the radial velocity oscillations along the inner and outer shear-layers, Case 2 in Table 6.2. ....................................................................................... 181

Figure 6.10: Time averaged axial velocity, turbulent kinetic energy (TKE), and oxygen mass fraction fields of Cases 1 and 2 in Table 6.2. ................................................................................. 182

Figure 6.11: Comparison of the radial distributions of the time averaged density, oxygen mass fraction, axial velocity, and turbulent kinetic energy at the different axial locations for Cases 1 and 2 in Table 6.2. ......................................................................................... 183

Figure 6.12: Time-averaged velocity vector distributions near the LOX post of Cases 1 and 2 in Table 6.2 ......................................................................................................................... 184

Figure 6.13: Axial distributions of time-averaged density, oxygen mass fraction, axial velocity, and turbulent kinetic energy along the centerline. ......................................................... 185

Figure 7.1: Schematic of simplex swirl injector employed in the present study, 1-injector casing; 2-vortex chamber; 3-discharge nozzle, 4-tangential passages. ...............................187

Figure 7.2: Schematic of 2D axi-symmetric grid system at one-third of the original grid density. ................................................................................................................................. 188

Figure 7.3: Mean density and velocity components fields (p_\omega = 10 MPa, T_{inj} = 120 K, T_\omega = 300 K, \dot{m} = 0.2 kg/s, K = 3.2). ................................................................................................. 205
Figure 7.4: Radial distributions of mean velocity components, temperature, density, and
compressibility factor at various axial locations (\( \dot{m} = 0.2 \text{ kg/s}, K = 3.2 \)). .................206

Figure 7.5: The dense fluid film thickness along the injector inner wall (\( p_\infty = 10 \text{ MPa} \),
\( T_{\infty} = 120 \text{ K}, T_{\infty} = 300 \text{ K}, \dot{m} = 0.2 \text{ kg/s}, K = 3.2 \)). .......................................................207

Figure 7.6: Temporal evolution of temperature field over one cycle of the dominant
vortex shedding process (\( p_\infty = 10 \text{ MPa} \), \( T_{\infty} = 120 \text{ K}, T_{\infty} = 300 \text{ K}, \dot{m} = 0.2 \text{ kg/s} \),
\( K = 3.2 \)). ........................................................................................................................................208

Figure 7.7: Power spectral densities of the pressure fluctuations at six different axial
locations (\( p_\infty = 10 \text{ MPa} \), \( T_{\infty} = 120 \text{ K}, T_{\infty} = 300 \text{ K}, \dot{m} = 0.2 \text{ kg/s} \),
\( K = 3.2 \)). ........................................................................................................................................209

Figure 7.8: Effect of mass flowrate on the film thickness. .................................................................210

Figure 7.9: Effect of mass flowrate on the temperature fields............................................................211

Figure 7.10: Effect of mass flowrate on the power spectral density of the pressure
oscillations. ........................................................................................................................................212

Figure 7.11: Effect of slit position on the film thickness.................................................................213

Figure 7.12: Effect of slit position on the pseudo streamline patterns near the head end........214

Figure 7.13: Comparison of liquid film thickness predicted from different theoretical
models and the simulation results. ........................................................................................................215

Figure 7.14: Effect of the swirl strength on the film thickness........................................................215

Figure 7.15: Effect of swirl strength on the pseudo streamline patterns.................................216

Figure 7.16: The power spectral density of pressure oscillations at different axial
locations(\( p_\infty = 10 \text{ MPa} \), \( T_{\infty} = 120 \text{ K}, T_{\infty} = 300 \text{ K}, \dot{m} = 0.2 \text{ kg/s} \), \( K = 4.2 \)). .................216

Figure 7.17: Schematic of displacement effect in a swirl injector..................................................217
# LIST OF TABLES

Table 1.1: Engine Operation Conditions and Critical Properties of Propellants ................. 1

Table 2.1: Coefficients of $A_n$ ................................................................. 45

Table 2.2: Semi-empirical Constants Based on Methane ................................................. 45

Table 2.3: Coefficients for Shape Factor Correlations...................................................... 55

Table 4.1: Simulation Conditions .................................................................................... 109

Table 4.2: Conditional averaged temperatures (K) in regions with $|\nabla \rho| >$ cutoff value .......... 111

Table 4.3: Temperatures at inflection points on isobaric $\rho - T$ curves at different pressures...................................................................................................................... 112

Table 5.1: Simulation Conditions .................................................................................... 134

Table 5.2: Conditional averaged temperatures (K) in regions with $|\nabla \rho| >$ cutoff value. .... 137

Table 5.3: Temperatures at inflection points on isobaric $\rho - T$ curves at different pressures...................................................................................................................... 137

Table 5.4: Physical parameters of the experimental data used for comparison ................... 144

Table 6.1: The critical points of methane and oxygen ....................................................... 165

Table 6.2: Simulation conditions for the analysis of high-pressure LOX/methane injection and mixing process. Subscript 1 denotes the oxygen stream, and subscript 2 denotes the methane stream........................................................................................................... 167

Table 6.3: The predicted initial vortex shedding frequency of each shear layer in Cases 1 and 2 .............................................................................................................................................. 172

Table 7.1: Geometric parameters of the studied swirl injector .......................................... 187

Table 7.2: Test Conditions* ............................................................................................ 191

Table 7.3: Effect of mass flowrate on dense fluid film thickness and spray cone angle. ...... 197

Table 7.4: Effect of slit position on film thickness and spray cone angle. ......................... 198

Table 7.5: Effect of LOX post length on the dense fluid film thickness and spray cone angle ........................................................................................................................................... 199

Table 7.6: Effect of swirl strength on the dense fluid film thickness and spray cone angle... 200
Sincere thanks and gratitude go to my advisor, Dr. Vigor Yang, for his invaluable support, guidance, and encouragement throughout my doctorate study in the past five years at Penn. State. Working with him, as one of his disciples, has been a pleasant and memorable experience.

I would also like to thank Dr. Andre’ L. Boehman, Dr. James G. Brasseur, and Dr. Robert J. Santoro for kindly providing their expert guidance and for their interest in my work by serving as my Ph.D committee members.

I extend sincere appreciation to Dr. Hua Meng and Dr. Shih-Yang Hsieh for their help and suggestions. I also thank my colleagues, Dr. Shanwu Wang, Dr. Danning You, Dr. Fuhua Ma, Dr. Ying Huang, and Yanxing Wang, Tao Liu, Jian Li, Puneesh Puri, Piyush Thakre for their support and many enlightening discussions.

The research work reported in this thesis was sponsored in part by the Air Force Office of Scientific Research under Grant No. F49620-01-1-0114.

To my parent, Baoxiang Zong and Shouqing Xu, I wish to express thanks and love for all that they have given me and continue to give. My appreciation and love also go to my elder sister, Yun Zong, for her invaluable love and support.

My deepest appreciation and love go to my girlfriend, Lei Zhao, who is always there to support me and provide me with endless love and pride.
Chapter 1

Introduction

1.1 Motivation and Objectives

Understanding the fundamental physicochemical mechanisms associated with mixing and combustion of cryogenic propellants in supercritical environment, in which both the pressure and temperature exceed the thermodynamic critical states, have long been matters of serious practical concern in combustion science and technology, mainly due to the necessity of developing high-pressure combustion devices, such as liquid-propellant rocket, gas turbine, and diesel engines. The propellants are usually delivered to combustion chambers at subcritical temperature, which then undergo a sequence of vaporization/diffusion, mixing, ignition, and combustion processes at pressure and temperature levels well above the thermodynamic critical points of the substances (see Table 1.1). Under these conditions, the propellants are heated and transit into the supercritical state (Prausnitz et al., 1986). The mixing and combustion processes exhibit many features distinct from those under subcritical conditions, thereby rendering conventional approaches developed for the devices operating at low-pressure invalid.

Table 1.1: Engine Operation Conditions and Critical Properties of Propellants

<table>
<thead>
<tr>
<th>Engines/Combustors</th>
<th>Propellants</th>
<th>Operation Conditions</th>
<th>Critical Properties of Propellants</th>
</tr>
</thead>
<tbody>
<tr>
<td>Space Shuttle Main Engine</td>
<td>Oxygen, Hydrogen</td>
<td>225 atm, 13 atm, 33.2 K</td>
<td>49.7 atm, 154.6K</td>
</tr>
<tr>
<td>Diesel Engine</td>
<td>Diesel Oil</td>
<td>&gt; 50 atm</td>
<td>~30 atm, ~650K</td>
</tr>
</tbody>
</table>

Under supercritical conditions, the sharp distinction between liquid and gas phases vanishes due to the diminution of surface tension and enthalpy of vaporization, and questions
Figure 1.1: Schematic diagram illustrating the basic phenomena associated with injection and combustion of LOX and \( \text{GH}_2 \) at low heating value (subcritical chamber pressures) and high heating value (supercritical chamber pressures).
arise with respect to correctly characterize propellant injection, mixing, and combustion processes. Figure 1.1 schematically compares the basic phenomena of a liquid-oxygen-gaseous-hydrogen (LOX/GH₂) shear-coaxial injector element operated at sub- and supercritical pressures (Oefelein and Yang, 1998). At subcritical chamber pressures, injected liquid jets undergo the classical cascade of processes associated with atomization. For this situation, dynamic forces and surface tension promote the formation of a heterogeneous spray that evolves continuously over a wide range of thermophysical regimes. Spray flames form and are lifted away from the injector faceplate in a manner consistent with the combustion mechanism exhibited by local droplet clusters. When chamber pressures approach or exceed the critical value of a particular propellant, the injected fluid jets undergo a “transcritical” change of state as the interfacial fluid temperatures rise above the saturation or critical temperature of the local mixture. For this situation, diminution of intermolecular forces promotes diffusion dominated processes prior to atomization and respective jets vaporize, forming a continuous fluid in the presence of exceedingly large gradients. Well-mixed diffusion flames evolve and are anchored by small but intensive recirculation zones generated by the shear-layers imposed by adjacent propellant streams. These flames produce wakes that extend far downstream.

Simulating the high-pressure phenomena described above inherently poses a variety of challenges which involve all of the classical closure problems and a unique set of problems imposed by thermodynamic non-idealities and transport anomalies. First, from the classical point of view, reacting multiphase flow introduces the complicating factors of chemical kinetics, highly nonlinear source terms, and a variety of subgrid-scale (sgs) velocity and scalar-mixing interactions. Second, thermodynamic and transport anomalies, such as divergence of constant-pressure specific heat, may occur during the temperature transition across the critical value, especially when the pressure approaches the critical point, a phenomenon commonly referred to as near-critical enhancement (Levelt Senger, 1991). 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 an important role in dictating the flow evolution (Yang, 2000). Third, the fluid properties and their spatial gradients vary continuously throughout the entire field. The resultant coupling dynamics becomes transient between the injected and the surrounding fluids, and involves an array of physiochemical processes with widely disparate time and length scales. Fourth, the flow Reynolds number increases with pressure. For oxygen and hydrogen, an increase in pressure from 1 to 100 atmospheres results in a reduction of the corresponding kinematic viscosity by a factor of two orders of magnitude. Based on the Kolmogorov universal equilibrium theory, the Kolmogorov and Taylor microscales may decrease by 1.5 and 1.0 orders of magnitude, respectively. These reductions of the characteristic scales of turbulent motions have a direct impact to the flow evolution and the numerical grid density required to resolve key processes. Finally, exceedingly large density-gradients emerge during high-pressure injection and mixing. At 100 atmospheres, the density ratio associated with a 100 K oxygen jet and a 300 K gaseous hydrogen stream (a typical operating condition in liquid rocket engine) is approximately 144. In a shear-coaxial element, this change occurs over an interval smaller than the thickness of the annular post, which is on the order of 0.1 mm. Resolving a gradient of such size numerically requires the use of extremely dense grids. Comprehensive reviews of the state of knowledge on supercritical mixing and combustion were recently 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 dissertation represents an attempt to address key issues related to modeling and understanding unsteady fluid dynamic and physicochemical processes at supercritical conditions. The objectives are as follows: 1) to provide insight into the fundamental concepts associated with modeling turbulent, chemically reacting, real-fluid mixtures at high-pressures; 2) to establish a unified theoretical framework which could
accommodate full conservation laws, turbulence closure, real-fluid thermodynamics, and transport anomalous; 3) to systematically investigate the fundamental flow dynamics and physiochemical processes at near and supercritical conditions; 4) 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.

1.2 Review of Relevant Literature

1.2.1 Supercritical Fluid

According to classical thermodynamic theory (Prausnitz et al., 1986), a fluid is in its supercritical state when both the temperature and pressure exceed the critical values (see Fig. 1.2). Because surface tension and enthalpy of vaporization that indicate the liquid/gas boundary approach zero, there is no longer the possibility of a two-phase region, but instead a single phase exists. The general term for the substance at this state is supercritical fluid.

Figure 1.2: P-T phase diagram of a pure propellant and the operating conditions of different combustion devices.
At near- and supercritical conditions, fluid properties possess liquid-like density, gas-like diffusivity, and pressure-dependent solubility. Surface tension and enthalpy of vaporization vanish, and isothermal compressibility and specific heat increase significantly. In addition, fluid properties and their gradients vary continuously. The departure from ideal gas behavior becomes even more significant when the fluid state approaches the critical condition. In the vicinity of the critical point, the thermophysical properties of fluids exhibit anomalous variations and are very sensitive to both temperature and pressure, a phenomenon commonly referred to as near critical enhancement (Levelt Senger, 1991). Those phenomena, coupled with intense chemical reaction and turbulence, have significant impacts on the dynamics of a given combustion system.

1.2.2 Experimental Study on High-Pressure Cryogenic Fluid Injection and Mixing

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 whole process is so complex that its mechanism cannot be thoroughly understood without extensive theoretical and experimental works conducted on simplified configurations and under well-controlled conditions. In this subsection, the experimental work on high-pressure fluid injection and mixing is reviewed.

Experimental investigation into supercritical fluid jet dynamics dates back to 1971. Newman and Brzustowski (1971) studied the injection of CO$_2$ fluid with an inlet temperature of 295K into a chamber filled with CO$_2$ and N$_2$ mixtures at near critical conditions. The critical temperature and pressure of CO$_2$ are 304 K and 73 atm, respectively, and those of N$_2$ are 126 K and 34 atm, respectively. The chamber temperature and pressure were preconditioned in the range of 295-330 K and 62-90 atm, respectively, and the CO$_2$ mass fraction varied from 0 to 50%. The shadowgraph visualization technique was employed to investigate the jet flow evolution and
its interaction with the surrounding fluid. Results indicated that over the pressure range considered, the jet surface structure and spray formation were suppressed with increasing temperature and CO₂ concentration in the chamber, mainly due to the diminished surface tension and enhanced CO₂ evaporation at near and above the critical temperature. Droplets were observed around the jet boundary, but their sizes decreased with an increase in the ambient temperature. The jet could be globally treated as a variable-density, single-phase turbulent submerged jet at both subcritical and supercritical pressures when the ambient temperature remained supercritical.

Motivated by the development of high-pressure cryogenic-propellant rocket engines, extensive experimental studies have been conducted to provide direct insight into supercritical fluid injection and mixing. The work included injection of liquid nitrogen and co-injection of liquid nitrogen and gaseous helium into gaseous nitrogen environments over a wide range of pressures. Chehroudi et al. (1999, 2000, 2002a, 2002b, 2003) studied the injection of liquid nitrogen initially at a subcritical temperature into an environment at a fixed supercritical temperature (300 K) and various pressures ranging from sub- to supercritical values (7.8 to 93 atm). Shadowgraph imaging, fractal analysis, and Raman scattering measurement were employed to examine the structures of the jet and the shear-layer between the injected and ambient fluids. The results based on the flow visualization confirmed the findings by Newman and Brzustowski. Drastic changes in jet surface phenomena took place across the critical pressure. Ligaments and droplets formed at subcritical pressures, but disappeared at supercritical conditions, due to the prevalence of turbulent motions and vanishing of surface tension, as shown in Fig. 1.3. Fractal analysis indicated that the jet surface topology at supercritical pressure bears a strong resemblance to its gaseous counterpart. The fractal dimension, however, dropped rapidly to a value close to that of a liquid spray as the pressure was reduced below the critical point.
To quantitatively characterize high-pressure cryogenic jet, its initial growth rate was measured and compared with the results of a large number of other flows, including atomized liquid sprays, turbulent incompressible gaseous jets, supersonic jets, and incompressible variable density jets/mixing layers covering over four-order of magnitude in the density ratio of injected to ambient flows (Chehroudi et al., 2002a). The growth rate of supercritical jet agreed well with that of the incompressible, variable density, gaseous mixing layers at low pressures. This was the first time a quantitative parameter was defined and used to demonstrate the similarity between these two flows beyond their physical appearance. Since the fluid jet exhibited distinct features at sub- and supercritical pressures, a unified model for the initial growth rate of jet, which could consider both the droplet gasification at low pressure and the interfacial bulge formation/separation at high-pressure, was proposed (Chehroudi et al., 2002b). Its prediction showed good agreement with the measured data.

Systematical cold flow experiments were conducted by Mayer and his colleagues at DLR of Germany (Mayer et al., 1996, 1998, 2000). The injection of liquid nitrogen into gaseous
nitrogen/helium environment with and without co-flow gas helium was performed. The chamber pressure varied from 10 to 60 atmospheres, and its temperature was fixed at 300 K. The injection temperature of nitrogen reached as low as 90 K, whereas that of gaseous helium ranged from 100 to 370 K. Similar changes in the jet surface structures were observed in shadowgraph images as pressure increased from sub- to super-critical values. Due to the fade of surface tension, the atomization mechanism changed to shear-layer instability, and the mixing of the injected dense nitrogen fluid with the helium co-flow or ambient gas behaved like a variable density, turbulent shear-layer at near- and supercritical conditions. Since mixing was strongly related to the large-scale vortices within the shear-layer, their length scales were quantitatively measured based on the flashlight photography and high-speed cinematography (Branam and Mayer, 2003). For pure nitrogen injection at a near critical temperature (123 K), the length scales in radial direction were two to three times greater than the radial ones near the injector exit due to the strong density gradient around the jet surface. This asymmetry decayed as the fluid was convected downstream, and it also became unpronounced when the injection temperature exceeded the critical value. It was also indicated that the resolved scales were comparable in magnitude to the Taylor micro scale in turbulent flow.

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 jet flows. The centerline density and temperature distributions of cryogenic jet at a near critical pressure (40 atm) were acquired by Oschwald and Schick (1999). They noted that the density decay becomes faster as the fluid temperature increases from sub-
supercritical values. The temperature, however, remains a relatively flat profile even far downstream. This was attributed to the anomalous thermophysical property variations near the critical point of nitrogen. Those quantitative measurement conducted at high-pressures provided indispensable basis for CFD model validation.

Chehroudi et al. (2002c, 2004) studied the effects of acoustic waves on the single nitrogen jet and the coaxial injection of liquid nitrogen and gaseous nitrogen over a wide range of chamber pressures. The strength of the acoustic wave was up to 180 dB, and the resonant frequencies of the assembly were at 2700 and 4800 Hz. The influence was substantial at subcritical conditions but became unnoticeable as pressure increased and exceeded the critical point. The phenomenon may be attributed to the formation of high-frequency vortices in the shear-layer and the weaker characteristic acoustic impedances of injected fluid under supercritical pressure. In addition, the co-axial subcritical jets at higher velocity ratios were more apt to be influenced. Since the sensitivity of coaxial jet to the external acoustic oscillations might correspond to the causes of combustion instability in liquid rocket engine, 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.

1.2.3 Experimental Study on High-Pressure Cryogenic Propellants Combustion

Typical applications of cryogenic propellants combustion in rocket engine have been illustrated in Fig. 1.1. Reactants are introduced into the combustion chamber through coaxial injectors. Liquid oxygen (LOX) generally is delivered through the inner LOX post at low speed, while gaseous hydrogen (GH2) is fed through the outer annular duct.

At a subcritical pressure, atomization starts at the confluence of the liquid and gaseous streams. The liquid core diminishes progressively as the spray is formed. The initial ligaments
are torn away from the LOX jet by the hydrogen stream, which finally experiences a secondary atomization and break up into finer droplets because their sizes are too large to sustain the shearing stresses associated with the velocity difference between the two streams. The atomization quality is determined by two important parameters (Candel et al., 1998). The momentum ratio between the two streams controls the stripping of the liquid core and determines its length, whereas the sizes of the droplets after secondary breakup are sensitive to the Weber number (We) defined based their diameter. When the Reynolds numbers of the two streams are sufficiently large, gaseous oxygen, formed after droplet vaporization, reacts with hydrogen in a highly turbulent flowfield.

The three characteristic time scales associated with vaporization, mixing, and combustion could be used to define two Damkhöler numbers: the chemical reaction Damkhöler number that compares the mixing time with the chemical time

\[
Da_c = \frac{\text{Mixing Time}}{\text{Chemical Reaction Time}}
\]  

and the vaporization Damkhöler number, which is the ratio of the mixing to vaporization times

\[
Da_v = \frac{\text{Mixing Time}}{\text{Vaporization Time}}
\]  

Snyder et al. (1997) estimated the magnitude of these numbers for a shear-coaxial injector at elevated chamber pressure. The chemical Damkhöler number is always greater than unity, whereas the vaporization Damkhöler number is generally lower than unity. Therefore, vaporization of LOX droplets controls the combustion process at subcritical pressure. If the droplets are too large, they may escape the combustion chamber without being fully vaporized. The greater chemical reaction Damkhöler number indicates that combustion occurs only in thin reactive zones and that the regime of combustion is of the flamelet type.
When chamber pressure is near or above the critical points of the injected propellants, surface tension and enthalpy of vaporization diminish. The vanishing of intermolecular forces promotes diffusion dominant processes, and the injected fluid forms a continuous flow regime in the presence of exceedingly large gradients. The magnitude of the LOX jet gasification rate is at least one order 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 becomes the slowest and therefore is the most influential process.

Candel et al. (1998) and Herding et al. (1998) carried out extensive experiments on the jet flame formed from a single coaxial injector at elevated chamber pressures (5-10 atm) over a wide range of mass and momentum ratios. The injection temperature of hydrogen was fixed at 289 K, and that of oxygen was around 100 K. Several important diagnostic techniques were developed. Flow visualization was achieved through emission images of OH radicals. The intensive reaction zone (flame) was simultaneously identified by planar Laser-Induced Fluorescence (LIF) of OH and O₂. The interface between gas and liquid and the breakup length of LOX jet were measured by the Elastic Light Scattering (ELS) technique. Quantitive temperature measurement was measured using the Coherent Anti-Stokes Raman Spectroscopy (CARS). The mean flame surface structures deduced from the Abel Transformation of the averaged OH emission image were compared with that measured by the OH-LIF images. Good agreement was obtained. The mean flame began at the LOX post tip, which was initially a thin, nearly cylindrical surface around the inner jet and expanded downstream into a thick shell surrounding the LOX spray. The initial expansion angle increased with increasing momentum ratio. Further downstream, the mean flame became annular. The inner and outer diameters of the flame volume slowly decreased with axial distance as the oxygen convected into the central region was being consumed. Statistics of flame location obtained from O₂-LIF showed that the wrinkling and
flapping of flame were smaller close to the injector exit and increased downstream. In addition, the large temperature fluctuations at the near-field were detected by the CARS spectrum of H₂, which indicated the presence of an unsteady mixing layer between oxygen jet and hydrogen flow.

Flame stabilization is a crucial issue in a propulsion system. In liquid-propellant rocket engines, it is achieved by recessing the LOX post with respect to the injector face plate. The detailed mechanisms of recess on cryogenic flame stabilization were investigated by Kendrick et al. (1999) at an elevated pressure (10 atm). The injection temperatures of LOX and gaseous hydrogen were approximately 100 K and 297 K, respectively. The momentum ratio between the annular and inner streams varied from 6.5 to 14.5. The flowfield was visualized by the OH emission image. When the LOX post was recessed, the flame was stabilized inside the injector, and its expansion angle was augmented. The thickness of the flame brush and the size of the reaction zone were also enhanced. The recess effect was more substantial at lower momentum ratio. A simple one dimensional model was constructed to explain the observed phenomena. Since the flame was formed inside the injector, hot products were produced and occupied a certain fraction of the available duct area. As a result, the annular hydrogen stream was accelerated, and the gas to liquid momentum ratio was enhanced. The strengthened momentum ratio, in turn, gave rise a faster breakup of the liquid core and a correspondingly enlarged flame blooming angle.

Combustion of LOX and GH₂ at both sub- and supercritical chamber pressures (5 to 70 atm) was investigated by Juniper et al. (2000). The injection temperatures of LOX and GH₂ were 80 K and 280 K, respectively. The gas to liquid momentum ratio ranged from 6 to 14.5. At subcritical pressures, ligaments and droplets appeared at the edge of the LOX jet. However, they were no longer evident at 70 atmospheres, where the dense oxygen was in the form of pocket with indistinguishable boundary. The atomization and vaporization was inhibited. Although the flame still attached to the LOX post tip at supercritical pressures, the initial expansion angle was
reduced and became less dependent on the momentum ratio. The combustion was dominant by the large-scale turbulent mixing, which was associated with the velocity ratio of the two streams. To retain the same momentum ratio at higher pressure, the velocity ratio was reduced, which caused the turbulent mixing to diminish and the flame to narrow.

Another notable and important work on high-pressure combustion was conducted by Mayer and his colleagues (Mayer and Tamura, 1996; Mayer et al., 2001; Ivancic and Mayer, 2002). Subscale shear-coaxial injectors with and without recess were employed. The hot firing test conditions covered a wide range of pressure (10-100 atm). The injection velocity of LOX was 10-30 m/s, and the temperature was 100 K. The velocity of GH₂ stream was fixed at 300 m/s, and its temperature varied from 150 to 300 K. Those conditions were comparable to the operating state of a liquid rocket engine. The flow visualization was achieved by shadowgraph imaging. The most important results of their work were presented in Fig. 1.4. A LOX post wake flame and its interaction with the H₂/O₂ shear-layer were clearly observed. The flame always attached instantaneously to the LOX post after ignition. A bright flame spot observed close to the LOX post tip suggested that a well-mixed flame with strong radiation was anchored in an intensive recirculation zone. This flow pattern could be observed over the entire range of test conditions for injector with and without recess, and even for a post tip thickness of 0.3 mm.

The flame anchoring mechanism was illustrated in Fig. 1.5. Several small recirculation eddies were generated in the vicinity of the LOX-post tip, which consisted of partly preburned hydrogen rich gas. As the evaporating LOX mixed and reacted with the hydrogen gas in these eddies, the hot product again mixed with hydrogen stream and circulated back. Since the flow velocities in this region were so low, stationary combustion was possible.
Figure 1.4: Near Injector region of a liquid-oxygen-gaseous-hydrogen shear-coaxial injector, a) flame; and b) corresponding flowfield. Oxygen and hydrogen velocities are 30 and 300 m/s, respectively. The injection temperatures are 100 and 300 K for oxygen and hydrogen streams, respectively, and the chamber pressure is 4.5 MPa (Adopted from Mayer and Tamura, 1996).
Ignition poses many problems to launch vehicles. For example, an accidentally high-pressure peak generated due to the ignition delay may trigger combustion instabilities with the risk of a serious damage of the combustor. The transient ignition of a cryogenic GH2/LOX system was recently investigated by Gurliat et al. (2003). A subscale shear-coaxial injector without recess was employed. Both the hydrogen and oxygen streams were delivered to the chamber at 77 K. The combustion was triggered by the intensive energy input from a pulsed laser at a certain axial location downstream of the faceplate. The detailed temporal behavior of the ignition was available for the first time through high-speed Schlieren image. The process could be characterized as consisting of four different phases. The primary ignition phase began at the time of energy inputing. During this phase, the flame front was convected downstream by the flow and expanded in the shear-layer. After the flame reached the edge of the shear-layer, the flame propagation phase started, where its front propagated upstream through the recirculation zone and consumed the premixed propellants. After reaching the faceplate and depleting all premixed propellants in the recirculation zone, it had to move downstream away from the injector until it achieved a maximum distance in the flame lift-off phase. The flame was finally anchored by the wake region near the injector faceplate. The existence of those steps during the ignition was also
confirmed by the chamber pressure history; however, the time scale of each phase may vary depending on different operating conditions.

1.2.4 Theoretical and Experimental Study on Swirl Coaxial Injector Design

Figure 1.6 schematically shows the configuration of a typical swirl coaxial injector widely employed in contemporary liquid-propellant rocket injection systems for liquid/liquid and gas/liquid mixtures. Liquid oxygen is introduced tangentially 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 post in the form of a thin sheet and impinges on the surrounding fuel stream. The swirl atomization process basically involves two mechanisms: disintegration of the liquid sheet as it swirls and stretches; and sheet breaks up due to the interaction with the surrounding coaxial flow.

![Figure 1.6: Schematic of swirl coaxial injector.](image-url)
Compared with jet injector, a liquid swirl injector distinguishes itself in many aspects (Bazarov et al., 2004). First, for the same pressure drop and liquid flowrate, the average median diameter of droplet is 2.2 to 2.5-fold smaller than that of jet injectors. This advantage prevails for high flowrates and abates when counter pressure (i.e., the sum of the combustion chamber pressure and the centrifugal pressure created by liquid swirling motion) grows. Second, swirl injectors are not so sensitive to manufacturing errors such as deviation from the prescribed diameter and surface misalignment. In addition, the flow passage areas of swirl injectors are much larger than those of jet injectors with the same flowrates and, consequently, they are less susceptible to choking or cavitation. Thirdly, the central post of rocket swirl injector features large aspect ratios (i.e. L/D up to 20) owing to propellant supply manifolding considerations. The viscous loss along the wall exerts significant influence on the flow evolution and consequently alters the spray distribution and atomization.

The fundamentals of inviscid swirl injector theory were established more than 60 years ago by Abramovich in 1944 and independently by Taylor in 1947. The up-to-date discussion of the classical theory and the injector design criterion, which was particularly easy of implementation, were presented by Bazarov et al. (2005) and Bayvel and Orzechowski (1993). Besides the theoretical analysis, a series of experiments were conducted to provide an essential reference frame of swirl injector design, especially for liquid rocket applications.

Hulka et al. (1991, 1993a, 1993b) conducted a series of cold-flow studies using water and inert gases as propellant simulants to characterize several liquid rocket swirl injector elements. There were three basic types of tests, including still photography of free oxidizer sprays, mass and mixture ratio distribution measurements of water only and water/nitrogen sprays, and the Rupe mixing efficiency measurement at atmospheric pressure using water and a sucrose solution over a broad range of mixture and velocity ratios. Rupe mixing efficiency, \( E_m \), is calculated as a summation of the mass weighted mixture ratio over the number of collected samples.
where, \( N \) is the number of collected samples, \( X_{oi} \) is the mass fraction of an oxidizer rich sample, \( X_{fi} \) is the mass fraction of a fuel rich sample, \( R_o \) is the overall oxidizer mass fraction, and \( R_i \) is the oxidizer mass fraction of a sample. 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 initial spreading angle, which was achieved by reducing the tangential inlet area or increasing the central post-exit diameter. The oxidizer mass flowrate had insignificant influence on the single element mixing efficiency, suggesting a larger oxidizer swirl element with a mass flowrate greater than that of a shear-coaxial injector could still obtain better intraelement mixing efficiency.

Rahman et al. (1995) visualized water/air spray injection at room conditions. The instantaneous shadowgraph 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 became closer to the injector exit as the mass flowrate increased. Due to the momentum loss along the injector wall, the spreading angle of the conical sheet decreased with the increase in the aspect ratio of the post length to its diameter.

A similar cold flow test with water/nitrogen as injectants was studied by Sasaki et al. (1997), with particular attention paid to the effect of the central post recess distance. In a recessed injector, because the liquid sheet generated by the swirl motion impinged on the outer wall of the annular fuel passage, its spray angle narrowed with a deformed pattern. The liquid sheet, which blocked the annular passage, was blown off in the shape of a mushroom and with a
screaming sound known as self-pulsation phenomena. 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 simultants for oxidizer and fuel, respectively. With the use of phase Doppler particle analyzer (PDPA) and mechanical patternator, the median droplet size, spray angle, and breakup length were measured. Their results indicated that an optimal recess length existed to obtain a maximum mixing efficiency.

The dynamic characteristics of the swirl injector were thoroughly studied by Bazarov and Yang (1998). The overall response function of the swirl injector could be represented in terms of the transfer characteristics of each individual element (tangential passage, vortex chamber, and discharge nozzle) and 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 the engine combustion dynamics by changing the injector dynamics alone without modifying the 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.

Most of the existing studies were conducted at low pressures, and thus did not simulate many of the important scaling parameters of the 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. Recently, 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 simultants. For high momentum ratio, the spreading angle of the spray was much less than that reported in previous
studies at one-atmosphere 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) (Tamura et al., 1997; Elm, 1991). 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.

1.2.5 Numerical Works on High-Pressure Fluid Mixing and Combustion

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

The most comprehensive numerical models were established by Oefelein and Yang (1998). They modeled two-dimensional mixing and combustion of oxygen and hydrogen streams at supercritical conditions by means of a large-eddy-simulation technique. The formulation accommodated real-fluid thermodynamics and transport phenomena. All the thermophysical properties were evaluated directly from fundamental thermodynamics theories over the entire fluid states of concern. Furthermore, a unified treatment of numerical algorithms based on general fluid thermodynamics was established to improve computational accuracy and efficiency (Meng and Yang, 2003). The results indicated that the density gradient dominated the evolution of the mixing layer and the mass diffusion rate greatly diminished near the critical point.

The dominance of density gradient was observed in the direct numerical simulation (DNS) conducted by Bellan and colleagues (Miller et al., 2001; Okong'o and Bellan, 2002; Okong’o et al., 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 one 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 minimal. This suggested that turbulent models for supercritical fluids should primarily focus on duplicating the species mass flux rather than the typical momentum flux.

Ivancic and Mayer (2002), Branam et al. (2003), and Barata et al. (2003) simulated cryogenic fluid injection and combustion at both sub- and supercritical pressures. The two-dimensional steady calculations were performed, which included the \( k-\varepsilon \) turbulence model and real gas properties evaluation for the injected cryogenic fluid. Since the treated processes were inherently transient, their drastic steady state assumption might yield inaccurate results and could not reveal the distinct features of high-pressure real-fluid dynamics.

The extinction limits of the flame generated around the LOX jet boundary were theoretically studied by Juniper et al. (2003). A one-dimensional counterflow diffusion flame model was constructed. The results indicated that the flame was very stable in the near injector region. It could not be extinct by strain rate, even for a very low hydrogen stream temperature. Since the typical strain rates encountered in rocket engine 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, 2004). 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.
1.3 Work Scope and Method of Approach

The present study investigates the high-pressure cryogenic fluid injection and mixing dynamics by means of large-eddy-simulation. The flow evolution under consideration is extremely complicated, involving thermodynamic nonidealities, transport anomaly, and high Reynolds number turbulent flow. 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 the simplified configurations and well controlled experimental conditions. The approach follows three fundamental steps: 1) the development of a generalized theoretical framework with the accurate property evaluation schemes and closure methodologies; 2) the implementation of an efficient and robust numerical algorithm for general fluid mixture, in which the real-fluid thermodynamics are treated consistently with full account of pressure effects; 3) the systematic investigation of a series of cases associated with trans- and supercritical injection and mixing dynamics. These steps are carried out in Chapters 2 through 7, respectively, with relevant conclusions and recommendations presented in Chapter 8.

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, 1999) and a modified Soave-Redlich-Kwong (SRK) equation of state that is reasonably accurate and easy for implementation (Graboski and
Daubert, 1978a, 1978b). Transport properties, such as viscosity and thermal conductivity, are estimated with an extended corresponding state principle with a 32-term Benedict-Webb-Rubin (BWR) equation of state (Ely and Hanley, 1981, 1983).

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 definition of partial mass and partial density properties are introduced. This framework takes full account of thermodynamic nonidealities and transport anomalies and 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) are adopted for temporal discretization. Spatial discretization employs the fourth-order accurate flux differencing methodologies developed by Rai and Chakravarthy (1994). A fourth-order scalar 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.

Chapters 4, 5, 6, and 7 present a series of case studies. In Chapters 4 and 5, injections of cryogenic nitrogen fluid initially at a subcritical temperature into a supercritical environment, in which both the pressure and temperature exceed the thermodynamic critical point, are investigated over a broad range of ambient pressures. The unique processes, which have substantial influence on the supercritical jet dynamics, are identified and analyzed in detail. The
results are compared with experimental data to establish the accuracy and credibility of the numerical method.

The validated model is applied in Chapter 6 to examine key phenomena associated with high-pressure injection and mixing of LOX and methane. Emphasis is placed on the thermophysical processes and transport which occur in the vicinity of the splitter plate and the impact of the different injection conditions. The simulation is conducted on a fixed pressure of 100 atmospheres, with the injection temperature selected to produce an optimal matrix of transcritical and supercritical conditions. Results highlight the effect of the velocity ratio on the shear-layer dynamics, the dominating effect of the density gradient, and the influence of the injection temperature on the flow evolution.

Swirl injection of high-pressure cryogenic oxygen into a supercritical gaseous oxygen environment is studied in Chapter 7. The influences of various geometric parameters and operation conditions, including mass flowrate, tangential slit position, injector post length, and swirl strength, on the injector dynamics and performance are investigated systematically. Both the internal flow dynamics and the external mixing process are explored. The distinct features between high- and low-pressure swirl injections are identified. To help understand the physical phenomena involved, a theoretical model is established. Its predictions are consistent with the simulation results.

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

Theoretical Formulation and Property Evaluation

2.1 Governing Equations

The theoretical formulation is based on the full conservation equations of mass, momentum, energy, and species concentration in Cartesian coordinates.

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

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

\[
\frac{\partial \rho E}{\partial t} + \frac{\partial [(\rho E + p)u_i]}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial (u_j \tau_{ij})}{\partial x_j} \tag{2.3}
\]

\[
\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho Y_k u_j}{\partial x_j} = \omega_k - \frac{\partial \rho Y_k U_{k,j}}{\partial x_j} , \quad k = 1, \ldots, N-1 \tag{2.4}
\]

where \(i, j\), and \(k\) are the spatial coordinate index, the dummy index to spatial coordinate, and the species index, respectively. The variables \(\rho, u_i, p, E, \tau_{ij}\), and \(q_i\) represent the density, velocity components, pressure, specific total energy, viscous stress tensor, and heat flux, respectively. \(N\) is the total number of species. \(Y_k\) and \(U_{k,j}\) are mass fraction and diffusion velocities of species \(k\), respectively. The viscous stress tensor \(\tau_{ij}\) for a Newtonian fluid (with Stokes assumption) and the heat flux vector \(q_j\) are defined as
\begin{align}
\tau_{ij} &= \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_i}{\partial x_j} \right) \tag{2.5} \\
q_j &= -\lambda \frac{\partial T}{\partial x_j} + \rho \sum_{k=1}^{N} \hat{Y}_k h_k U_{k,j} \tag{2.6}
\end{align}

where \( \mu \) and \( \lambda \) are the coefficients of viscosity and thermal conductivity, respectively. \( T \) is temperature. In the present work, viscosity and thermal conductivity are estimated with an extended-corresponding-state-principle with a 32-term Benedict-Webb-Rubin (BWR) equation of state (Jacobsen and Stewart, 1973). The specific total energy \( E \) is given by

\[ E = e + \frac{u_j^T u_j}{2} \tag{2.7} \]

The specific internal energy, \( e \), is obtained as

\[ e = h - \frac{p}{\rho} \tag{2.8} \]

The specific enthalpy of mixture, \( h \), containing contributions from its constituent species, can be written as

\[ h = \sum_{k=1}^{N} Y_k \hat{h}_k \tag{2.9} \]

where \( \hat{h}_k \) is partial mass enthalpy of species \( k \), which will be defined in the following sections.

The formulation is closed by a modified Soave-Redlich-Kwong (SRK) equation of state for real fluid mixture (Soave, 1972; Graboski and Daubert, 1978a, 1978b).

To obtain the expression for the chemical reaction source term, consider an \( L \)-step reaction mechanism with \( N \) species, which can be written as (Kuo, 1986)
where \( v_{ki}' \) and \( v_{ki}'' \) are the stoichiometric coefficients on the reactants and products side for species \( k \) in the \( i^{th} \) reaction. \( \chi_k \) represents the chemical formula of species \( k \). \( k_f \) and \( k_b \) are the reaction rate constants of the forward and backward reactions, respectively. They may take the following form

\[
k_i(T) = A_i T^b \exp\left(-E_i / R_u T\right)
\]

where \( A_i, b, \) and \( E_i \) are empirical parameters and \( E_i \) represents the activation energy of reaction \( i \).

The following relationship expresses the net production rate \( \dot{\omega} \) of each species in a multi-step mechanism

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

where \( W_k \) and \( [\chi_k] \) represent the molecular weight and molar concentration of species \( k \). Note that the expression for the net production rate, Eq. 2.12, is valid only for elementary reactions. Since some researchers may use a global kinetic mechanism, the exponents for molar concentrations may differ from their stoichiometric coefficients.

### 2.2 Turbulence Closure: Large-Eddy-Simulation

Turbulence remains a challenge in fluid mechanics research due to its strong nonlinear behavior, although this topic has been studied for more than one hundred years. Numerical simulation of turbulent motions can be classified into three major categories, as illustrated in Fig. 2.1.
The most straightforward method is direct numerical simulation (DNS). Given sufficient computing resources, the equations governing flow evolution are solved without a model, and the entire spectrum of turbulence scales is resolved on the grid. DNS is the most complete numerical tool for studying turbulence; however, its computational cost increases rapidly with the Reynolds number (approximately as $Re^{9/4}$). This approach is restricted to flows at low-to-moderate Reynolds number. The burden for directly simulating most practical engineering problems is far beyond the current computer capabilities.

The Reynolds-averaged Navier-Stokes equations (RANS) have been used for most engineering applications. In this approach, RANS equations are solved to determine only the mean flow fields. The computational cost for RANS models is much less than that for DNS because of its much lower grid resolution requirements at high Reynolds number. However, owing to the different behavior between large- and small-scale turbulent motions, it is impossible to achieve a universal model that can cover all types of turbulent flows (Piomelli, 1999).

Large-eddy-simulation (LES) (Deardorff, 1970) is an intermediate approach between the two aforementioned methods. In LES, the dynamics of the large, energy-carrying flow motions, which are directly affected by the geometry and flow conditions and are the least universal, are
resolved, and only the motions with length scales smaller than the resolved scales are modeled.
Since the small-scale flow motions are relatively homogeneous and universal, and less affected
by the boundary conditions than the large-scale ones, the hope is that LES can be applied to a
wide range of flows in comparison with RANS simulation (Pope, 2000). Similar to DNS, LES
provides a three-dimensional, time-dependent solution of the governing equations. However,
because only the energy containing flow motions are resolved in LES, the vast computational cost
of explicitly resolving the smallest-scale motions is avoided.

For three-dimensional flows generally encountered in engineering applications, the
numerical task of solving the LES equation is still substantial. Although many commercial CFD
codes (i.e. Fluent) offer LES functionality, the calculations, as carried out on grids generally
employed, are often better classified as very-large-eddy-simulation (VLES). In LES, the filtered
velocity field accounts for the bulk turbulent kinetic energy everywhere in the flowfield, whereas,
the grid and filter of VLES are too large to resolve all energy-containing motions, and instead a
significant portion of energy resides in subgrid motions. Since VLES is performed on coarser
grids, it is less expensive than LES. The simulation, however, is strongly dependent on the
modeling of the residual motions (Piomelli, 1999; Pope, 2000), and traditional LES models for
subgrid quantities do not perform well.

In LES, because the dissipative scales of turbulence are not adequately or totally
resolved, subfilter scale (SFS) modeling is required. The role of the traditional SFS model is to
mimic the drain of energy through energy cascade, and thereby to transfer energy (or variances)
from the resolved scales to the unresolved subfilter scales. In other words, the effects of
unresolved scales on resolved scales are modeled with energy drain being the most important (but
not the only) effect. Many SGS models have been developed since the late 1980s. Commonly
used SGS models include the Smagorinsky eddy viscosity model, the dynamic eddy viscosity
model, the similarity model and the mixed model.
The Smagorinsky SGS model (Smagorinsky, 1963) is widely used because it successfully models the drain of energy from resolved scale to unresolved flow motions. It can predict fairly accurately the integral scale flow motions and global dissipation when the grid is sufficiently fine to resolve most energy containing motions. This model, however, has obvious deficiencies. Firstly, an empirical model coefficient, which actually is flow and filter-width dependent (Pope, 2000), is required as initial input. Thus, the optimal model constant must be changed in different flows. Secondly, this model does not have the correct limiting behavior near the wall (Junela and Brasseur, 1999). Actually, as will be discussed in detail hereafter, all eddy-viscosity and similarity SFS models inherent possess the same problem in the near wall region (Junela and Brasseur, 1999). Thirdly, for laminar shear flow or viscous sub-layers close to the solid wall, in which the residual stresses are zero, the Smagorinsky model gives rise to spurious residual stresses tensor. Finally, the model does not account for backscatter of energy from small to large scales, which has been shown to be of importance in transitional turbulence.

To avoid the empirical coefficients in the algebraic Smagorinsky model, a dynamic eddy viscosity model (Germano et al., 1991) was proposed. In this model, the Smagorinsky coefficient is determined from the resolved-scale information, which is allowed to vary in both time and space. This is achieved by filtering the resolved-scale velocity with a test-filter at a scale larger than the effective LES filter. The coefficients of the dynamic model are assumed to be the same in both filters and are computed dynamically during the calculation. When model coefficient is negative, backscatter of energy occurs locally. The dynamic model can yield good predictions of energy transferring process, and most importantly, the subfilter stresses vanish in the transition to laminar flow. However, in this procedure, an additional spatial averaging is performed to avoid excessive fluctuations in the calculated model coefficients, which reduces its spatial variability (Moin, 1991; Lilly, 1992).
A weakness of all eddy viscosity models is that they assume the residual stress is proportional to strain rate tensor (It turns the principle axis of the strain-rate and residual stress tensor to align.). A scale-similar model that does not have this property was introduced by Bardina et al. (1980). A dynamic mixed model with a scale-similar part was applied by Zang et al. (1993). Unlike eddy viscosity models which close only the deviatoric part of SGS stress tensor, similarity models close the full SGS stress tensor. This kind of model has proved to be successful in simulations of the turbulent-mixing layer (Vreman, 1997).

As mentioned above, both eddy viscosity and similarity models inherently possess a significant deficiency near surfaces in high Reynolds number flows (Juneja and Brasseur, 1999). The error may arise from the poor performance of algebraic SFS model at the first several grid levels, where integral scales are necessarily under-resolved and the turbulence is highly anisotropic. Under this condition, the models create a spurious feedback loop between predicted resolved-scale (RS) velocity and modeled SFS acceleration, and are unable to simultaneously capture SFS acceleration and RS-SFS energy flux. To fix this problem, Zhou et al. (2001) introduced a modeling strategy in which the grid-resolved subfilter velocity is estimated from a separate dynamical equation containing the essential inertial interactions between subfilter-scale and resolve scale (RS) velocities. This method successfully suppresses the spurious feedback loop between RS velocity and SFS acceleration, and greatly improves the predictions of anisotropic structures and resolved velocity fields. The resolvable subfilter-scale (RSFS) model accurately captures SFS acceleration intensity and RS-SFS energy flux, even during the nonequilibrium transient (Zhou et al., 2001). There are other types of SFS models, such as Lagrangian dynamic model (Meneveau et al., 1996) and Monotonically Integrated LES (MILES) (Fureby and Grinstein, 1999; 2002; Grinstein et al., 2002), which can not be discussed in detail herein.
The successful application of LES depends not only on SFS model, but also relies heavily on many other important issues (Moin, 2002), including filtering and governing equation, wall layer modeling, accuracy of numerical algorithm, and boundary conditions. The scope is so broad that far beyond the contents of this brief section. The comprehensive review on LES can be found in Piomelli (1999) and Moin (2002).

2.2.1 Filtering

In large-eddy-simulation, a filtering operation is performed so that the resulting filtered velocity field can be adequately resolved on a relative coarse grid. Specifically, the required grid spacing is proportional to the filter width. A filtered (or resolved) variable is defined as

$$\tilde{f}(x) = \int_{\infty}^{x} f(x)G_f(x - x')dx'$$  \hspace{1cm} (2.13)

where $G$ is the filter function and $\int_{\infty}^{x} G(x)dx = 1$. Leonard (1974) indicated that if $G$ is only a function of $x - x'$, the differentiation and filtering operations could commute with each other. Commutation of the filtering operation with spatial differentiation is strictly valid only for uniform grid systems (Ghosal and Moin, 1995; Ven, 1995). The commutation error is usually neglected for moderately stretched grids, and can be lumped with the subgrid model (Ribault et al., 1999; Moin, 1997). The modeling error is found to be generally smaller than the discretization error (Ribault et al., 1999).

The filter function $G$ could be any function defined in an infinite domain and satisfies the following requirements

$$G(x) = G(-x);$$

$$\int_{\infty}^{x} G(x)dx = 1;$$
where $\Delta$ stands for the filter size. The most commonly used filter functions are summarized as follows.

- **Tophat:**
  This filter is popularly employed in the physical space, defined as
  \[
  G_f(x) = \begin{cases} 
  1/\Delta & \text{if } |x| \leq \Delta/2 \\
  0 & \text{otherwise} 
  \end{cases}
  \]  
  (2.14)

For example, in the finite-volume approach, the cell-averaged variables are defined as

\[
\tilde{f} = \frac{1}{\Delta V} \int_{\Delta V} f(x) dx
\]  
(2.15)

Thus, the cell average in the finite volume method, which will be implemented in the current study, belongs to the Top-hat filter.

- **Gaussian filter:**
  The Gaussian filter function is the Gaussian distribution with zero mean and variance
  \[
  \sigma^2 = \Delta^2 / 12
  \]
  \[
  G_f(x) = \frac{6}{\pi \Delta^2} \exp(-\frac{6|x|^2}{\Delta^2})
  \]  
  (2.16)

- **Cutoff Filter:**
  \[
  \hat{G}_f(k) = \begin{cases} 
  1 & \text{if } |k_c| < \pi/\Delta \\
  0 & \text{otherwise} 
  \end{cases}
  \]  
  (2.17)

The cutoff filter is a tophat filter in spectral space. A detailed description of properties of various filters can be found in the textbook (Pope, 2000).
2.2.2 Filtered Governing Equations

To capture all of the flow scales resolved by a given grid system, and to model the effects of unresolved scales, the concepts of decomposition and filtering are introduced. Based on the Favre-averaging (Favre, 1969), any instantaneous variable \( f \) can be expressed as the sum of a Favre-averaged filtered scale \( \bar{f} \) and a sub-filter scale \( f' \)

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

where

\[
\bar{f} = \frac{\rho \bar{f}}{\rho}
\]

Because of \( \bar{f}' \neq 0 \) and \( \bar{f}'' \neq 0 \) in this spatial filtering process, the filter operation in LES is different from the conventional Reynolds average in time domain. Therefore, the relationships derived from the time averaging in the RANS concept are not always true in the filter operations of LES (see Appendix A).

The filtered Favre-averaged mass, momentum, energy and species conservation equations can be written as

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

\[
\frac{\partial \rho \bar{u}_i}{\partial t} + \frac{\partial(\rho \bar{u}_i \bar{u}_j + \rho \delta_{ij})}{\partial x_j} = \frac{\partial (\bar{\tau}_{ij} - \tau_{ij}^{\text{sgs}})}{\partial x_j}
\]

\[
\frac{\partial \rho \bar{E}}{\partial t} + \frac{\partial((\rho \bar{E} + \rho \bar{u}_i \bar{u}_j))}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \bar{u}_j \bar{\tau}_{ij} + \lambda \frac{\partial \bar{T}}{\partial x_i} - H_i^{\text{sgs}} + \sigma_i^{\text{sgs}} \right)
\]

\[
\frac{\partial \rho \tilde{Y}_k}{\partial t} + \frac{\partial \left( \rho \tilde{u}_j \tilde{Y}_k \right)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho \bar{U}_{k,j} \tilde{Y}_k - \Phi_{k,j}^{\text{sgs}} - \theta_{k,j}^{\text{sgs}} \right) + \tilde{\omega}_k
\]
The unclosed sub-filter terms are defined:

\[ \tau_{ij}^{\text{sgs}} = (\overline{\rho u_i u_j} - \overline{\rho \tilde{u}_i \tilde{u}_j}) \] (2.24)

\[ H_i^{\text{sgs}} = (\rho E_i - \overline{\rho \tilde{E}_i}) + (\overline{pu_i} - \overline{\rho \tilde{u}_i}) \] (2.25)

\[ \sigma_{ij}^{\text{sgs}} = (u_j \tilde{\tau}_{ij} - \overline{u_j \tilde{\tau}_{ij}}) \] (2.26)

\[ \Phi_{k,j}^{\text{sgs}} = (\rho Y_k u_j - \overline{\rho \tilde{Y}_k \tilde{u}_j}) \] (2.27)

\[ \Theta_{k,j}^{\text{sgs}} = (\rho Y_k U_{k,j} - \overline{\rho \tilde{Y}_k \tilde{U}_{k,j}}) \] (2.28)

The SGS stresses term \( \tau_{ij}^{\text{sgs}} \), SGS energy fluxes term \( H_i^{\text{sgs}} \) and SGS species fluxes \( \Phi_{k,j}^{\text{sgs}} \) result from filtering these convective terms. The SGS viscous work term, \( \sigma_{ij}^{\text{sgs}} \), comes from correlations of the velocity field with the viscous stress tensor, and the SGS species diffusive fluxes term, \( \Theta_{k,j}^{\text{sgs}} \), comes from correlations of the velocity field with the species mass fractions with the diffusion velocities. The resolved-scale species mass production rate, \( \tilde{\omega}_k \), 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 be filtered. Filtering the equation of state gives us

\[ \overline{p} = R_u \tilde{Z} \overline{\rho T} + R_u (\tilde{Z} \overline{\rho T} - \tilde{Z} \overline{\rho \tilde{T}}) \] (2.29)

where \( Z \) is the compressibility factor. The first term on the right hand side uses only resolved variables (i.e. \( \tilde{Z} \), \( \overline{\rho} \), \( \overline{T} \)) and can be computed directly. The second term includes a correlation of the temperature, compressibility, and density (\( \tilde{Z} \overline{\rho \tilde{T}} \)). This term is difficult to model. For ideal gas \( (Z = 1) \) with low heat release, this term is negligible (Calhoon and Menon, 1996). This may be not true for high-pressure real-fluid mixture. Tramecourt et al. (2004) recently evaluated
the contributions of the two terms in the directly simulation of supercritical heptane/nitrogen mixing layer. They reported that the contribution of the second terms was always less than 0.2% of that of the first term. Based on this observation, the second term is neglected in the present simulation.

The filtered total energy $\tilde{E}$ can be approximated as

$$\tilde{E} = \tilde{h} - \frac{\tilde{p}}{\rho} + \frac{\tilde{u}_k^2}{2} + k^{gs} = \tilde{\psi} + \int_{p_0}^{p} \left[ \frac{1}{\rho} + \frac{T}{\rho^2} \left( \frac{\partial \rho}{\partial T} \right)_p \right] dp - \frac{\tilde{p}}{\rho} + \frac{\tilde{u}_k^2}{2} + k^{gs}$$  \hspace{1cm} (2.30)

where $\psi = \sum_{i=1}^{N} Y_i h_i^0$ and $k^{gs} = \tau^{gs}_{kk} / 2\tilde{\rho} = \frac{1}{2} \left( \rho u_k u_k / \tilde{\rho} - \tilde{u}_k^2 \right)$.

### 2.2.3 Subgrid-Scale Models

The SGS modeling for the unresolved terms in Eqs. (2.24)-(2.28) is one of the important issues in LES. Because the small eddies, which are less than the filter size and unresolved in LES, dissipate most turbulent kinetic energy, SGS models are introduced to allow for the transferring of energy from resolved to unresolved scales and to mimic the drain of energy associated with the energy cascade. Most of the SGS models are based on an eddy-viscosity type model, in which the SGS stress $\tau^{gs}_{ij}$ is related to the large-scale strain-rate tensor $\tilde{S}_{ij}$ as follows

$$\tau^{gs}_{ij} - \frac{\delta_{ij}}{3} \tau^{gs}_{kk} = -2\nu_t \tilde{S}_{ij}$$  \hspace{1cm} (2.31)

where $\nu_t$ is the eddy viscosity and $\tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_j}{\partial x_i} + \frac{\partial \tilde{u}_i}{\partial x_j} \right)$.
2.2.3.1 Algebraic Smagorinsky Type Model

In this kind of model, the eddy viscosity $v_t$ is obtained algebraically to avoid solving additional equations. Usually the equilibrium hypothesis is made to simplify the problem and to obtain an algebraic model. The equilibrium hypothesis 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 SGS kinetic energy production and viscous dissipation rate term: $-\tau_{ij}^{sgr} \tilde{S}_{ij} = \varepsilon_v$.

The Smagorinsky model based on the equilibrium hypothesis is written

$$v_t = (C_s \Delta)^2 |\tilde{S}|$$  \hspace{1cm} (2.32)

where $\Delta$ is the filter width and $|\tilde{S}| = (2\tilde{S}_{ij}\tilde{S}_{ij})^{1/2}$. The filter width is chosen as $(\nabla \forall)^{1/3}$, where $\nabla \forall$ is cell volume. The coefficient $C_s$ can be specified from the isotropic turbulence decay or a prioric test. Erlebacher et al. (1992) extended the above model to include flow compressibility

$$\tau_{ij}^{sgr} = -2\nu_t \tilde{\rho}(\tilde{S}_{ij} - \frac{\tilde{S}_{kk} \delta_{ij}}{3}) + \frac{2}{3} \tilde{\rho}k^{sgr} \delta_{ij}$$  \hspace{1cm} (2.33)

where $\nu_t$ is the eddy viscosity.

$$\nu_t = C_{sC} (\Delta D)^2 |\tilde{S}|$$  \hspace{1cm} (2.34)

$$k^{sgr} = C_t (\Delta D)^2 \tilde{S}_{ij} \tilde{S}_{ij}$$  \hspace{1cm} (2.35)

where the dimensionless quantities $C_{sC}$ and $C_t$ 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
where \( y^* = y u_c / \nu \) and \( u_c \) is friction velocity.

Since no chemical reaction is considered in the present simulation, the subgrid energy flux (\( H_{ij}^{sgs} \)) and the convective species flux (\( \Phi_{ik}^{sgs} \)) terms is modeled based on the gradient transport assumption (Oefelein and Yang, 1998)

\[
H_{ij}^{sgs} = -\bar{\rho} \frac{v_i}{Pr_i} \left( \frac{\partial \tilde{h}}{\partial x_j} + \tilde{u}_i \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{1}{2} \frac{\partial k_{ij}^{sgs}}{\partial x_j} \right) \tag{2.37}
\]

where \( Pr_i \) represents the turbulent Prandtl number, a standard value 0.7 is used (Zang et al., 1992). The SGS viscous work term, \( \sigma_{ij}^{sgs} \), is neglected due to its small contribution to the total energy equation (Martin et al., 1999).

The convective species flux term (\( \Phi_{ik}^{sgs} \)) is usually approximated as

\[
\Phi_{ik}^{sgs} = -\bar{\rho} \frac{v_i}{Sc_i} \frac{\partial \tilde{Y}_k}{\partial x_i} \tag{2.38}
\]

where \( Sc_i \) is the turbulent Schmidt number. It should be noted that the use of the gradient transport assumption for reactive species is questionable. The SGS species diffusive fluxes term, \( \Theta_{k,j}^{sgs} \), usually is neglected (Calhoon and Menon, 1996; Oefelein and Yang, 1998).

The algebraic Smagorinsky type model described above is the most widely used model in LES. However, as pointed out by Moin et al. (1991), it has several limitations. First, the optimal model constant must be changed for a different class of flows. Second, the model does not have the correct limiting behavior near a 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.

### 2.2.3.2 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). The dynamic model uses resolved-scale information at the grid-filter level and a coarser test-filter $\hat{G}_j$ with characteristic $\hat{\Delta} > \Delta$ (typically, $\hat{\Delta} = 2\Delta$) in order to compute the model parameters $C_R$ and $C_I$ as a function of space and time (Germano et al., 1991). Formally, the dynamical procedure is based on the Germano identity (Germano, 1992)

\[
\langle \rho \hat{u}_i \hat{u}_j \rangle = \langle \rho \hat{u}_i \hat{u}_j \rangle - \langle \rho \rangle \langle \hat{u}_i \hat{u}_j \rangle
\]

where $L_{ij} = \langle \rho \hat{u}_i \hat{u}_j \rangle - \langle \rho \rangle \langle \hat{u}_i \hat{u}_j \rangle$ and $T_{ij} = \langle \rho \hat{u}_i \hat{u}_j \rangle - \langle \rho \rangle \langle \hat{u}_i \hat{u}_j \rangle$. Here a Favre-filtered variable under a test-filter is defined as $\langle \tilde{f} \rangle = \langle \rho \tilde{f} \rangle / \langle \tilde{\rho} \rangle$. The brackets $\langle \cdot \rangle$ denote the averaging operation based on the test filter. 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.

\[
L_{ij} = T_{ij} - \langle \tau_{ij}^{\text{SGS}} \rangle \tag{2.39}
\]
\[ C_R = \frac{<L_{ij}M_{ij}>_a}{<M_{ij}M_{ij}>_a} - \frac{1}{3} \frac{<L_{ij}M_{ij}>_a}{<M_{ij}M_{ij}>_a} \]  
(2.40)

\[ C_i = \frac{<L_{ik}>_a}{<\beta - <\alpha>>_a} \]  
(2.41)

where \(<\cdot>_a\) denote an appropriate spatial average, generally taken over the homogeneous directions to ensure the numerical stability (Moin et al. 1991; Germano et al., 1991; Lilly, 1992). This additional averaging reduces the spatial variability of the model constant.

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

\[ M_{ij} = \beta_{ij} - <\alpha_{ij}> \]  
(2.42)

\[ \beta_{ij} = -2\Delta^2 <\bar{\rho}> |\bar{S}| (\bar{S}_{ij} - \frac{\delta_{ij}}{3} \bar{S}_{kk}); \alpha_{ij} = -2\Delta^2 \bar{\rho} |\bar{S}| (\bar{S}_{ij} - \frac{\delta_{ij}}{3} \bar{S}_{kk}) \]  
(2.43)

\[ \beta = 2 <\bar{\rho}> \Delta^2 |\bar{S}|^2; \alpha = 2 \bar{\rho} \Delta^2 |\bar{S}|^2 \]  
(2.44)

The same idea for modeling the SGS turbulent stress can be employed to dynamically calculate the turbulent Prandtl number and Schmidt number in Eq. 2.37 and Eq. 2.38 (Wang, 2002).

We implemented the algebraic Smagorinsky model in the current study although it may not be the best SGS model. There are two reasons: first, the best SGS model for real-fluid flows is still unknown; and second, the grid requirement for other models such as the dynamical model is normally stricter than the algebraic Smagorinsky model due to its double filters, both of which are required to be located in the inertial range.

### 2.3 Equation of State

In order to evaluate thermophysical properties for real-fluid mixture, an equation of state capable of handling real fluid behavior at high-pressure and low-temperature regime is required.
The most common equation of state utilized for calculating high-pressure fluid properties is the cubic equations of state, which includes Redlich-Kwong (Reid et al, 1986), Peng-Robinson (Peng and Robinson, 1976), and the modified Soave-Redlich-Kwong (SRK) equations of state (Soave, 1972; Graboski and Daubert, 1978a, 1978b). The modified SRK equation of state, which is capable of handling the quantum gas behavior of hydrogen, is adopted here for the calculation of thermodynamic properties and derivation of numerical relationships. The consistent treatment of thermodynamic properties using one equation of state produces an efficient numerical algorithm. A more complicated Benedict-Webb-Rubin (BWR) equation of state, combined with the extended corresponding states theory, is utilized for estimating transport properties, as suggested by Ely and Hanly (1981; 1983). Both the modified SRK and the BWR equations of state are capable of representing liquid and gas phase behaviors. The BWR equation of state can be applied over broader temperature and pressure ranges, but the SRK equation of state is easy to apply, especially for deriving the thermodynamic differential relationships.

2.3.1 Modified Soave-Redlich-Kwong (SRK) Equation of State

The modified SRK equation of state is considered to be both simple and fairly accurate, which takes the following form (Soave, 1972; Graboski and Daubert, 1978a, 1978b)

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

where \( R_u \) is the universal gas constant. The parameters ‘a’ and ‘b’ account for the effects of the attractive and repulsive forces between molecules, respectively. ‘\( \alpha \)’ is the third parameter, which is a function of temperature and acentric factor. For mixtures, they are calculated from the following mixing rules.
The cross parameter $\alpha_{ij} a_{ij}$ in Eq. 2.46 is given by

$$\alpha_{ij} a_{ij} = \sum_{i=1}^{N} \sum_{j=1}^{N} x_i x_j \alpha_{ij} a_{ij} \alpha_{ji} a_{ji} (1 - \kappa_{ij})$$

(2.48)

where $x_i$ is the mole fraction of species $i$. $\kappa_{ij}$ is the binary interaction coefficient, which can be calculated from a known data set (Graboski and Daubert, 1978a, 1978b). The constants $a_i, b_i$ can be determined from the following universal relationships (Moran and Shapiro, 1999)

$$a_i = 0.42747 \frac{R_u^2 T_{ci}^2}{p_{ci}}$$

(2.49)

$$b_i = 0.08664 \frac{R_u T_{ci}}{p_{ci}}$$

(2.50)

The third parameter for species $i$ is given as (Meng, 2000)

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

(2.51)

where $T_{ci}, p_{ci}$, are the critical temperature and pressure for species $i$. $T_n$ is the reduced temperature for species $i$, and $S_i$ is another variable. These parameters are given by the following formulas

$$T_n = \frac{T}{T_{ci}}$$

(2.52)

$$S_i = 0.48508 + 1.5517 \omega_i - 0.15613 \omega_i^2$$

(2.53)
Equations 2.51 and 2.53 are not capable of accurately correlating hydrogen systems due to its quantum gas behavior. A modified expression of $\alpha$ for hydrogen is further established (Graboski and Daubert, 1978a; 1978b)

$$\alpha_{H_2} = 1.202 \exp(-0.30228T_c)$$

(2.54)

This correlation is expected to be accurate for hydrogen at reduced temperatures greater than about 2.5 (the critical temperature of hydrogen is 33.2K). No mixture of technical interests lies below this temperature. When Eq. 2.54 is used, the binary interaction coefficients $\kappa_{ij}$ involving hydrogen species should be set to 0.

2.3.2 Benedict-Webb-Rubin (BWR) Equation of State

The BWR equation of state of methane is presented here, which is proposed by Jacobsen and Stewart (1973) based on very broad ranges of experimental data to ensure the proper extrapolation to low-temperature and high-pressure regions. Its expression is

$$p = \sum_{n=1}^{9} A_n(T) \rho^n + \sum_{n=10}^{15} A_n(T) \rho^{2n-17} e^{-\gamma \rho^2}$$

(2.55)

where the 15 coefficients $A_n$ are given in Table 2.1, which are functions of temperature. The 32 semi-empirical constants of $N_s$ are listed in Table 2.2. The units for pressure, density, and temperature are given in bar, mol/liter, and K. The stain-rate $\gamma$ is 0.0096 (mol/liter)$^2$ (Meng, 2000).
Table 2.1: Coefficients of $A_n$

<table>
<thead>
<tr>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$A_4$</th>
<th>$A_5$</th>
<th>$A_6$</th>
<th>$A_7$</th>
<th>$A_8$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_1T$</td>
<td>$N_1T + N_2T^{1/2} + N_3 + N_4T + N_5/T^{2}$</td>
<td>$N_6T + N_7 + N_8/T + N_9/T^{2}$</td>
<td>$N_{10}T + N_{11} + N_{12}/T$</td>
<td>$N_{13}$</td>
<td>$N_{14}/T + N_{15}/T^{2}$</td>
<td>$N_{16}/T$</td>
<td>$N_{17}/T + N_{18}/T^{2}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$A_9$</th>
<th>$A_{10}$</th>
<th>$A_{11}$</th>
<th>$A_{12}$</th>
<th>$A_{13}$</th>
<th>$A_{14}$</th>
<th>$A_{15}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_{19}/T^{2}$</td>
<td>$N_{20}/T^{2} + N_{21}/T^{3}$</td>
<td>$N_{22}/T^{2} + N_{23}/T^{4}$</td>
<td>$N_{24}/T^{2} + N_{25}/T^{3}$</td>
<td>$N_{26}/T^{2} + N_{27}/T^{4}$</td>
<td>$N_{28}/T^{2} + N_{29}/T^{3}$</td>
<td>$N_{30}/T^{2} + N_{31}/T^{3} + N_{32}/T^{4}$</td>
</tr>
</tbody>
</table>

Table 2.2: Semi-empirical Constants Based on Methane

<table>
<thead>
<tr>
<th>$N_1$</th>
<th>$N_2$</th>
<th>$N_3$</th>
<th>$N_4$</th>
<th>$N_5$</th>
<th>$N_6$</th>
<th>$N_7$</th>
<th>$N_8$</th>
<th>$N_9$</th>
<th>$N_{10}$</th>
<th>$N_{11}$</th>
<th>$N_{12}$</th>
<th>$N_{13}$</th>
<th>$N_{14}$</th>
<th>$N_{15}$</th>
<th>$N_{16}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-1.184347314485E-2$</td>
<td>$7.540377272657E-1$</td>
<td>$-1.225769717554E+1$</td>
<td>$6.260681393432E+2$</td>
<td>$-3.490654409121E+4$</td>
<td>$5.301046385532E-4$</td>
<td>$-2.875764479978E-1$</td>
<td>$5.011947936427E+1$</td>
<td>$-3.174982181302E-3$</td>
<td>$2.064957753744E+5$</td>
<td>$1.285951844828E-2$</td>
<td>$-1.106266656726E+0$</td>
<td>$3.060813353408E-4$</td>
<td>$-3.174982181302E-3$</td>
<td>$5.191608004779E+0$</td>
<td>$-3.074944210271E-4$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$N_{17}$</th>
<th>$N_{18}$</th>
<th>$N_{19}$</th>
<th>$N_{20}$</th>
<th>$N_{21}$</th>
<th>$N_{22}$</th>
<th>$N_{23}$</th>
<th>$N_{24}$</th>
<th>$N_{25}$</th>
<th>$N_{26}$</th>
<th>$N_{27}$</th>
<th>$N_{28}$</th>
<th>$N_{29}$</th>
<th>$N_{30}$</th>
<th>$N_{31}$</th>
<th>$N_{32}$</th>
</tr>
</thead>
</table>
2.4 Thermodynamic Properties

In order to solve the conservation equations, additional relationships relating thermodynamic properties to temperature and, in high-pressure cases, pressure, are required. The thermodynamic properties to be evaluated are density, internal energy, enthalpy, entropy, partial molar enthalpy, and chemical potential of each species. These properties can be derived directly from fundamental thermodynamic relationships, which is valid over all thermodynamic states (Moran and Shapiro, 1999; Yang, 2000; Meng and Yang, 2003)

\[ e(T, \rho) = e_0(T) + \int_{\rho_0}^{\rho} \left[ \frac{p}{\rho^2} - \frac{T}{\rho} \left( \frac{\partial p}{\partial T} \right)_T \right] d\rho \tag{2.56} \]

\[ h(T, p) = h_0(T) + \int_{p_0}^{p} \left[ \frac{1}{\rho} + \frac{T}{\rho^2} \left( \frac{\partial p}{\partial T} \right)_T \right] dp \tag{2.57} \]

\[ s(T, \rho) = s_0(T, \rho_0) - \int_{\rho_0}^{\rho} \left[ \frac{1}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_T \right] d\rho \tag{2.58} \]

\[ C_p(T, \rho) = C_{V0}(T) - \int_{\rho_0}^{\rho} \left[ \frac{T}{\rho^2} \left( \frac{\partial^2 p}{\partial T^2} \right)_T \right] d\rho + \frac{T}{\rho^2} \left( \frac{\partial p}{\partial T} \right)_T^2 \left( \frac{\partial p}{\partial \rho} \right)_T \tag{2.59} \]

where the \( e, h, s, C_p, C_V \) are internal energy, enthalpy, entropy, constant-pressure heat capacity, and constant-volume heat capacity, respectively. The subscript 0 refers to an ideal state at a low pressure and integral terms are the departure functions. All the partial derivatives in these relations are calculated based on the modified Soave-Redlich-Kwong equation of state:

\[ \left( \frac{\partial \rho}{\partial T} \right)_{\rho_j} = \frac{\rho R_u}{(M_w - b \rho)} - \frac{1}{M_w} \left[ \frac{\partial}{\partial T} \left( a \alpha \right) \right]_{\rho, \gamma_i} \left( \frac{\rho^2}{M_w + b \rho} \right) \tag{2.60} \]

\[ \left( \frac{\partial \rho}{\partial \rho} \right)_{T, \gamma_i} = \frac{M_w R_u T}{(M_w - b \rho)^2} - \frac{a \alpha \rho (2M_w + b \rho)}{M_w (M_w + b \rho)^2} \tag{2.61} \]
where the derivative $\frac{\partial}{\partial T}(aa)$ is given in Appendix C.

### 2.4.1 Partial Molar and Partial Density Properties

At standard pressure, gas mixtures behave ideally, where the mixture properties are simply the molar-weighted sum of the properties of each component. High-pressure fluid mixtures, however, do not obey Raoult’s law (Moran and Shapiro, 1999). Their properties, such as total volume, internal energy, enthalpy, and Gibbs free energy, depend on both the temperature, pressure, and composition. If any of the above properties are denoted by $F(x_1, x_2, \cdots, p, T)$, then the partial molar property $\bar{F}_i$ is defined as

$$\bar{F}_i = (\partial F / \partial x_i)_{p,T,x_{j\neq i}}$$

For a binary mixture, the partial molar properties in terms of the mole fraction of the first component ($x_1$) is

$$\bar{F}_1 = (\partial F / \partial x_1)_{p,T}$$

$$\bar{F}_2 = F - x_1(\partial F / \partial x_1)_{p,T}$$

Figure 2.2 shows a plot of the volume of one molar mixture as a function of $x_1$. The partial molar volume, $\bar{V}_1$ and $\bar{V}_2$, at a given mole fraction $x_1^*$ are obtained by drawing a tangent to the volume curve at $x_1^*$ and reading off the intercepts of the tangent with the vertical axis at
$x_i = 0.1$. The plot also shows the excess volume $V^E$, defined as the difference between the actual volume and the molar fraction-averaged volume of the two pure components at the same pressure and temperature.

![Figure 2.2: Molar volume of a mixture as function of composition at fixed pressure and temperature.](image)

As being demonstrated in the early works regarding high-pressure droplet vaporization and combustion (Manrique and Borman, 1969; Hsieh et al., 1991), in order to find faithful results, the properties of each component in a non-ideal mixture have to be calculated based on the partial molar properties. In a general CFD code, all flow properties are derived in a mass or density based manner, which rends the evaluation of partial molar properties inconvenient. Thus, the concepts of partial mass and partial density properties were recently established by Lafon et al. (1995) and Meng (2000). According to fundamental thermodynamics, any thermodynamic property $\phi$ in a mixture is a function of temperature, pressure, and masses of the constituent species

$$m\phi = m\phi(T, p, m_i)$$

(2.65)
Therefore, the partial mass property is defined as

\[
\hat{\phi}_i = \left( \frac{\partial m\phi}{\partial m_i} \right)_{T,p,m_{ji}}
\]  

(2.66)

where \( i, j = 1, \cdots, N \), and \( \phi \) refers to any proper thermodynamic property per unit mass of a mixture, such as enthalpy and internal energy.

In fluid mechanics, density is more convenient to use instead of mass. Therefore, it is better to define the mixture thermodynamic properties per unit volume

\[
\rho \phi = \rho \phi(T, \rho_i)
\]  

(2.67)

This leads naturally to the definition of the partial density property \( \tilde{\phi}_i \)

\[
\tilde{\phi}_i = \left( \frac{\partial \rho \phi}{\partial \rho_i} \right)_{T,\rho_{ji}}
\]  

(2.68)

According to this definition, the partial density internal energy, enthalpy, and entropy are expressed as

\[
\tilde{e}_i = \left( \frac{\partial \rho e}{\partial \rho_i} \right)_{T,\rho_{ji}}
\]  

(2.69)

\[
\tilde{h}_i = \left( \frac{\partial \rho h}{\partial \rho_i} \right)_{T,\rho_{ji}}
\]  

(2.70)

\[
\tilde{s}_i = \left( \frac{\partial \rho s}{\partial \rho_i} \right)_{T,\rho_{ji}}
\]  

(2.71)

where calculations of \( \tilde{e}_i \), \( \tilde{h}_i \), and \( \tilde{s}_i \) require the thermodynamic relations presented in Eq. 2.56 to 2.60, and the SRK equation of state. In addition, a relationship between the partial density property and the partial mass property is derived as

\[
\hat{\phi}_i = \hat{\phi}_i + \rho \left( \frac{\partial \phi}{\partial p} \right)_{T,Y_i} \left( \frac{\partial p}{\partial \rho_i} \right)_{T,\rho_{ji}}
\]  

(2.72)
Utilizing fundamental thermodynamic theories, including Euler equation and Gibbs-Duhem relation, the following relationship regarding chemical potential of each species, which is required for the treatment of thermodynamic phase equilibrium, can be derived

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

The details for calculating thermodynamic properties are presented in Appendix B. As a specific example, the partial density internal energy and enthalpy of species \( i \), \( \tilde{e}_i \) and \( \tilde{h}_i \), are derived here. According to the definition presented in Eq. 2.69, we first need to derive an expression for the internal energy \( e \). Using Eq. 2.56 and the derivative expressions presented in Appendix B, the following relation is found

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

where the expression of \( \frac{\partial a \alpha / T}{\partial T} \) is presented in Appendix C.

Based on the definition, the partial density internal energy \( \tilde{e}_i \) can be expressed as

\[ \tilde{e}_i = e_{i,0} + \frac{2}{b M_w} \left[ \sum_j x_j \left( T \frac{\partial}{\partial T} \left( a_y \alpha_y - a_y \alpha_y \right) \right) \ln \left( 1 + \frac{b \rho}{M_w} \right) \right] + \frac{b_i}{b M_w} \left[ T \frac{\partial}{\partial T} (a \alpha) - a \alpha \right] \frac{\rho}{M_w + b \rho} - \frac{1}{b} \ln \left( 1 + \frac{b \rho}{M_w} \right) \]  

Utilizing Eq. 2.75, the expression for the internal energy, Eq. 2.74 can be related to the partial density internal energy

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

According to thermodynamics

\[ \rho h = \rho e + p \]
Following the definition for the partial density property, the expression for partial density enthalpy can be found by taking derivative of the partial density of species $i$ at both sides of the Eq. 2.77 and keeping temperature and all the other partial densities constant

$$\left( \frac{\partial \rho_{h}}{\partial \rho_{i}} \right)_{T, \rho_{j \neq i}} = \left( \frac{\partial e}{\partial \rho_{i}} \right)_{T, \rho_{j \neq i}} + \left( \frac{\partial p}{\partial \rho_{i}} \right)_{T, \rho_{j \neq i}}$$

(2.78)

It is recognized that Eq. 2.78 is equivalent to Eq. 2.79

$$\hat{h}_{i} = \tilde{e}_{i} + \left( \frac{\partial p}{\partial \rho_{i}} \right)_{T, \rho_{j \neq i}}$$

(2.79)

Substituting Eq. 2.72 into Eq. 2.79, and taking use of the fundamental expressions of enthalpy, which are available in any thermodynamics textbook, the following relationship regarding the partial mass enthalpy, $\hat{h}_{i}$, can be derived

$$\hat{h}_{i} = \tilde{e}_{i} + \frac{\rho}{\left( \frac{\partial p}{\partial \rho_{i}} \right)_{T, \rho_{j \neq i}}} \left( \frac{\partial p}{\partial \rho_{j}} \right)_{T, \rho_{j \neq i}}$$

(2.80)

### 2.4.2 Critical Point of Fluid Mixture

The thermodynamic critical point of a pure fluid is fixed and corresponds to the maximum temperature and pressure where the vapor-liquid equilibrium (VLE) with two distinct phases can coexist. However, when the system consists of more than one component, the critical temperature and pressure are functions of the composition (as shown in Fig 2.3). Since a fluid mixture reaches a stability limit at the critical point, the Gibbs criteria should be satisfied to guarantee a concave distribution of the Helmholtz free energy as its composition varies. Due to
the different physical criteria for criticality in a pure fluid and a mixture, the properties that diverge strongly in pure fluids near the critical region only diverge weakly in mixtures.

In general, the Gibbs Criteria requires the two determines defined below equal zero at the critical point of mixture (Reid et al., 1986)

\[
L = \begin{vmatrix}
A_{11} & A_{12} & \cdots & A_{1n} \\
A_{21} & A_{22} & \cdots & A_{2n} \\
\vdots & \vdots & \ddots & \vdots \\
A_{n1} & A_{n2} & \cdots & A_{nn}
\end{vmatrix} = 0 \quad (2.81)
\]

and

\[
M = \begin{vmatrix}
A_{11} & A_{12} & \cdots & \cdots & A_{1n} \\
A_{21} & A_{22} & \cdots & \cdots & A_{2n} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
A_{n-1,1} & A_{n-1,2} & \cdots & \cdots & A_{n-1,n} \\
\frac{\partial L}{\partial N_1} & \frac{\partial L}{\partial N_2} & \cdots & \cdots & \frac{\partial L}{\partial N_n}
\end{vmatrix} = 0 \quad (2.82)
\]

Figure 2.3: T-V phase diagram of multi-component mixture with different compositions (x₁=0.4, 0.6).
where \( A \) is the Helmholtz free energy, and 
\[
A_j = \left( \frac{\partial^2 A}{\partial N_i \partial N_j} \right)_{T,V}.
\]

With a proper equation of state, the above equations can be solved simultaneously to find the critical temperature and volume. The critical pressure of mixture is then determined based on the pre-specified \( P - V - T \) relationship.

### 2.5 Transport Properties

Transport properties to be evaluated include viscosity, thermal conductivity and binary mass diffusivity. Accurate estimations of these properties are very important for high-pressure fluid mixing and combustion computation, since they determine not only the flow dynamics, but also the heat and mass transfer rates (Vesovic and Wakeham, 1991). As proved in the literature, pressure effects have to be taken into account to accurately estimate these properties.

#### 2.5.1 Corresponding States Theories

The law of corresponding state, which was originally proposed by van der Waals in 1873, expresses that the equilibrium properties of different fluids can be related to their critical properties in a universal way. For example, if pressure, temperature, and volume are related to their critical properties, the PVT function relating the reduced pressure, temperature, and volume becomes identical for all substances. The reduced property is defined as

\[
p_r = \frac{p}{p_c}, T_r = \frac{T}{T_c}, V_r = \frac{V}{V_c}
\]  

(2.83)

The corresponding states theory also holds for other properties, including viscosity, and thermal conductivity. Based on the corresponding states argument, a property of any fluid can be
estimated by relating to its counterpart of a reference substance, whose property can be easily
determined (Ely and Hanly, 1981).

\[ \eta_x(T, \rho) = \eta_0(T_0, \rho_0) F_\eta \]  

(2.84)

where the subscript \( x \) refers to the fluid of interest, \( 0 \) to the reference fluid

\[ F_\eta = \left( \frac{M_{w_x}}{M_{w_0}} \right)^{1/2} f_{x,0}^{1/2} h_{x,0}^{-2/3} \]  

(2.85)

Here, \( M_w \) is the molecular weight. \( T_0 \) and \( \rho_0 \) of the reference fluid are calculated by

\[ T_0 = T / f_{x,0} \]
\[ \rho_0 = \rho h_{x,0} \]  

(2.86)

In general corresponding states theory, the parameters \( f_{x,0} \) and \( h_{x,0} \) is the ratio of the
critical temperature and volume. However, the range of its applicability can be broadened
considerably by introducing the extended corresponding states (EXCST) model, where the
equivalent parameters of \( f_{x,0} \) and \( h_{x,0} \) become

\[ f_{x,0} = \left( \frac{T_{c,x}}{T_{c,0}} \right) \phi(T_{r,x}, V_{r,x}, \omega_x) \]  

(2.87)

\[ h_{x,0} = \left( \frac{V_{c,x}}{V_{c,0}} \right) \phi(T_{r,x}, V_{r,x}, \omega_x) \]  

(2.88)

In Eq. 2.87 and Eq. 2.88, \( \theta \) and \( \phi \) are the so-called shape factors, which are functions of
Pitzer’s acentric factor \( \omega_x \) and the reduced temperature and volume. These functions can be
calculated by the following correlations

\[ \theta(T_{r,x}, V_{r,x}, \omega_x) = 1 + (\omega_x - \omega_0) F(T_{r,x}, V_{r,x}) \]  

(2.89)

\[ \phi(T_{r,x}, V_{r,x}, \omega_x) = [1 + (\omega_x - \omega_0) G(T_{r,x}, V_{r,x})] Z_{c,0} / Z_{c,x} \]  

(2.90)

where \( Z \) is the compressibility factor.
The extended corresponding states theory will be utilized with appropriate mixing rules to estimate the transport properties of mixtures.

### 2.5.2 Mixing Rules for Mixtures

In order to apply the corresponding states theory to a mixture, the variables of that mixture have to be calculated from the corresponding parameters of its components using appropriate mixing rules.

Typically, the mixing rule expresses a mixture parameter $Q_m$ in terms of composition and pure component parameters according to

\[
Q_m = \sum_i \sum_j x_i x_j Q_j
\]

(2.95)

The coefficients in Eq. 2.91 and Eq. 2.92 are listed in Table 2.3 (Ely and Hanly, 1981)

Table 2.3: Coefficients for Shape Factor Correlations

<table>
<thead>
<tr>
<th>Coefficients in Eq. 2.91</th>
<th>Coefficients in Eq. 2.92</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_1=0.090569$</td>
<td>$a_2=0.394901$</td>
</tr>
<tr>
<td>$b_1=-0.862762$</td>
<td>$b_2=-1.023545$</td>
</tr>
<tr>
<td>$c_1=0.316636$</td>
<td>$c_2=-0.932813$</td>
</tr>
<tr>
<td>$d_1=-0.465684$</td>
<td>$d_2=-0.754639$</td>
</tr>
</tbody>
</table>
where $x_i$ and $x_j$ are the molar fractions of compounds $i$ and $j$, respectively. The interaction term $Q_{ij}$ is calculated from composition properties $Q_i$ and $Q_j$ based on a combining rule. The simplest combining rule is either arithmetic average or geometric mean, in which the double summation in Eq. 2.95 is reduced

$$Q_{ij} = \frac{Q_i + Q_j}{2} \quad \text{and} \quad Q_m = \sum_i x_i Q_i \quad (2.96)$$

$$Q_{ij} = (Q_i Q_j)^{1/2} \quad \text{and} \quad Q_m = (\sum_i x_i Q_i^{1/2})^2 \quad (2.97)$$

To improve performance, it is customary to included a binary interaction parameters $k_{ij}$ into the expressions for $Q_{ij}$. One possibility could be

$$Q_{ij} = \frac{k_{ij}(Q_i + Q_j)}{2} \quad (2.98)$$

The value of $k_{ij}$ is unity, and values of $k_{ij}$ for all possible binary pairs should be determined by regressing experimental data. The partial molar properties are very sensitive to the values of $k_{ij}$ (Reid et al., 1986).

The theory of mixing rules is discussed elsewhere (Reid et al., 1986) and will not be treated deeply here. The following mixing rules are defined for calculating transport properties (Ely and Hanly, 1981)

$$h_{x,0} = \sum_i \sum_j x_i x_j h_{ij,0} \quad (2.99)$$

$$f_{x,0} = h_{x,0}^{-1} \sum_i \sum_j x_i x_j f_{ij,0} h_{ij,0} \quad (2.100)$$

The molecular weight of the mixture can be found by Eq. 2.101

$$Mw_x^{1/2} = h_{x,0}^{-4/3} f_{x,0}^{-1/2} \sum_i \sum_j x_i x_j h_{ij,0}^{4/3} f_{ij,0}^{1/2} Mw_{ij,0}^{1/2} \quad (2.101)$$
where the indexes, i and j, represent the species components in the mixture. The following combining rules are chosen

\[
 f_{ij,0} = \left( f_{i,0} f_{j,0} \right)^{1/2} (1 - \kappa_{ij}) \\
 h_{ij,0} = \frac{1}{8} \left( h_{i,0}^{1/3} + h_{j,0}^{1/3} \right)^3 (1 - l_{ij}) \\
 M_{wj} = 2M_{w_i}M_{w_j} / (M_{w_i} + M_{w_j})
\]

(2.102)  (2.103)  (2.104)

where the variables, \( \kappa_{ij} \) and \( l_{ij} \), are the binary interaction parameters with values close to zero, which are set to zero for estimating transport properties.

### 2.5.3 Viscosity of Mixtures

The extended corresponding states one fluid model (Ely and Hanly, 1981) is applied here for estimating the viscosity of a mixture. The basic idea is straightforward. First, it is assumed that the viscosity of a single-phase mixture is equated to that of a hypothetical pure fluid

\[
 \mu_{mix}(T, \rho) = \mu_x(T, \rho)
\]

(2.105)

where the subscripts, mix and x, refer to the mixture and the hypothetical pure fluid, respectively.

The corresponding states theory for transport properties is then used to evaluate the viscosity of the hypothetical pure fluid with respect to a given reference fluid

\[
 \mu_x(T, \rho) = \mu_0(T_0, \rho_0) F_\mu
\]

(2.106)

where the subscript, 0, refers to the reference fluid

\[
 F_\mu = \left( \frac{M_{w_x}}{M_{w_0}} \right)^{1/2} f_{x,0}^{-1/2} h_{x,0}^{-2/3}
\]

(2.107)
The variables, \( f_{X,0}, h_{X,0}, \) and \( Mw_x \) are then evaluated by the extended corresponding states (EXCST) theory and the mixing rules.

Methane is chosen as the reference fluid, because of the existence of its PVT and viscosity data over the entire range of fluid states. The data fitted methane viscosity correlation is

\[
\mu_0(\rho_0, T_0) = \mu_0^{(1)}(T_0) + \mu_0^{(2)}(T_0)\rho_0 + \Delta\mu_0(\rho_0, T_0)X_\mu
\]

(2.108)

where the first two terms represent the dilute gas and first density correction, respectively, while the last term is a remainder which dominates in high-density region. The factor, \( X_\mu \), is a correction of the possible non-correspondence of viscosity. The details about this correlation can be found in the paper of Ely and Hanly (1981).

### 2.5.4 Thermal Conductivity of Mixtures

Estimating the thermal conductivity of a mixture is more complicated, since it is affected by two factors, one arising from the transfer of energy from pure collision or translation effect, \( \lambda' \), and another from the transfer of energy via the internal degree of freedom, \( \lambda'' \) (Ely and Hanly, 1983). The latter term is, in general, independent of density. Therefore, only the collision or translation part is evaluated using the extended corresponding states one fluid model, which takes the same procedure as that for estimating the viscosity of a mixture. First, the thermal conductivity of a mixture is equated to that of a hypothetical pure fluid as

\[
\lambda'_{\text{mix}}(\rho, T) = \lambda'_X(\rho, T)
\]

(2.109)

The corresponding states theory is then applied to calculate the thermal conductivity of the hypothetical pure fluid via

\[
\lambda'_X(T, \rho) = \lambda'_0(T_0, \rho_0)F_{\lambda'}X_\lambda
\]

(2.110)
where \( F_\lambda \) takes the same form as in Eq. 2.107, whose calculation requires the extended corresponding states theory and the mixing rules, and \( X_\lambda \) is the correction term for non-correspondence.

Finally, the thermal conductivity of a mixture can be expressed as

\[
\lambda_{\text{mix}}(\rho, T) = \lambda'_0(\rho_0, T_0)F_\lambda X_\lambda + \lambda''_{\text{mix}}(T)
\]  

(2.111)

In Eq. 2.111 the thermal conductivity of the reference fluid, methane, is evaluated via an empirical correlation. The second term in Eq. 2.111, which is related to internal degree of freedom, can be calculated via the modified Eucken correlation with mixing rules (Ely and Hanly, 1983), which are

\[
\frac{\lambda^*_i M_{\text{wi}}}{\mu^g_i} = 1.32\left(C_{p,i}^g - \frac{5R_u}{2}\right)
\]  

(2.112)

and

\[
\lambda^*_{\text{mix}}(T) = \sum_i \sum_j x_i x_j \lambda^*_ij
\]  

(2.113)

\[
(\lambda^*_ij)^{-1} = 2[(\lambda^*_i)^{-1} + (\lambda^*_j)^{-1}]
\]  

(2.114)

where the indexes, \( i \) and \( j \), refer to the components in the mixture, \( \mu^g_i \) is the dilute gas viscosity of component \( i \), \( C_{p,i}^g \) is the ideal gas heat capacity of component \( i \), and \( R_u \) is the universal gas constant.

### 2.5.5 Binary Mass Diffusivity

Evaluation Binary mass diffusivity presents more of a challenge than viscosity and thermal conductivity because of the following two reasons. 1. There are only limited
experimental data existent for binary mass diffusivity at high pressures, which results in few estimation methods.  2. There is no satisfactory liquid state theory available for calculating binary mass diffusivity in the liquid phase.

In this work, the binary mass diffusivity in gaseous phase at low pressure is evaluated using empirical correlation of Fuller et al., which is recommended by Reid et al. (1986). It takes the following form

$$D_{ij} = \frac{0.001437^{1.75}}{pM_{ij}^{1/2}[(\Sigma_{v})_{i}^{1/3} + (\Sigma_{v})_{j}^{1/3}]^2}$$  \hspace{1cm} (2.115)

where $D_{ij}$ is binary mass diffusivity, cm$^2$/s

T is temperature, K

p is pressure, bar

$M_{ij}$ is the combined molecular weight, as expressed in Eq. 2.104

and $\Sigma_{v}$ is found for each component by summing atomic diffusion volumes, which is tabulated in Reid et al. (1986, Table 11-1).

High-pressure effect on binary mass diffusivity is evaluated by the method proposed by Takahashi (1974), which is based on a simple corresponding state method

$$\frac{D_{ij}P}{(D_{ij}p)^+} = f(T_r, P_r)$$  \hspace{1cm} (2.116)

where the superscript $^+$ indicates the low-pressure values given by Eq. 2.115. The function $f(T_r, P_r)$ represents a scaling factor of pressure based on the reduced temperature and pressure, which is tabulated by Takahashi and also shown in Reid et al. (1986, Fig. 11-3). In order to calculate the reduced parameters, the following combing rules for pseudocritical properties of a mixture are used.
The binary mass diffusivities in liquids are evaluated by the method of Tyn and Calus, as recommended by Reid et al. (1986). For a binary mixture of solute i in solvent j, it is

\[
T_c = x_i T_{c,i} + x_j T_{c,j} \tag{2.117}
\]

\[
p_c = x_i p_{c,i} + x_j p_{c,j} \tag{2.118}
\]

The binary mass diffusivities in liquids are evaluated by the method of Tyn and Calus, as recommended by Reid et al. (1986). For a binary mixture of solute i in solvent j, it is

\[
D_{ij} = 8.93 \times 10^{-8} \left( \frac{V_i}{V_j^2} \right)^{1/6} \left( \frac{P_j}{P_i} \right)^{0.6} \frac{T}{\mu_j} \tag{2.119}
\]

where \( V \) is the molar volume at the normal boiling temperature, cm\(^3\)/mol

T is temperature, K

\( \mu_j \) is the viscosity of solvent, cP

\( P_i \) and \( P_j \) are parachors for the solute and solvent, and the calculation methods are given in Reid et al. (1986).

There is no correlation currently available for estimating the pressure effect on binary mass diffusivity in the liquid phase.
Chapter 3
Numerical Methodology

Analysis of the fluid dynamic and physico-chemical processes described in Chapter 1 poses a variety of numerical challenges. This chapter outlines the inherent difficulties and the numerical framework selected to handle these problems. The basic algorithm treats three-dimensional flowfield in a time-accurate manner using a unified treatment of general fluid thermodynamics with preconditioned, density-based, finite-volume approach and dual-time stepping integration. A multiblock domain decomposition technique, along with static load balance, is used to facilitate the application of efficient parallel computation with message passing interfaces (MPI) at the domain boundaries.

3.1 Basic Approach

Present analysis of high-pressure real-fluid mixing and combustion dynamics bears two severe numerical challenges. First, thermodynamic non-idealities and transport anomalies take place as the fluid transits through the transcritical regime. 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 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.

The application of time derivative preconditioning techniques (Turkel, 1992; Shuen et al., 1993; Choi and Merkel, 1993; Hsieh and Yang, 1997) coupled with recently developed
methodologies for handling general fluid thermodynamics (Meng and Yang, 2003) has largely negated the difficulties outlined above. The current work employs these methodologies, takes full account of thermodynamic nonidealities and transport anomalies in the whole fluid state of concern and accommodates any arbitrary equation of state. The unified treatment of general fluid thermodynamics based on the partial mass and partial density properties is employed coupling the preconditioning techniques developed by Hsieh and Yang (1997). Temporal discretization is obtained using a second-order accurate dual-time stepping integration. Spatial discretization employs the fourth-order accurate flux differencing methodologies developed by Rai and Chakravarthy (1994). A fourth-order scalar 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 the 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.

### 3.2 Three-Dimensional Cartesian System

The three-dimensional, unsteady, density-weighted, filtered forms of the compressible Navier-Stokes equations (without body forces) and species conservation equation can be expressed as

\[
\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial (\mathbf{E} - \mathbf{F}_v)}{\partial x} + \frac{\partial (\mathbf{F} - \mathbf{F}_v)}{\partial y} + \frac{\partial (\mathbf{G} - \mathbf{G}_v)}{\partial z} = \mathbf{H}
\]  

(3.1)

where the vectors \( \mathbf{Q}, \mathbf{E}, \mathbf{F}, \mathbf{G}, \mathbf{E}_v, \mathbf{F}_v, \mathbf{G}_v \) and \( \mathbf{H} \) are defined as
Each nomenclature is defined beforehand and the superscript $T$ stands for the transpose of the vector.

3.3 A Unified Preconditioning Scheme for General Fluid Mixtures

It is well known that time-marching algorithms are efficient for solving the transonic, supersonic, and hypersonic compressible flow problems. However, they encounter convergence difficulties for the low-Mach number flows due to the pressure singularities in the momentum equation and the system stiffness arising from the ill-conditioned eigenvalues.
To circumvent the pressure singularity problem, the static pressure is decomposed into a constant reference pressure, $\bar{p}_0$, and a gauge pressure, $\bar{p}_g$ (Choi and Merkel, 1993; Shuen et al., 1993)

$$\bar{p} = \bar{p}_0 + \bar{p}_g \quad \text{(3.10)}$$

To maximize the benefit of this method, $\bar{p}_0$ should be taken to comprise the majority of $\bar{p}$. Physically, the gauge pressure $\bar{p}_g$ amounts to the dynamic pressure responsible for the velocity-pressure coupling in the momentum equation, and is that part of pressure driving the flow motions. With this decomposition, the static pressure, $\bar{p}$, inside the momentum equation is replaced by the gauge pressure, $\bar{p}_g$.

To solve the system eigenvalue disparities and implement the dual-time stepping procedure, pseudo-time derivatives are added to Eq. 3.1 yielding an equation of the form as

$$\Gamma \frac{\partial Z}{\partial \tau} + \frac{\partial Q}{\partial t} + \frac{\partial(E - E_v)}{\partial x} + \frac{\partial(F - F_y)}{\partial y} + \frac{\partial(G - G_y)}{\partial z} = H \quad \text{(3.11)}$$

Here $\Gamma$ represents the preconditioning matrix and $\tau$ the pseudo-time variable. By judicious selection of the primitive variable $Z$ and the preconditioning methodology, convergence in pseudo-time can be optimized for a wide variety of conditions to any desired level of temporal accuracy.

Selection of the primitive variables and the preconditioning matrix is dependent upon two criteria: 1) the eigenvalues must be well conditioned, real, and maintaining their directional characteristics; and 2) diffusion processes must not be reversed. Based on these criteria, the primitive variable vector is defined as

$$Z = (\bar{p}_g, \bar{u}, \bar{v}, \bar{w}, \bar{T}, \bar{Y}_1, \cdots, \bar{Y}_{N-1}) \quad \text{(3.12)}$$
The choice of pressure $\bar{p}$ as one of the primitive variables is crucial for two reasons. It singles out the propagation of acoustic waves in the pseudo-time and facilitates the elimination of the pressure singularity problem. The velocity components $\bar{u}$, $\bar{v}$, and $\bar{w}$ are also logical choices since these quantities appear in the diffusion operators. Similarly, the temperature $\bar{T}$ and species $\bar{Y}_1, \ldots, \bar{Y}_{N-1}$ have been selected because they also appear in the diffusion operators. The choice of temperature is primarily a matter of convenience. Using this term greatly simplifies the computation of Jacobian matrices and eliminates the need to iteratively solve for temperature as a function of enthalpy.

The preconditioning Jacobian matrix defined in the subsequent sections is derived based on fundamental thermodynamic theories, which is valid over the entire fluid state of concern and can accommodate any arbitrary equation of state. The key thermodynamic relations associated with this approach are list in the next sub-section.

### 3.3.1 Important Thermodynamic Relationships

All the relationships required in the numerical algorithm, including Jacobian matrices and fluid properties, are derived using fundamental thermodynamic theories, which can be calculated based on any equation of state. The partial mass and partial density properties of a real fluid mixture, as defined in Chapter 2, are utilized in the derivations.

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

$$p = p(T, \rho)$$  \hspace{1cm} (3.13)
where \( i = 1, \cdots, N \).

Only the differential form is interested, then it can be expressed as

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

Rearrange it, we have the Eq. 3.15

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

Since \( \rho_i = \rho Y_i \)

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

Substituting Eq. 3.16 into Eq. 3.15 leads to following expression

\[
dp = A_T dT + A_Y dY_i + A_\rho d\rho
\]

where

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

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

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

A very useful formulation can be derived from Eq. 3.17, which is

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

Next, a thermodynamic relationship correlating internal energy as a function of pressure, density, and mass fractions is derived. We begin with the following one
\[ \rho e = \rho e(T, \rho_i) \] (3.22)

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

\[ d\rho e = \rho \left( \frac{\partial \rho e}{\partial T} \right)_{\rho_i} dT + \sum_{i=1}^{N} \left( \frac{\partial \rho e}{\partial \rho_i} \right)_{T, \rho_j \neq i} d\rho_i \] (3.23)

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

\[ e_i = \left( \frac{\partial \rho e}{\partial \rho_i} \right)_{T, \rho_j \neq i} \] (3.24)

which is the partial density internal energy of species \( i \) in the mixture. The first derivative in Eq. 3.23 is the constant volume heat capacity \( C_V \). Substituting the partial density internal energy of each species into Eq. 3.23 leads to the following expression

\[ d\rho e = \rho C_V dT + \sum_{i=1}^{N} e_i d\rho_i \] (3.25)

Inserting Eq. 3.16 into Eq. 3.25

\[ d\rho e = \rho C_V dT + \sum_{i=1}^{N} \bar{e}_i \rho dY_i + \sum_{i=1}^{N} \bar{e}_i Y_i d\rho \] (3.26)

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

\[ de = C_V dT + \sum_{i=1}^{N-1} (e_i - \bar{e}) dY_i + \frac{1}{\rho} \left( \sum_{i=1}^{N} Y_i \bar{e}_i - e \right) d\rho \] (3.27)

Substituting Eq. 3.26 into Eq. 3.27, we can establish Eq. 3.28

\[ de = B_v dT + B_p d\rho + \sum_{i=1}^{N-1} B_i dY_i \] (3.28)

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

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

(3.29)

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

(3.30)

\[ B_{Y_i} = \left( \hat{e}_i - \hat{e}_N - \sum_{i=1}^{N} Y_i \hat{e}_i - e \right) \left( \frac{\partial \rho}{\partial \rho_i} \right)_{T, \rho_{i, m}} \left( \frac{\partial p}{\partial \rho_i} \right)_{T, \rho_{m, n}} \]

(3.31)

Substituting Eq. 3.28 into Eq. 3.32, the following expression is derived after some straightforward manipulations

\[ dh = de + \frac{1}{\rho} dp - \frac{p}{\rho^2} d\rho \]

(3.32)

Finally a relationship regarding the speed of sound in the mixture is derived. According to the definition of the speed of sound in thermodynamics, we recognize that the coefficient \( D_T \) equals to the constant pressure heat capacity \( C_p \) of a fluid mixture,

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

(3.37)

According to the definition in thermodynamics, we recognize that the coefficient \( D_Y \) equals to the constant pressure heat capacity \( C_p \) of a fluid mixture,
Based on the Eq. 3.17, the following expression is obtained in a straightforward manner.

\[
\left( \frac{\partial p}{\partial \rho} \right)_{s,Y_i} = \left( \frac{\partial p}{\partial T} \right)_{\rho_i} \left( \frac{\partial T}{\partial \rho} \right)_{s,Y_i} + \left( \frac{\partial p}{\partial \rho} \right)_{T,Y_i}
\]  

(3.39)

In thermodynamics, the following relationship exists

\[
s = s(T, \rho, Y_i)
\]

(3.40)

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

After utilizing some fundamental thermodynamic relationships, the following differential form of Eq. 3.40 can be obtained

\[
ds = \frac{C_v}{T} \, dT - \frac{1}{\rho^2} \left( \frac{\partial p}{\partial T} \right)_{\rho_i} \, d\rho + \sum_{i=1}^{N-1} \left( \frac{\partial s}{\partial Y_i} \right)_{T,\rho,Y_{j\neq i}} \, dY_i
\]

(3.41)

Based on Eq. 3.41, the following expression is further derived

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

(3.42)

Substituting Eq. 3.42 into Eq. 3.39, an expression of the speed of sound in the general fluid mixture is established as

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

(3.43)

Equations 3.17, 3.28, 3.33, and Eq. 3.43 are the important thermodynamic relationships required in the numerical derivations below.
3.3.2 Preconditioning Matrix

With those fundamental thermodynamic relations, the transformation matrix \( T = \frac{\partial Q}{\partial Z} \),

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

are well defined and listed in Appendix D. Each element of the first column of the matrix \( T \) has a common term \( \left( \frac{\partial \rho}{\partial \rho} \right)_{T,Y} \), which can be expressed as

\[
\left( \frac{\partial \rho}{\partial \rho} \right)_{T,Y} = \frac{C_p}{C_v} \left( \frac{\partial p}{\partial \rho} \right)_{T,Y} = \frac{\gamma}{a^2}
\]  

(3.44)

The preconditioning matrix is established after replacing the speed of sound in this term by a scaling factor \( \beta \).

\[
\Gamma = \begin{pmatrix}
\frac{\gamma}{\beta} & 0 & 0 & \cdots & 0 & -\frac{A_{y_1}}{A_p} & -\frac{A_{y_2}}{A_p} & \cdots & -\frac{A_{y_n}}{A_p} \\
\frac{\gamma \tilde{u}}{\beta} & \tilde{\rho} & 0 & \cdots & 0 & -\frac{A_{y_1} \tilde{u}}{A_p} & -\frac{A_{y_2} \tilde{u}}{A_p} & \cdots & -\frac{A_{y_n} \tilde{u}}{A_p} \\
\frac{\gamma \tilde{v}}{\beta} & 0 & \tilde{\rho} & \cdots & 0 & -\frac{A_{y_1} \tilde{v}}{A_p} & -\frac{A_{y_2} \tilde{v}}{A_p} & \cdots & -\frac{A_{y_n} \tilde{v}}{A_p} \\
\frac{\gamma \tilde{w}}{\beta} & 0 & 0 & \cdots & \tilde{\rho} & -\frac{A_{y_1} \tilde{w}}{A_p} & -\frac{A_{y_2} \tilde{w}}{A_p} & \cdots & -\frac{A_{y_n} \tilde{w}}{A_p} \\
\frac{\gamma \hat{h}}{\beta} + \left( \sum_{i=1}^{N} \gamma \dot{e}_i - e \frac{\rho}{\rho} \frac{\partial \rho}{\partial \rho} \right)_{T,Y} & \tilde{p} \tilde{\rho} & \tilde{p} \tilde{\rho} & \tilde{p} \tilde{\rho} & \tilde{p} \tilde{\rho} & \tilde{p} \tilde{\rho} & \tilde{p} \tilde{\rho} & \tilde{p} \tilde{\rho} & \tilde{p} \tilde{\rho} & \cdots & -\frac{A_{e_i} \dot{e}_i}{A_p}
\end{pmatrix}
\]  

(3.45)

where \( A_T, A_p, A_{y_i}, B_T, B_{y_i} \) are defined in the previous subsection. The scaling factor \( \beta \) takes the form

\[
\beta = \frac{\gamma e a^2}{1 + (\gamma - 1) e}
\]  

(3.46)
Here $\epsilon$ ($0 < \epsilon \leq 1$) is the preconditioning factor, which is proportional to the square of the local Mach number, $M^2$, and gives good control of both the convection and diffusion time scales. In contrast to the form $\Gamma$ defined by other researchers, all of the off-diagonal terms in Eq. 3.45 have been retained. By keeping these terms, the unaltered system is identically restored as $\epsilon \to 1$:

$$\lim_{\epsilon \to 1} \Gamma = T \quad (3.47)$$

The criteria employed to select optimal values for $\epsilon$ are present in the next subsection.

The system eigenvalues associated with the pseudo-time domain are obtained by taking the determinant of the matrices $\Gamma^{-1}A$, $\Gamma^{-1}B$, $\Gamma^{-1}C$. The calculation is straightforward, and the eigenvalues are

$$\lambda = \text{diag}(\lambda_1, \lambda_2, \tilde{u}, \tilde{u}, \tilde{u}, \cdots) \quad (3.48)$$

where $\lambda_1$ and $\lambda_2$ represent the rescaled acoustic eigenvalues. These terms are given by

$$\lambda_1 = \frac{1}{2} \left[ U(\epsilon + 1) + \sqrt{U^2(1-\epsilon)^2 + 4\epsilon a^2} \right]$$

$$\lambda_2 = \frac{1}{2} \left[ U(\epsilon + 1) - \sqrt{U^2(1-\epsilon)^2 + 4\epsilon a^2} \right] \quad (3.49)$$

$U$ represents $\tilde{u}$, $\tilde{v}$, and $\tilde{w}$ in x-, y- and z-direction respectively. As $\epsilon \to 1$, Eq. 3.49 approaches the values given by the non-preconditioned system. Obviously, all of the eigenvalues are in the same order of magnitude, which proves that the choice of preconditioning matrix $\Gamma$ and primitive variable vector is appropriate. Furthermore, since all the numerical Jacobians are calculated based on the fundamental thermodynamics theories, those results are independent of equation of state and can be apply to any fluid state of concern without empiricism.
3.3.3 Convergence Optimization

Associated with each finite-volume cell are various fundamental time scales which characterize propagation rates of competing convective and diffusive processes in each of the coordinate directions. The convective propagation rates are characterized by the Courant-Friedrichs-Lewy (CFL) numbers

\[
CFL_x = \frac{\rho(\lambda_x)\Delta \tau}{\Delta x}, \quad CFL_y = \frac{\rho(\lambda_y)\Delta \tau}{\Delta y}, \quad CFL_z = \frac{\rho(\lambda_z)\Delta \tau}{\Delta z}
\]  

(3.50)

where \( \rho(\lambda_x), \rho(\lambda_y), \rho(\lambda_z) \) are the spectral radii associated with

\[
\rho(\lambda_x) = \frac{1}{2} \left[ |u| (1 + \varepsilon) + \sqrt{u^2 (1 - \varepsilon)^2 + 4\varepsilon a^2} \right]
\]

\[
\rho(\lambda_y) = \frac{1}{2} \left[ |v| (1 + \varepsilon) + \sqrt{v^2 (1 - \varepsilon)^2 + 4\varepsilon a^2} \right] \quad (3.51)
\]

\[
\rho(\lambda_z) = \frac{1}{2} \left[ |w| (1 + \varepsilon) + \sqrt{w^2 (1 - \varepsilon)^2 + 4\varepsilon a^2} \right]
\]

The diffusive propagation rates are characterized by the von Neumann numbers

\[
VNN_x = \frac{\nu\Delta \tau}{\Delta x^2}, \quad VNN_y = \frac{\nu\Delta \tau}{\Delta y^2}, \quad VNN_z = \frac{\nu\Delta \tau}{\Delta z^2}
\]  

(3.52)

Buelow et al. (1994, 1995) have shown that the maximum CFL number associated with a given cell scales with the grid aspect ratio, whereas the minimum CFL number remains fixed. When source and sink terms are not present, optimum pseudo-time step corresponds to the minimum CFL number. This criteria is enforced in a three-dimensional domain by selecting

\[
\Delta \tau = \max \left( \frac{CFL \Delta x}{\rho(\lambda_x)}, \frac{CFL \Delta y}{\rho(\lambda_y)}, \frac{CFL \Delta z}{\rho(\lambda_z)} \right)
\]  

(3.53)

The time step definition given by this equation incorporates the preconditioning factor as a function of the spectral radii given by Eq. 3.49.
The optimal value of the preconditioning factor is dependent upon the local Mach number and the cell Reynolds numbers

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

(3.54)

the cell Prandtl number \( \text{Pr} = \nu / \alpha \), the cell Schmidt number \( \text{Sc}_j = \nu / D_{\text{in}} \ (i = 1, \cdots, N) \), and

the physical time step employed in the calculation procedure. If the respective quantities \( \text{Re} \), \( \text{RePr} \), \( \text{ReSc} \) exceed a value of unity in either of the coordinate direction, convective effects dominant and the conservation equations exhibit a hyperbolic character. For this situation an inviscid criterion must be employed. If \( \text{Re} \), \( \text{RePr} \), and \( \text{ReSc} \) 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 when employing the dual-time stepping methodology is the effect of the physical time derivatives on the pseudo-time system. The first term in Eq. 3.11 behaves as a sink in the pseudo-time system with a magnitude that is directly proportional to the pseudo-time step and inversely proportional to the physical time step. It is well known that such terms promote favorable damping characteristics in time-marching schemes and accelerate convergence. Venkateswaran and Merkel (1995) have shown that a limit exists where preconditioning the pseudo-time derivatives negates the favorable damping characteristics induced by these sink terms.

In the current work, the preconditioning factor is selected using the methodologies developed by Choi and Merkel (1993), Buelow et al.(1995), and Venkateswaran and Merkel (1995). Optimal values are specified locally by the relation

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

(3.55)
The subscripts “inv”, “Δt”, and “vis” refer to the inviscid, unsteady, and viscous preconditioning factors, respectively. The criteria employed to evaluate these terms are given below.

### 3.3.3.1 Inviscid Preconditioning Factor

Choi and Merkel (1993) have demonstrated that an effective convective criterion which insures that acoustics speeds and flow velocities are the same order of magnitude is obtained when $\epsilon$ is assigned a value proportional to the local Mach number. To obtain the correct functional form, it is necessary to examine the characteristic condition number, which is defined as the ratio of the largest to smallest absolute eigenvalue. The optimum condition number is unity.

![Figure 3.1: Contours of the condition number as a function of the Mach number squared and the preconditioning factor.](image-url)
A plot of the condition number associated with Eq. 3.49 is given in Fig. 3.1. Here, \( \log_{10} \) contours are plotted as a function of the Mach number squared and the preconditioning factor \( \epsilon \). In the limit as \( M^2 \to 0 \), a minimum condition number of 2 is obtained, with local minima corresponding to the relation \( \epsilon = 2M^2 \). To achieve the correct limiting behavior at low Mach numbers, the inviscid criteria for the preconditioning factor is specified as

\[
\epsilon_{inv} = \begin{cases} 
\frac{\epsilon^2}{2} & M \leq \epsilon \\
2M^2 & \epsilon < M < 1 \\
1 & M \geq 1
\end{cases}
\] (3.56)

The term \( \epsilon \) is included to avoid singularities in stagnation regions where \( M = 0 \). Typically, \( \epsilon = 10^{-5} \). For infinitely large physical CFL numbers (the steady state limit) and in the absence of strong local diffusion processes, this choice yields minimal disparities in the system eigenvalues and optimal damping rates. The convergence rates are entirely dependent on the magnitude of the pseudo CFL number.

### 3.3.3.2 Unsteady Preconditioning Factor

Venkateswaran and Merkel (1995) have employed von Neumann stability theory to gain insight into the characteristics of the dual-time system and the effects of the physical CFL number on the numerical attributes of the pseudo-time system. Results demonstrate the effects of small physical time steps on the system eigenvalues. In contrast to the steady state limit described above, the limit of infinitely small physical CFL numbers alters the system eigenvalues such that the choice \( \epsilon = 1 \) renders minimal disparities. This effect is caused by the physical time derivatives that appear as sink terms in the pseudo-time equations.
The trends presented by them indicated that the optimal choice for the unsteady preprocessing factor is bounded by the interval \( \epsilon_{\text{inv}} \leq \epsilon_{\Delta t} \leq 1 \) and inversely related to the value of the local physical CFL number. By examining the eigenvalues and making a series of simplifying assumptions, a factor of the form

\[
\epsilon_{\Delta t} = \frac{1}{a^2} \left[ \left( \frac{l_x}{\pi \Delta t} \right) + \left( \frac{l_y}{\pi \Delta t} \right) \right] + M^2
\]

(3.57)

was derived. Here, \( l_x \) and \( l_y \) represent the characteristic dimensions of the computational domain and \( M \) is the Mach number. Equation 3.57 is tuned to damp the low wavenumber modes which are typically the most difficult to treat.

### 3.3.3.3 Viscous Preconditioning Factor

In regions where diffusion processes dominate, the criteria outlined in the last two sections must be modified to account for interactions associated with the parabolic system. 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, Buelow et al. (1994, 1995) have developed a preconditioning factor based on local length scales which is tuned to damp the low wavenumber modes. This definition requires a priori assumption regarding the orientation of dominate convective and diffusion processes within a given grid configuration and the choice for \( \varepsilon_{\text{vis}} \) is somewhat more involved. In three dimensions, there are three possible CFL numbers, and two possible VNN numbers, and six possible values of \( \varepsilon_{\text{vis}} \) exist. 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.

Most grid configurations are stretched such that predominate diffusion processes are resolved in a direction normal to the predominate convective processes. 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 definition given by Eq. 3.53, this quantity must be optimized with respect to the minimum CFL number. In three-dimensional this achieved by: 1) equating Eq. 3.50 with Eq. 3.52, respectively; 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

\[
\varepsilon_{\text{vis}} = \left[ \frac{\bar{u}^2 \delta_x (\delta_x - 1)}{\bar{u}^2 \delta_x^2 + a^2}, \frac{\bar{v}^2 \delta_y (\delta_y - 1)}{\bar{v}^2 \delta_y^2 + a^2}, \frac{\bar{w}^2 \delta_z (\delta_z - 1)}{\bar{w}^2 \delta_z^2 + a^2} \right]
\]

where
This equation takes into account the effects of momentum, energy, and mass diffusion processes on the overall convergence rate.

3.4 Spatial Discretization: Finite Volume Approach

3.4.1 Finite Volume Approach

The governing equations are solved numerically by means of a finite-volume approach. This method allows for the treatment of arbitrary geometry. To utilize the finite-volume approach, the governing equation is integrated over the control volume $V$ enclosed by the surface $S$ in the physical domain as

$$\iiint_V \left( \Gamma \frac{\partial Z}{\partial \tau} + \frac{\partial Q}{\partial t} + \frac{\partial (E - E_v)}{\partial x} + \frac{\partial (F - F_v)}{\partial y} + \frac{\partial (G - G_v)}{\partial z} - H \right) dV = 0 \quad (3.60)$$

Using the Gauss divergence theorem, the integral conservation equation takes the following form for the three-dimensional cell with six surfaces, as shown in Fig. 3.2.

$$\iiint_V (\Gamma \frac{\partial Z}{\partial \tau} + \frac{\partial Q}{\partial t}) dV + \int_{S_y} \vec{W} \bullet \vec{n}_y dS_y + \int_{S_z} \vec{W} \bullet \vec{n}_z dS_z + \int_{S_y} \vec{W} \bullet \vec{n}_y dS_y + \int_{S_z} \vec{W} \bullet \vec{n}_z dS_z = \iiint_V H dV \quad (3.61)$$
where

\[ \vec{\tilde{W}} = (\vec{E} - \vec{E}_v)\hat{i} + (\vec{F} - \vec{F}_v)\hat{j} + (\vec{G} - \vec{G}_v)\hat{k} \] (3.62)

and \( \vec{n}_\xi, \vec{n}_\eta, \) and \( \vec{n}_\zeta \) are unit normal vectors to the surface in the \( \xi-, \eta-, \) and \( \zeta-\)directions, respectively. The unit normal vectors are related to cell surface area \( S_\xi, S_\eta, \) and \( S_\zeta \) as

\[ \vec{n}_\xi = \left( S_{\xi x} \hat{i} + S_{\xi y} \hat{j} + S_{\xi z} \hat{k} \right) \left| \vec{n}_\xi \right| \]  

\[ \vec{n}_\eta = \left( S_{\eta x} \hat{i} + S_{\eta y} \hat{j} + S_{\eta z} \hat{k} \right) \left| \vec{n}_\eta \right| \] (3.63)

\[ \vec{n}_\zeta = \left( S_{\zeta x} \hat{i} + S_{\zeta y} \hat{j} + S_{\zeta z} \hat{k} \right) \left| \vec{n}_\zeta \right| \]

The cell surface areas are defined as
The magnitude of each surface vector can be obtained by

\[ \vec{S}_\xi = \frac{1}{2} (\vec{r}_{72} \times \vec{r}_{56}) = \frac{1}{2} \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ x_2 - x_7 & y_2 - y_7 & z_2 - z_7 \\ x_6 - x_3 & y_6 - y_3 & z_6 - z_3 \end{vmatrix} = S_{\xi x} \vec{i} + S_{\xi y} \vec{j} + S_{\xi z} \vec{k} \]

\[ \vec{S}_\eta = \frac{1}{2} (\vec{r}_{86} \times \vec{r}_{75}) = \frac{1}{2} \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ x_6 - x_8 & y_6 - y_8 & z_6 - z_8 \\ x_5 - x_7 & y_5 - y_7 & z_5 - z_7 \end{vmatrix} = S_{\eta x} \vec{i} + S_{\eta y} \vec{j} + S_{\eta z} \vec{k} \quad (3.64) \]

\[ \vec{S}_\zeta = \frac{1}{2} (\vec{r}_{74} \times \vec{r}_{83}) = \frac{1}{2} \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ x_4 - x_7 & y_4 - y_7 & z_4 - z_7 \\ x_3 - x_8 & y_3 - y_8 & z_3 - z_8 \end{vmatrix} = S_{\zeta x} \vec{i} + S_{\zeta y} \vec{j} + S_{\zeta z} \vec{k} \]

The magnitude of each surface vector can be obtained by

\[ |\vec{S}_\xi| = \left( S_{\xi x}^2 + S_{\xi y}^2 + S_{\xi z}^2 \right)^{1/2} \]

\[ |\vec{S}_\eta| = \left( S_{\eta x}^2 + S_{\eta y}^2 + S_{\eta z}^2 \right)^{1/2} \]

\[ |\vec{S}_\zeta| = \left( S_{\zeta x}^2 + S_{\zeta y}^2 + S_{\zeta z}^2 \right)^{1/2} \quad (3.65) \]

The cell volume \( \Delta V \) associated with each cell can be evaluated using Kordulla and Vinokur (1983) formula

\[ \Delta V = \frac{1}{2} \vec{r}_{11} \cdot \left( \vec{S}_\xi + \vec{S}_\eta + \vec{S}_\zeta \right) \quad (3.66) \]

We also define cell surface areas per cell volume as

\[ \tilde{S}_\xi = \frac{\vec{S}_\xi}{\Delta V} , \quad \tilde{S}_\eta = \frac{\vec{S}_\eta}{\Delta V} , \quad \tilde{S}_\zeta = \frac{\vec{S}_\zeta}{\Delta V} \]

Assuming the increments \( \Delta \xi = \Delta \eta = \Delta \zeta = 1 \) in the body-fitted coordinate system and substituting Eq. 3.62 and Eq. 3.63 into Eq. 3.61 yields the following governing equation in the general coordinates
where the vectors $E_{\xi}, F_{\eta}, G_{\zeta}, E_{\bar{\xi}}, F_{\bar{\eta}}, G_{\bar{\zeta}}$ are defined as

$$E_{\xi} = \left(\tilde{S}_{\xi x} E + \tilde{S}_{\xi y} F + \tilde{S}_{\xi z} G\right) \quad E_{\bar{\xi}} = \left(\tilde{S}_{\bar{\xi} x} E_{\bar{\xi}} + \tilde{S}_{\bar{\xi} y} F_{\bar{\xi}} + \tilde{S}_{\bar{\xi} z} G_{\bar{\xi}}\right)$$

$$F_{\eta} = \left(\tilde{S}_{\eta x} E + \tilde{S}_{\eta y} F + \tilde{S}_{\eta z} G\right) \quad F_{\bar{\eta}} = \left(\tilde{S}_{\bar{\eta} x} E_{\bar{\eta}} + \tilde{S}_{\bar{\eta} y} F_{\bar{\eta}} + \tilde{S}_{\bar{\eta} z} G_{\bar{\eta}}\right)$$

$$G_{\zeta} = \left(\tilde{S}_{\zeta x} E + \tilde{S}_{\zeta y} F + \tilde{S}_{\zeta z} G\right) \quad G_{\bar{\zeta}} = \left(\tilde{S}_{\bar{\zeta} x} E_{\bar{\zeta}} + \tilde{S}_{\bar{\zeta} y} F_{\bar{\zeta}} + \tilde{S}_{\bar{\zeta} z} G_{\bar{\zeta}}\right)$$

The quantities $E_{\xi, j=1/2, j, k}, E_{\bar{\xi} v, j=1/2, j, k}, F_{\eta, j=1/2, j, k}, F_{\bar{\eta} v, j=1/2, j, k}, G_{\zeta, j=1/2, j, k}, G_{\bar{\zeta} v, j=1/2, j, k}$ and $G_{\bar{\zeta} v, i, j, k=1/2}$ represent the numerical fluxes associated with each cell interface (as shown in Fig. 3.2). $\tilde{S}$ 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

$$\Delta \tau = \frac{\Delta \tau_{\xi} \Delta \tau_{\eta} \Delta \tau_{\zeta}}{\Delta \tau_{\xi} + \Delta \tau_{\eta} + \Delta \tau_{\zeta}}$$

where

$$\Delta \tau_{\xi} = \frac{CFL \cdot \Delta V}{\rho(\lambda_x) S_{\xi x} + \rho(\lambda_y) S_{\xi y} + \rho(\lambda_z) S_{\xi z}} / \tilde{S}_{\xi}$$

$$\Delta \tau_{\eta} = \frac{CFL \cdot \Delta V}{\rho(\lambda_x) S_{\eta x} + \rho(\lambda_y) S_{\eta y} + \rho(\lambda_z) S_{\eta z}} / \tilde{S}_{\eta}$$

$$\Delta \tau_{\zeta} = \frac{CFL \cdot \Delta V}{\rho(\lambda_x) S_{\zeta x} + \rho(\lambda_y) S_{\zeta y} + \rho(\lambda_z) S_{\zeta z}} / \tilde{S}_{\zeta}$$
3.4.2 Evaluation of Inviscid Fluxes

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

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

(3.70)

where the left and right stencils are used to give the desired accuracy. The above equation corresponds to the stencil illustrated in Fig. 3.3

![Schematic diagram of the stencil](image)

Figure 3.3: Schematic diagram of the stencil used in evaluating inviscid flux terms in the $x - y$ plane.

. 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. In the present work, the methodology proposed by Rai and Chakravarthy (1994) is used. Accordingly the numerical flux in Eq. 3.67 is computed as
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. 3.70 regarding the desired accuracy, the left and right state terms in Eq. 3.71 must be computed using the same or higher order accuracy. These terms are written as follows to facilitate easy switching and make the scheme TVD (total-variation-diminishing).

\[
\hat{E}_{j+1/2,j,k} = \hat{E}_{j+1/2,j,k} - \phi^{(4)}_{j+1/2,j,k} \left( \frac{\hat{E}_{j+3/2,j,k} - 2\hat{E}_{j+1/2,j,k} + \hat{E}_{j-1/2,j,k}}{24} \right) \tag{3.71}
\]

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 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.
3.4.3 Evaluation of Viscous and SGS Fluxes

A three-dimensional auxiliary cell is shown schematically by the dash-dotted lines in Fig. 3.4. 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

\[
\nabla \cdot \vec{f} = \frac{1}{\Delta V} \int_S \vec{f} \cdot \vec{n} dS \quad (3.75)
\]

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

\[
\left( \frac{\partial f}{\partial x} \right)_{i+1/2,j,k} = \frac{1}{\Delta V_{i+1/2,j,k}} \left[ f S_{\xi\xi} \bigg|_{i+1/2,j,k} - f S_{\xi\xi} \bigg|_{i,j,k} + f S_{\eta\eta} \bigg|_{i+1/2,j+1/2,k} - f S_{\eta\eta} \bigg|_{i+1/2,j,k+1/2} \right] \quad (3.76)
\]

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

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

$$f_{i+1/2,j+1/2,k} = \frac{1}{4}(f_{i,j,k} + f_{i+1,j,k} + f_{i+1,j+1,k} + f_{i,j+1,k})$$

$$f_{i+1/2,j-1/2,k} = \frac{1}{4}(f_{i,j,k} + f_{i+1,j,k} + f_{i+1,j-1,k} + f_{i,j-1,k})$$

The evaluation of SGS fluxes follows a similar procedure as for the viscous and diffusive fluxes.

### 3.4.4 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 to prevent oscillations near shock waves and in 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

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

(3.80)

where

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

(3.81)

where \( \varepsilon_2, \varepsilon_4, \varepsilon_6 \) 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. Also, the standard model has difficulties in hypersonic flow and density stratified supercritical fluid 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

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

(3.82)

The modified eigenvalues are given as

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

(3.83)

where \( \rho(\lambda) \) is the spectral radius of the flux Jacobian matrix \( \Gamma^{-1} A \).
The second-difference dissipation term given in Eq. 3.82 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.

### 3.5 Temporal Discretization

The physical time derivatives in Eq. 3.67 are evaluated by general backward differencing

$$\frac{\partial Q}{\partial t} = \frac{1}{\Delta t} [a_i Q^{n+1} - \phi(Q^n, Q^{n-1}, \cdots)] \quad (3.88)$$
The coefficient $a_i$ and function $\phi$ in Eq. 3.88 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

$$a_i = \frac{1}{2}, \quad \phi = \frac{1}{2}(4Q^n - Q^{n-1}) \quad (3.89)$$

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

$$Q^{m+1} = Q^n + T\Delta Z^{m+1} \quad (3.90)$$

Substituting Eq. 3.88 and Eq. 3.90 into Eq. 3.67 yields the following discretized system

$$\left\{ \Gamma + \frac{\Delta \tau}{\Delta t} T \right\} \Delta Z + \left( E_{\xi} - E_{\xi v} \right)_{i+1/2,j,k}^{m+1/2,j,k} + \left( F_{\eta} - F_{\eta m} \right)_{i,j-1/2,k}^{m+1/2,j,k} + \left( G_{\xi} - G_{\xi v} \right)_{i,j,k-1/2}^{i,j,k+1/2} = H^{m+1} - \frac{\Delta \tau}{\Delta t} (a_i Q^n - \phi) \quad (3.91)$$

A fourth-order Runge-Kutta (RK-4) scheme is used to solve the governing equation 3.91 in the pseudo-time space due to its higher temporal accuracy and relatively larger CFL number (i.e., $2\sqrt{2}$ for an Euler calculation using RK-4). A thorough investigation of the stability characteristics of the RK4 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
where

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

Superscripts ‘m’ and ‘m+1’ stand for the solution at the ‘mth’ and ‘m+1th’ 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)

\[ \alpha_1 = \frac{1}{4}, \quad \alpha_2 = \frac{1}{3}, \quad \alpha_3 = \frac{1}{2} \]  

The iterative solution of given governing equation 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.

3.6 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 noncatalytic 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.

3.6.1 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 Method-of-Characteristics (MOC) proposed by Poinsot and Lele (1992). In the absence of a significant diffusion processes, the MOC method provides the 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
All of the terms in Eq. 3.95 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

$$\tilde{\Omega}_{inlet} = \Delta V$$

$$L_{inlet} = \begin{pmatrix} 0 \\ \tilde{u} - \tilde{u}_{ref} \\ \tilde{v} - \tilde{v}_{ref} \\ \tilde{w} - \tilde{w}_{ref} \\ \tilde{T} - \tilde{T}_{ref} \\ \tilde{Y}_1 - \tilde{Y}_{1,ref} \\ \vdots \\ \tilde{Y}_N - \tilde{Y}_{N-1,ref} \end{pmatrix}$$

(3.95)

where $\tilde{u}_{ref}$, $\tilde{v}_{ref}$, $\tilde{w}_{ref}$, $\tilde{T}_{ref}$, $\tilde{Y}_{ref}$, ..., $\tilde{Y}_{N-1,ref}$ 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. (1994).

To simulate the far field boundary the incoming characteristic given by Eq. 3.95 is modified to provide a nonreflecting outflow condition. The equation of interest is given by the selection matrix

\[
L = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
\end{bmatrix}
\]  

Equation (3.97)

Associate with this equation is the term

\[
\Pi = \lambda_2 \left[ \frac{1}{\varepsilon} \frac{u}{a} \frac{\partial p}{\partial x} - \frac{\rho a}{\varepsilon} \frac{\partial u}{\partial x} \right]
\]  

Equation (3.98)

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. 3.49. 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. (1994) have proposed that Eq. 3.98 be replaced with the term

\[
\Pi^k_2 = k(p - p\infty)
\]  

Equation (3.99)
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

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

(3.100)

The factor presented here has been modified from that given by Rudy and Strikwerda (1980) to accommodate the dual-time preconditioned system. Here \( \bar{M}^2 \) 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. (1994) 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. 3.98. These conditions are given by

\[
\tilde{\Omega}_{\text{outlet}} = \Delta V
\]

\[
L_{\text{outlet}} = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 1 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 1 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & 0 & \cdots & 1
\end{pmatrix}
\]  

(3.101)
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.

3.7 Parallel Implementation

3.7.1 Parallel Architecture

Every computer, whether sequential or parallel, operates by executing instructions on data. Depending on whether there is one or several instruction streams and data streams, the computing architecture can be classified into four categories (Flynn, 1972).

1. Single Instruction stream, Single Data stream (SISD)
2. Multiple Instruction streams, Single Data stream (MISD)
3. Single Instruction stream, Multiple Data stream (SIMD)
4. Multiple Instruction stream, Multiple Data stream (MIMD)

SISD computers are the standard sequential computer with single processor. In MISD computers, each processor has its own control unit, but they share a common memory. However, MISD machines are seldom used in practice. For SIMD computers, all processors operate under the control of a single instruction stream. TMC CM-200, MasPar, ICL DAP can be regarded as SIMD machines. However, the most widely used computing architecture is the MIMD system, which is indicated schematically in Fig. 3.5. In this configuration, each processor has its own data set as well as a set of instructions to follow. These processors work independent of each other on these data sets and only communicate at some point during the computation where the data set and the results obtained are shared by two or more processors. MIMD-type computers include IBM SP-2, Cray T3E, CM5 and Beowulf Clustered computers.
For the SIMD or MIMD systems, it is usually necessary to exchange data between processors. This can be done in two ways: 1) shared memory systems, and 2) Distributed memory systems. The shared memory system consists of global address space, which is accessible by all processors and thus memory is shared among these processors. One processor can communicate with other processors by writing into or reading from the global memory. This architecture inherently solves the inter-processor communication problem, but introduces bottleneck problems created from simultaneous access to the memory by more than one processor. In the distributed memory systems, each processor has its own local (or private) memory and the global/shared memory is absent. The processors are connected externally to switches and a network of wires to allow communications among them. The efficiency of these systems is based on the communication time required among these processors, and enjoys several advantages such as hardware compatibility, functionality, and performance. The only drawback of this architecture is the enormous responsibility placed on software programmers. The programmers must provide an efficient scheme to distribute the data and set of instructions, and also explicitly provide the instruction set for communications among the various CPUs. This
requires reconstruction of the numerical algorithm and synchronization of the processors for efficient, parallel computing.

### 3.7.2 Beowulf Cluster Parallel Computers

A Beowulf system is a multi-computer architecture used for parallel computations. In a Beowulf system, one server computer and many other client computers are connected together via high-speed networks. It is a distributed memory, MIMD system built primarily using commodity hardware components, such as any PC capable of running the free operating system Linux, standard Ethernet adapters, and switches. The first Beowulf system was built by Donald and Becker (Sterling et al., 1993) and consisted of 16 486DX4-100MHz machines each with 16 MB of memory. The main advantage of a Beowulf system is its high performance/price ratio in comparison with other dedicated MPP systems. Another important characteristic of the Beowulf clusters is compatibility. Changes of hardware, including the node and network system, will not affect the programming model. A Beowulf system also uses commodity software, such as the Linux operating system, Message Passing Interface (MPI), and other available open-source software.

The work conducted for this study was implemented on an in-house Beowulf system, consisting of 500 Pentium II/III processors, a Giga-Bit switch and 100MB fast Ethernet Cards. The operating system was RedHat Linux. The Message Passing Interface (MPI) involves a library of functions and macros that can be used in C, FORTRAN, and C++ Program were used to exchange the information among processors. More detailed information about this Beowulf system can be found in (Wang, 2002).
3.7.3 Domain Decomposition

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 3.6 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.

3.8 Limitations of the Present Model

The present theoretical formulations are derived based on the full conservation laws and fundamental thermodynamics, which theoretically could be applied to any fluid states of concern without empiricism. However, several limitations are introduced when choosing different methodologies to close the governing system.
3.8.1 Limitations of Equation of State and Thermodynamic Property Evaluation

In order to accurately evaluate thermophysical properties of real-fluid mixture at low-temperature and high-pressure regime, a proper equation of state is indispensable. In balance of computational cost and accuracy, a modified Soave-Redlich-Kwong (SRK) equation of state (Graboski and Daubert, 1978a, 1978b) is employed in the present simulation. The coefficients of this EOS are obtained by fitting the vapor pressure data and thus very suitable for conditions where the reduced temperature is less than one. Compared with the complicated BWR equation of state (Jacobsen and Stewart, 1973), using the modified SRK equation of state results in an approximately 8 percent of density deviation in the present pressure and temperature ranges of concern (Yang, 2000). The relative error association with the SRK equation of state, however, may become significant when chemical reaction is involved and the temperature of product is

Figure 3.6: Schematic of a two-dimensional sub-domain with ghost cells (adopted from Wang, 2002).

Although the thermodynamic properties of the present simulation are evaluated based on the fundamental thermodynamics, deviations between calculated value and the experimental data exist at low-temperature region (i.e. temperature less than 120 K for nitrogen). For instance, a 16 percent deviation of the constant pressure specific heat between the predicted values and the data from NIST chemistry database is observed at 40 atm and 100 K for nitrogen. This deviation increases to 28 percent when temperature further decreases to 80 K. The relative error associated with two dataset can be reduced to approximately 15% when temperature ranges from 80 to 100 K and pressure remains at 40 atm by using the BWR equation of state. The errors associated with thermodynamic property are introduced from two aspects. Firstly, the fundamental thermodynamic theories can only qualitative describe the fluid behavior in high-pressure low temperature regime due to the lack of validation data. Secondly, the SRK equation of state can not very accurately represents the P-V-T behavior of a fluid in liquid phase.

3.8.2 Limitations of Transport Properties Evaluations

Several inherent limitations exist in evaluation the viscous flux and transport properties. Firstly, the second (i.e. bulk) viscosity is neglected in calculating the viscous stress tensor (Eq. 2.5) owing to the lack of reliable data within the range of fluid thermodynamic state of concerns. It is worth noting that the stress terms associated the second viscosity probably become significant for a supercritical fluid in which volume dilation plays an important role in dictating the flow evolution (Meng et al., 2005). This issue remains to be further investigated. Secondly, the non-equilibrium thermodynamic effects from which species concentrations diffuse due to temperature gradients (Soret effect, or “thermal-diffusion”) and thermal energy diffuse due to
concentration gradients (Dufour effect, or “diffusion-thermal”) are not considered in the present simulation because both theory and experimental data related to those effects are insufficient. Thirdly, the extended corresponding states one fluid model (Ely and Hanly, 1981, 1983) is employed here to estimate the molecular viscosity and thermal conductivity of a fluid mixture. This method is mainly developed and validated for hydrocarbon fuels. The method becomes inaccurate when the molar fraction of water is greater than 30%. In addition, the predicted results are not thoroughly validated against the experimental data in regime where fluid temperature exceeds 1000 K. Therefore, this correlation should be used with caution when applied to combustion system where water is the major product and the temperatures of products are always greater than 1000 K.

3.8.3 Limitations of Subgrid-scale Models

The algebraic Smagorinsky model is implemented in the current study. The deficiencies of this model have been discussed in Chapter 2. Besides those disadvantages, there are still many issues need to be further addressed regarding LES of real fluid mixture. Firstly, although the non-equilibrium thermodynamic effects has unnoticeable influence on the large energy containing flow motions (Oefelein, 2004), it could be very important for the energy and species transportations in the subgrid scale level (Miller, 2000). Secondly, the filtered equation of state is only calculated by the resolved variables, whereas the term including the correlation $\bar{Z}\rho T$ is neglected because its small contributions on the resolved pressure fields in the supercritical mixing layer simulation (Tramecourt et al., 2004). This assumption still needs to be revisited at different fluid states and flow conditions. Thirdly, the use of gradient diffusion terms to model turbulence energy and species transports is questionable due to the effect of heat release on the
subgrid-scale turbulence field in a combustion system. Development of accurate subgrid scale (sgs) model suitable for chemically reacting real fluid mixture remains difficult.

### 3.8.4 Limitations of Numerical Algorithm

The numerical framework employs a density-based, finite volume methodology along with a dual time-step integration technique. Temporal discretization is obtained using a second-order backward difference and the pseudo-time term is integrated with a four-step Runge-Kutta scheme. Spatial discretization is achieved with a fourth-order, central-difference scheme in generalized coordinates. Since the large density gradient regimes appear during the cryogenic fluid injection and mixing, a fourth-order scalar dissipation with a total-variation-diminishing switch developed by Swanson and Turkel (1992) is implemented to ensure computational stability and to prevent numerical oscillations in regions with steep gradients. The switch is automatically turned off in the smooth region. The effects of numerical dissipation on the overall solution accuracy within the context of LES were assessed following the approach suggested by Wang et al. (2005) for supercritical jet simulation (Chapters 4 and 5). When the sgs term was turned off, unphysical oscillations occurred in the flowfield, which finally resulted in an overflow of the calculation. When the sgs model was activated, the solution remained stable even if the numerical dissipation was reduced by half. This suggests that within the employed grid resolution, the sgs terms prevail, and the artificial dissipation only serves to obtain numerical robustness and stability. Another important issue should be noted is that a pseudo-time term is added to the governing system to overcome the low Mach system stiffness. In the dual time integration, the computation is first conducted in the pseudo time space until convergence is achieved ($\partial z/\partial \tau \approx 0$), then the solution advances one step in physical time. When the pseudo time term fully converges, its effect on the dynamic system is eliminated. The insufficient
convergence may smear the solution and finally cause the overflow of the calculation. Presently, the total residual of the pseudo time term is reduced by four orders of magnitude in each physical time loop to minimize its influence on the solution accuracy.

3.8.5 Applicability of Model

Since all the thermodynamic properties are evaluated based on fundamental thermodynamics, theoretically the present model could be applied to any fluid states of concern without empiricism. However, the one fluid assumption (surface tension and enthalpy of vaporization approach zero) is only valid for pure gas, pure liquid, and the fluid state where temperature or pressure exceeds the critical value. Under such conditions, no phase boundary exists or the fluid state transits continuously with the appearing of exceedingly large density gradient. When liquid to gas phase transition should be considered, the surface tracking method and atomization models is needed to take into account the evolution of the phase boundary and the break up of the liquid jet and droplets. In addition, the motion of each liquid droplet in the flowfield should be tracked in a Lagrangian frame and its effect on the carrier phase should be model. Those issues will be systematically investigated in the subsequent research work.
Chapter 4

Axi-symmetric Analysis of Supercritical Cryogenic Fluid Injection

4.1 Problem Description

Supercritical fluid jet and mixing layer are common in nature, such as gaseous planet (i.e. Jovian) atmospheres and volcanic lava streams, and are of great relevance to a wide range of engineering applications, including material processing, environmental control and cleanup, heat transfer, and combustion devices for propulsion and power-generation systems. The underlying flow processes exhibit many features distinct from those in an atmospherical environment (Zong et al., 2004). For instance, owing to the diminishment of surface tension and enthalpy of vaporization, the sharp distinction between the liquid and gas phases vanishes, and the fluid properties and their spatial gradients vary continuously throughout the entire field. Those phenomena, coupled with anomalous variations of thermophysical properties as fluid temperature transits through the transcritical regime (Levelt Senger, 1991), render conventional analysis developed for low pressure applications invalid (Yang, 2000).

To characterize supercritical fluid jet dynamics, cryogenic nitrogen fluid injection into supercritical gaseous nitrogen, simulating the experiments conducted by Chehroudi et al. (2002a, 2002b), were numerically investigated in this chapter. The physical model of concern is shown schematically in Fig 4.1. Cryogenic nitrogen fluid is injected into supercritical gaseous nitrogen through a circular duct with an inner diameter of 0.254 mm. Because of the enormous computational effort required for calculating the flowfield in the entire three-dimensional regime, only a cylindrical sector with periodic boundary conditions specified in the azimuthal direction is treated herein. The model established in the preceding chapters, which could accommodate full
conservation laws and real-fluid thermodynamics and transport phenomena over the entire range of fluid states of concern, is applied. The present analysis allows a detailed investigation into the temporal and spatial evolution of a cryogenic jet.

4.2 Computational Domain and Grid System

The computational domain downstream of the injector measures a length of $40D_{inj}$ and a radius of $6D_{inj}$. The dimensions are sufficient to minimize the effect of the far-field boundary conditions on the near-injector flow evolution. The entire grid system consists $225 \times 90$ points along the axial and radial directions, respectively. The grids are clustered in the shear-layer and near the injector to resolve rapid property variations in those regions. The mean grid size in the near field ($0 \leq x/D_{inj} \leq 20$) falls in the inertial sub-range of the turbulent kinetic energy spectrum, estimated using the Kolmogorov-Obukhow theory. The smallest grid width is $2 \mu m$. 

Figure 4.1: Schematic of fluid jet.
For clarity, a system with one-fourth of the original grid density is shown in Fig 4.2. The computational domain is divided into 45 blocks, with each calculated on a single processor of a distributed-memory parallel computer. The physical time step is $1 \times 10^{-3}$ ms and the maximum CFL number for the inner-loop pseudo-time integration is 0.7. For each case, simulation was conducted for 12 flow-through times (i.e., 15 ms) to obtain statistically meaningful data.

A grid independence study was performed as part of the validation procedure, in which the same numerical code, configuration, and flow condition (i.e. Case 1 in Table 1) were considered with two different grid resolutions: a fine ($270 \times 120$) and a coarse ($225 \times 90$) mesh. Figure 4.3 shows the radial distributions of the mean axial velocity, turbulent kinetic energy (TKE), compressibility factor $Z$, and viscosity (normalized by the value of the ambient gas) at different axial locations. Results from the two different grid systems agree well with each other, except for the small deviation of TKE.
4.3 Boundary Conditions

At the injector exit, a fully developed turbulent pipe flow is assumed. The mean velocity follows the one-seventh-power law and the temperature is specified with a top-hat profile. The pressure is determined using a one-dimensional approximation to the momentum equation in the axial direction. Turbulence is provided by superimposing broad-band white noise onto the mean velocity profile. The disturbances are generated by a Gaussian random-number generator with an
intensity of 12% of the mean quantity. At the downstream boundary, extrapolation of primitive
variables from the interior may cause undesired reflection of waves propagating into the
computational domain. Thus, the non-reflecting boundary conditions proposed by Poinsot and
Lele (1992) are applied, along with the specification of a reference pressure. Because the jet flow
is directly exhausted to an ambient condition, the surrounding fluid may be entrained into the
computational domain. At the radial boundary, the pressure, temperature, and axial velocity are
specified. The conservation law of mass is employed to determine the radial velocity. Finally,
the non-slip adiabatic conditions are enforced along the solid walls.

4.4 Results and Discussion

The theoretical model and numerical scheme established in the preceding sections were
implemented to study the injection and mixing of cryogenic fluid under supercritical conditions.
As a specific example, liquid nitrogen at a temperature of 120 K is injected through a circular
tube with a diameter of 254 µm into a supercritical nitrogen environment. A turbulent pipe flow
with a bulk velocity of 15 m/s is assumed at the injector exit. The ambient temperature remains
at 300 K, but the pressure varies from 42 to 93 atm, comparable to the chamber pressures of many
operational rocket engines. For reference, the critical temperature and pressure of nitrogen are
126 K and 34 atm, respectively. Three different flow conditions summarized in Table 4.1 are
considered, simulating the experiments conducted by Chehroudi and Talley (2002a), where the
subscripts ∞ and inj denote the injection and ambient conditions, respectively. The Reynolds
number is defined as $Re = \frac{\rho_{inj} u_{inj} D_{inj}}{\mu_{inj}}$. 

$\text{Re} = \frac{\rho_{inj} u_{inj} D_{inj}}{\mu_{inj}}$. 

Figure 4.4 shows the variations of nitrogen density and constant-pressure specific heat as functions of temperature at four different pressures. Two observations are noted here. First, the density decreases sharply near the critical point as the temperature increases. The effect of density stratification between the jet and the ambient fluid becomes much more substantial for $P_{\infty} = 4.3\, MPa$ compared with the other two cases. Second, the temperature sensitivity of the specific heat depends strongly on pressure. It increases rapidly as the fluid state approaches the critical point, and theoretically becomes infinite exactly at the critical point. This implies that much more thermal energy is needed to heat up the cold fluid jet in Case 1 (i.e., $P_{\infty} = 4.3\, MPa$) than the other two cases when the fluid temperature transits across the near-critical regime. The anomalous variations of fluid volumetric and thermal properties near the critical point and their dependence on pressure have profound influences on fluid jet development at high pressures.

### 4.4.1 Instantaneous Flowfield

For a constant-density jet, the shear-layer between the jet and the ambient fluid is susceptible to the Kelvin-Helmholz instability and experiences vortex rolling, paring, and
breakup. A cryogenic supercritical jet undergoes qualitatively the same process, but with additional mechanisms arising from volume dilation and baroclinic torque.

Figure 4.5 shows snapshots of the density, density-gradient, temperature, and vorticity-magnitude fields at three different ambient pressures. The small vortical structures in the core region result from the imposed turbulent motions at the injector exit. For Case 1, in which the ambient pressure of 4.3 MPa is closer to the critical value, the jet surface is straight near the injector with only tiny instability waves in the downstream region. As the ambient pressure increases, the velocity fluctuation in the radial direction becomes more vigorous. Large-scale instability waves develop in the near-injector region, which then grow up and roll into a succession of ring vortices as the injected fluid moves downstream. The resultant vortical flow motions facilitate the entrainment of the ambient gaseous nitrogen into the cold jet fluid. The initial density-stratification layer is only slightly stretched in Case 1, but severely twisted in higher-pressure cases. As a general trend, the higher the ambient pressure, the stronger vortical motions and radial velocity fluctuations near the jet surface.

It has been established that the evolution and interaction of large coherent structures strongly influence the mixing and entrainment of a shear-layer (Crow and Champagne, 1971). Figure 4.6 shows the temporal evolution of the jet surface structures of Case 3 \( (p_\infty = 9.3 \text{ MPa}) \). Both the temperature and density fields clearly demonstrate the entrainment of lighter and warmer ambient gaseous nitrogen into the jet flow through vortical motions, along with a series of thread-like entities emerging from the jet surface. The same phenomena were observed in the experiments by Chehroudi and co-works (2002a) under the same flow condition.
4.4.2 Effect of Density Stratification

To explore the formation and influence of the density-stratification layer near the jet boundary, conditional-averaged temperatures over the regions where the density-gradient magnitudes exceed pre-specified cutoff values are determined. The result is listed in Table 4.2, where $|\nabla \rho|_{\text{max}}$ is the maximum density gradient in the entire field, around $1.15 \times 10^7$ kg/m$^4$ for Case 3. The conditional fluid temperature decreases with increasing cutoff density-gradient, and approaches the inflection point on the isobaric $\rho - T$ curve shown in Fig. 4.4. Table 4.3 summarizes the inflection temperatures for the three different pressures considered herein. It is noteworthy that fluid properties usually undergo rapid variations across the temperature inflection point for an isobaric process, and the specific heat reaches its maximum at this point. For example, the density of nitrogen decreases more than three times in Case 1 as the temperature increases from 125 to 135 K. Thus, the formation of the steep density-gradient region is closely related to property variations, which to a large extent are dictated by real-fluid thermodynamics. Turbulent diffusion and mixing tend to introduce warm ambient gases into the cold jet, and subsequently smooth the density-stratification effect. The drastic volume dilation during the mixing process when the temperature transits across the inflection point, however, prevents the entrainment of the surrounding fluid, and thereby facilitates the formation of steep density-gradient regimes.

Table 4.2: Conditional averaged temperatures (K) in regions with $|\nabla \rho| >$ cutoff value.

<table>
<thead>
<tr>
<th>Cutoff</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0.1 \times</td>
<td>\nabla \rho</td>
<td>_{\text{max}}$</td>
<td>131.7</td>
</tr>
<tr>
<td>$0.2 \times</td>
<td>\nabla \rho</td>
<td>_{\text{max}}$</td>
<td>131.1</td>
</tr>
<tr>
<td>$0.3 \times</td>
<td>\nabla \rho</td>
<td>_{\text{max}}$</td>
<td>130.6</td>
</tr>
</tbody>
</table>
The effect of density stratification on the evolution of a planar mixing layer was studied by Atsavapranee and Gharib (1997). Because the higher density stratification increasingly inhibits instability-wave growth and vortex pairing, the flow topography is considerably simplified, as evidenced in Fig. 4.5. In addition, the total yield of mixed fluid is reduced with high density stratification due to the combined effect of weakened fluid entrainment into the Kelvin-Helmholtz vortices, decreased frequency of vortex pairing, and arrest of turbulence during flow restratification.

Figure 4.7 shows the power spectral densities (PSD) of the axial and radial velocity fluctuations at various radial locations of $r/D_{inj} = 0.6, 0.7, \text{ and } 0.8$ in the mixing layer for $p_z = 9.3 \text{ MPa}$. The axial position of $x/D_{inj} = 16$ is near the end of the potential core, where a sharp density gradient exists at $r = 0.1 D_{inj}$ (see Fig. 4.5). In the low-frequency regime, in which large-scale structures prevail, the axial velocity fluctuation increases as the density stratification layer is approached. The trend for the radial velocity fluctuation, however, is opposite. The velocity fluctuations in the high-frequency range remain basically insensitive to the radial position. Density stratification exerts a strong influence on large-scale flow motions. It acts like a solid wall in the flow that amplifies the axial turbulent fluctuation but damps the radial one. The same PSD results are also observed for Cases 1 and 2, which are not presented here.

A similar phenomenon was reported by Hannoun et al. (1988) in their experiments on grid-induced shear-free turbulence near a sharp density interface. As a consequence of the strong

<table>
<thead>
<tr>
<th>$p_z$ (MPa)</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$ (K)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.3</td>
<td>130.3</td>
<td>142.1</td>
<td>148.6</td>
</tr>
<tr>
<td>6.9</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9.3</td>
<td></td>
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</tbody>
</table>

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A similar phenomenon was reported by Hannoun et al. (1988) in their experiments on grid-induced shear-free turbulence near a sharp density interface. As a consequence of the strong
anisotropy of the turbulence near the density interface, large eddies of integral length scales become flattened, and the vertical component of the turbulent kinetic energy is transferred to its horizontal quantity. Such an energy redistribution among its spatial components considerably modifies the amount of energy available for fluid mixing at the density interface. Thus, the existence of strong density stratification suppresses radial velocity fluctuations in the flowfield and inhibits the development of instability waves. In the present study, the initial density ratio and the strength of density stratification decrease as the ambient pressure increases, so do their damping effects on the shear-layers. The jet surface is nearly straight in Case 1, with only tiny instability waves developing in the downstream region. The shear-layers, however, are highly twisted in both Cases 2 and 3, as shown in Fig. 4.5.

The frequency spectra of velocity fluctuations shown in Fig. 4.7 do not indicate the standard $5/3$ law for the turbulent kinetic energy spectrum based on the Kolmogorov theory, which characterizes the inertial subrange. Apte and Yang (2001) mentioned in their two-dimensional simulations of unsteady flow evolution in a porous-walled chamber that the exponent of the wave number in the inertial subrange of the turbulent energy spectrum varies between $f^{-3}$ and $f^{-4}$, with $f$ being the frequency. Gilbert (1988) proposed that the kinetic energy spectrum can be obtained from spiral vortex distributions within coherent vortices and should follow the $f^{-11/3}$ law. In this work, the frequency dependence in the inertial subrange lies between $f^{-5/3}$ and $f^{-3}$.

The present two-dimensional large-eddy simulation inherently neglects the vortex stretching mechanism, which is responsible for the transfer of energy from large to small scales through energy cascade and the continuous generation of small-scale vortical structures. Since these structures redistribute and dissipate energy at the smallest scales, the lack of vortex
stretching leads to lower energy-dissipation and turbulence-production rates during the flow evolution. This issue will be addressed in subsequent three-dimensional calculations.

4.4.3 Shear-Layer Instability

To study the vortical dynamics and flow instability in the mixing layer, the power spectral densities of the radial velocity oscillations at two different axial locations are presented in Fig. 4.8. The radial position is fixed at r/D_{inj} = 0.5. A dominant frequency around 35 kHz, corresponding to the most amplified frequency of the shear layer instability, is observed at an upstream location of x/D_{inj} = 8 for both Cases 2 and 3. This frequency is weakly dependent on the ambient pressure (or the density ratio). When the fluid is convected downstream to x/D_{inj} = 18, the dominant frequency decreases to 15.9 kHz for Case 2 and 18.6 kHz for Case 3, nearly one half of the value of the most amplified shear instability mode. The vortex pairing process is clearly demonstrated. The situation with Case 1, however, is considerably different. Owing to the low compressibility factor (i.e. 0.21) of the injected fluid and the large density ratio of 12.24, the jet exhibits a liquid-like fluid behavior distinct from the other high-pressure cases. The dominant frequencies become 20 and 10 kHz at x/D_{inj} = 8 and 18, respectively.

The flow instabilities and vortex shedding in constant-density shear layers were reviewed by Schadow and Gutmark (1992). Based on their work, the initial vortex shedding frequency, f_i, can be scaled with the shear-layer momentum thickness θ_0 and a characteristic velocity \overline{U}, normally taken as the average bulk velocity of the two streams. The result yields a non-dimensional frequency or Strouhal number, S_{St} = f_i θ_0 / \overline{U}, which ranges from 0.044 to 0.048 for a planar turbulent shear layer. As the vortices move downstream, they merge together to oscillate at the sub-harmonics of the initial vortex shedding frequency, f_i / N (N = 2, 3, 4, ...).
Although the above analysis was formulated for planar flows, it can be applied with good accuracy to mixing layers in axisymmetric configurations if the thickness of the shear layer is much smaller than the radius of the injector. In the present work, $\bar{U} \approx 8 \, m/s$ and the initial momentum thickness $\theta_0$ estimated for a fully developed turbulent pipe flow is 0.011 mm. If the Strouhal number is chosen to be $St = 0.048$, then the most amplified frequency becomes $f_1 = 34.9 \, kHz$ and the corresponding second harmonic frequency is 17.5 kHz. Those values agree well with the calculated vortex-shedding frequencies based on the radial velocity oscillations in Cases 2 and 3.

To provide more insight into observed flow phenomena, a linear stability analysis is carried out of the effects of ambient pressure on the fluid jet evolution. The work extends the approaches described by Yu and Monkewitz (1990) and Soteriou and Ghoniem (1995) to include real-fluid thermodynamics. The SRK equation of state is implemented in the formulation. Each dependent variable is decomposed into a base and a perturbation quantity. The former is adopted directly from the present simulation. The latter takes the following general form for a planar jet

$$\hat{\phi}(x, y, t) = \phi(y) \exp \{i(kx - \omega t)\} \quad (4.1)$$

where $k$ and $\omega$ are the wave number and frequency, respectively. For a spatial instability problem, $k$ is a complex variable and its negative imaginary part represents the spatial growth rate. After substitution of the decomposed variables into the conservation laws and linearization of the result, a dispersion equation characterizing the relationship between the wave number and frequency can be derived in terms of pressure fluctuation as follow

$$\frac{d^2 \hat{p}}{dy^2} - \left( \frac{1}{\bar{\rho}} \frac{d \bar{\rho}}{dy} + \frac{2}{\bar{u} - \omega/k} \frac{d \bar{u}}{dy} \right) \frac{d \hat{p}}{dy} - k^2 \hat{p} = 0 \quad (4.2)$$
The problem now becomes solving Eq. 4.2 for the eigenvalues $k$ and $\omega$ subject to appropriate boundary conditions. A complete discussion of the stability analysis is given by Liu et al. (2004).

Figure 4.9 shows the spatial growth rates of the instability waves as a function of the normalized frequency (i.e., the Strouhal number) for the three different pressures considered in the present study. The growth rate of the shear wave increases with increasing pressure. The strong density stratification in the lower pressure case suppresses the growth of the wave and stabilizes the mixing layer. The theoretically predicted frequencies of the most unstable oscillations are 23.2, 28.8 and 29.6 KHz for Cases 1, 2, and 3, respectively. These values are slightly underestimated for Cases 2 and 3, but overestimated for Case 1. The maximum deviation from the numerical simulation is 15%. The frequency of the most unstable mode exhibits a weak pressure dependence at high pressures. It, however, decreases significantly in the near-critical regime due to the enhanced effect of density stratification and increased mixing-layer momentum thickness.

4.4.4 Vortical Dynamics

As a consequence of the large velocity difference between the jet and ambient flow, a strong shear-layer is generated near the injector, which is then tilted and develops to large structures due to vortex interactions. The vortical dynamics can be best quantified using the transport equation given below

$$\frac{D\omega}{Dt} = (\omega \cdot \nabla)u - (\nabla \cdot u)\omega - \nabla \left( \frac{1}{\rho} \nabla \times \nabla p \right) + \nabla \times \left( \frac{1}{\rho} \nabla \cdot \tau \right)$$

\[ (4.3) \]
where $\frac{D}{Dt}$ stands for the substantial derivative. The first term on the right-hand side represents vortex stretching, which vanishes in the present two-dimensional simulation. The second term describes the volume-dilatation effect, and the third term denotes the baroclinic torque produced by the misalignment between the pressure and density gradients. The last term arises from viscous dissipation. For cryogenic fluid injection under supercritical conditions, large volume expansion occurs when the jet is heated by the ambient gas. Thus, both baroclinic torque and volume dilatation may play an important role in determining vorticity transport.

Figure 4.10 shows an instantaneous vorticity budget in the radial direction at the axial position of $\frac{x}{D_{maj}} = 5$ for all the three cases. At this position, the large coherent structures are well developed in Cases 2 and 3. The results are normalized by the bulk velocity ($u_{maj}$) and momentum thickness ($\theta_u$) at the injector exit. The baroclinic torque and viscous dissipation locally rival in magnitude, and have opposite contributions in Eq. 4.3. These two terms attain their maxima in regions with large density gradients in which vigorous mixing between the jet and ambient flows occurs (see Fig. 4.5). In Case 1, much of the vorticity production takes place on the light fluid side. A similar phenomenon was noted by Okong’o and Bellan (2002) in their study of a supercritical binary mixing layer. As the ambient pressure increases (or the density ratio decreases), the location with intensive vorticity production slightly shifts toward the dense fluid, but still resides on the ambient gas side, since the radial position of the mixing region also changes. The magnitudes of all the three vorticity production terms increase with increasing ambient pressure due to strengthened vortical motions.
4.4.5 Mean Flow Properties

The mean flow properties are obtained by taking long-time average of the instantaneous quantities over 10 ms (about 8 flow-through times) after the calculated flowfield has reached its stationary state. Figure 4.11 shows the radial distributions of the normalized mean density, \( \rho' = (\bar{\rho} - \bar{\rho}_{c})/\bar{\rho}_{c} \), at six different axial locations. The subscript \( c \) refers to the quantity at the centerline. The radial coordinate is normalized by the full width of the radial profile measured where the flow property of concern (i.e., density in the present figure) is one half of its maximum value (FWHM), \( r_{1/2} \). Similar to incompressible fluid jets (Abramovich, 1963; Schetz, 1980), there exist three distinct regions in a cryogenic fluid jet under supercritical conditions: a potential core in the upstream where a flat-hat distribution around the centerline occurs, a transition region, and a fully developed self-similar region. The density profiles at \( x/D_{inj} > 25 \) merge to a single distribution for Cases 2 and 3, manifesting the existence of self-similarity in the downstream region. Such a self-similar profile, however, is not observed until \( x/D_{inj} > 30 \) for Case 1. The high-pressure condition facilitates the development of the self-similar behavior through its effect on reducing the density ratio of the injected fluid to the ambient flow.

Figure 4.12 shows the normalized axial velocity profiles in the radial direction. Self-similarity is achieved at the same location as that for the density distribution. It occurs at a relatively upstream position as the ambient pressure increases. Compared with the density field, the velocity profile exhibits a narrower distribution, with the jet boundary (defined as the radial position at which \( u = 0.01u_{c} \) ) situated at \( r/r_{1/2} \approx 2.5 \), a value consistent with the data reported by Branam and Mayer (2003). In addition, no flat-hat profile exists even in the upstream region due to the use of the one-seventh power distribution for a fully developed turbulent pipe flow at the injector exit.
Figure 4.13 presents the axial distributions of the normalized temperature, density and compressibility factor along the centerline for three different pressures. Evidently, the temperature decreases relatively slowly with decreasing pressure in the axial direction. It is well established that when a fluid reaches its thermodynamic critical state, the constant-pressure specific heat becomes infinite and the thermal diffusivity decreases to zero, a phenomenon known as the critical divergence. Because the ambient pressure for Case 1 \( (p_\infty = 4.3 \, MPa) \) is closer to the critical value, the specific heat increases drastically when the temperature transits across the inflection point on the isobaric \( \rho-T \) curve (see Fig. 4.4). This effect, combined with the lower thermal conductivity, causes a slower increase in temperature along the centerline in Case 1 as the injected fluid moves downstream. The compressibility factor indicates a monotonic decrease with decreasing pressure in the low-temperature regime, and a rapid increase across the inflection point on the isobaric \( \rho-T \) curve. The compressibility factor, thus, increases much more rapidly at a lower pressure, which amounts to a faster decrease in density. Although the centerline temperature varies laggardly in all the three cases, the rapid variation of the compressibility factor causes the density to undergo a fast decrease downstream of the potential core, especially for the case of \( p_\infty = 4.3 \, MPa \).

The rapid variations of thermophysical properties exert a significant influence on the jet flow evolution. Fig. 4.14 shows the radial distributions of the specific heat, thermal diffusivity, and kinematic viscosity at \( x/D_{inj} = 10 \), a location slightly upstream of the end of the potential core. A spike exists in the specific-heat profile at \( r/r_{1/2} = 0.6 \) in Case 1, mainly due to the temperature transition across the inflection point. The same phenomenon is observed for Cases 2 and 3, but with much lower amplitudes. The thermal diffusivity also exercises a large excursion of variation across the temperature inflection point. It increases considerably from the liquid core to the ambient flow by a factor of 14, 7, and 5 in Cases 1, 2, and 3, respectively. A similar
situation occurs with the kinematic viscosity. The intensive change of viscosity in the shear-layer gives rise to another vorticity production mechanism, as shown in Eq. 4.3. These observations, again, highlight the importance of thermophysical properties in dictating the behavior of a supercritical fluid jet.

4.5 Summary

A two-dimensional numerical study has been conducted to investigate cryogenic fluid injection and mixing under supercritical conditions. The model accommodates full conservation laws and real-fluid thermodynamics and transport phenomena over the entire range of fluid states of concern. Turbulent closure is achieved using a large-eddy-simulation technique. The present analysis allows a detailed investigation into the temporal and spatial evolution of a cryogenic jet. The near-field behavior is well captured.

The major results obtained are summarized below.

1. As a result of intensive property variations between the fluid jet and surroundings, a series of large density-gradient regions are formed around the jet surface. These regions act like a solid wall that amplifies the axial flow oscillations but damps the radial ones. The interfacial instability in the shear layer is effectively suppressed, especially for cases with large density ratios. As the ambient pressure increases, the strength of density stratification decreases, so does its damping effect. Thus, the jet expands rapidly with increasing pressure.

2. Various mechanisms dictating vorticity transport are analyzed. The baroclinic torque arising from the density stratification between the injected and ambient flows and viscous dissipation play an important role in determining the flow evolution.

3. The jet dynamics are largely dictated by the local thermodynamic state of the fluid. When the temperature transits across the inflection point in an isobaric process, the rapid property
variations qualitatively change the jet behavior compared with its counterpart at low pressures. In addition, an increase in the ambient pressure results in an earlier transition of the jet into the self-similar region.

4. The spatial growth rate of the surface instability wave increases as the ambient pressure increases. The frequency of the most unstable mode exhibits a weak pressure dependence at high pressures. It, however, decreases significantly in the near-critical regime due to the enhanced effect of density stratification and increased mixing-layer momentum thickness. The result agrees well with the linear stability analysis.
Figure 4.4: Density and constant-pressure specific heat of nitrogen as the functions of temperature and pressure.
Figure 4.5: Effect of pressure on density, density gradient, temperature and vorticity fields ($T_\infty = 300$ K, $u_{\text{inj}} = 15$ m/s, $T_{\text{inj}} = 120$ K, $D_{\text{inj}} = 254$ µm, $t = 1.55$ ms).
Figure 4.6: Time evolution of jet surface structures ($p_\infty = 9.3$ MPa, $T_\infty = 300$ K, $u_{inj} = 15$ m/s, $T_{inj} = 120$ K, $D_{inj} = 254$ µm).
Figure 4.7: Power spectral densities of velocity fluctuations at different radial locations with $x/D_{mj} = 16$ ($p_\infty = 9.3$ MPa, $T_\infty = 300$ K, $u_{inj} = 15$ m/s, $T_{inj} = 120$ K, $D_{mj} = 254$ µm).
Figure 4.8: Effect of pressure on power spectral densities of radial velocity fluctuations at two different axial locations with $r/D_{inj} = 0.5$. 
Figure 4.9: Spatial growth rate as function of Strouhal number at different pressures.
Figure 4.10: Vorticity budgets at different ambient pressures ($T_\infty = 300$ K, $u_{inj} = 15$ m/s, $T_{inj} = 120$ K, $D_{inj} = 254$ µm, $t = 1.55$ ms).
Figure 4.11: Effect of pressure on normalized density distribution in radial direction.
Figure 4.12: Effect of pressure on normalized velocity distribution in radial direction.
Figure 4.13: Effect of pressure on normalized density, normalized temperature, and compressibility factor along jet centerline.
Figure 4.14: Radial distributions of mean thermophysical properties at $x/D_{maj} = 10$. 
5.1 Problem Description

An axi-symmetric analysis was established to study the dynamics of a nitrogen jet initially at a subcritical temperature and injected into supercritical nitrogen over a broad range of pressures in Chapter 4. Results indicated that the jet evolution is largely dictated by the local thermodynamic state through its influence on the fluid thermophysical properties. Owing to the differences of fluid states and flow conditions between the jet and the surroundings, a string of strong density-gradient regimes is generated around the jet surface and exerts a stabilizing effect on the flow development. The surface layer acts like a solid wall that transfers the turbulent kinetic energy from its axial to radial component. The spatial growth rate of the surface instability wave increases with increasing pressure. The frequency of the most unstable mode exhibits a weak pressure dependence at high pressures. It, however, decreases significantly in the near-critical regime due to the enhanced effects of density stratification and increased mixing-layer momentum thickness.

Although much insight was obtained, the axi-symmetric simulation inevitably neglected the vortex stretching and tilting mechanisms that are responsible for the transfer of energy from large to small scales through energy cascade and the continuous generation of small-scale vortical structures. Consequently, turbulent kinetic energy (TKE) dissipation and turbulence-production rates are underpredicted during the flow evolution. The present work attempts to remedy this deficiency by conducting three-dimensional simulations of cryogenic nitrogen fluid jets in supercritical nitrogen environments. The theoretical formulation accommodates full conservation
laws, and takes into account real-fluid thermodynamics and transport phenomena. The main objectives of this chapter are: 1) to characterize three-dimensional fluid injection and mixing dynamics in supercritical environments, 2) to identify the underlying mechanisms and key parameters dictating the flow evolution.

The simulation conditions of Cases 2 and 3 in Chapter 4 are restudied. Liquid nitrogen initially at a subcritical temperature of 120 K is injected through a circular tube with a diameter of 254 µm into a supercritical nitrogen environment. A turbulent pipe flow with a bulk velocity of 15 m/s is assumed at the injector exit. The ambient temperature remains at 300 K, but the pressure varies from 69 to 93 atm, comparable to the chamber pressures of many operational rocket engines. The two simulation conditions are summarized in Table 5.1, matching the experiments conducted by Chehroudi et al. (2002a and 2002b), where the subscripts \( \infty \) and \( \text{inj} \) denote the injection and ambient conditions, respectively. The Reynolds number is defined as

\[
Re = \frac{\rho_{\text{inj}} \mu_{\text{inj}} D_{\text{inj}}}{\mu_{\text{inj}}}
\]

<table>
<thead>
<tr>
<th>Case 1</th>
<th>( p_\infty ) (MPa)</th>
<th>( T_{\text{inj}} ) (K)</th>
<th>( T_\infty ) (K)</th>
<th>( \rho_{\text{inj}} ) (kg/m(^3))</th>
<th>( \rho_\infty ) (kg/m(^3))</th>
<th>( \rho_{\text{inj}}/\rho_\infty )</th>
<th>( u_{\text{inj}} ) (m/s)</th>
<th>( \rho_{\text{inj}}/\rho_\infty )</th>
<th>( Re )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>6.9</td>
<td>120</td>
<td>300</td>
<td>603</td>
<td>77</td>
<td>15</td>
<td>7.83</td>
<td>44700</td>
<td></td>
</tr>
<tr>
<td>Case 2</td>
<td>9.3</td>
<td>120</td>
<td>300</td>
<td>626</td>
<td>103</td>
<td>15</td>
<td>6.07</td>
<td>42300</td>
<td></td>
</tr>
</tbody>
</table>

The computational domain downstream of the injector measures a length of \( 40 D_{\text{inj}} \) and a mean diameter of \( 12 D_{\text{inj}} \). The dimensions are sufficient to minimize the effect of the far-field boundary conditions on the near-injector flow evolution. A three-dimensional grid is generated by rotating the two-dimensional grid with respect to the centerline. The entire grid system consists of \( 225 \times 90 \times 72 \) points along the axial, radial, and azimuthal direction, respectively. The grids are clustered in the shear-layer and near the injector to resolve rapid property variations in those regions. The mean grid size falls in the inertial sub-range of the turbulent kinetic energy
spectrum, estimated using the Kolmogorov-Obukhow theory. The smallest grid width is 2 \mu m. The computational domain is divided into 54 blocks, with each calculated on a single processor of a distributed-memory parallel computer. The physical time step is $1 \times 10^{-5}$ ms and the maximum CFL number for the inner-loop pseudo-time integration is 0.7. For each case, the calculation is first conducted for an extended period until the flowfield reaches its stationary state. The time stamp is then reset, and data is collected for more than 12 flow-through times (i.e., 15 ms) to obtain statistically meaningful turbulence properties.

### 5.2 Results and Discussion

#### 5.2.1 Instantaneous Flow Field Dynamics

Figure 5.1 shows snapshots of the vorticity, temperature, and density-gradient fields at two different ambient pressures of 6.9 and 9.3 MPa. The non-dimensional time, $t^*$, is defined as $t^* = t \cdot u_{inj} / D_{inj}$, where $t$ represents the physical time recorded after the flowfield reaches the stationary state. The small structures in the vorticity field near the injector arise from the imposed turbulence at the inlet. In both cases, the jet surfaces exhibit tiny instability waves immediately downstream of the injector. These waves then grow up and roll into a succession of ring vortices. The resultant large-scale vortical motion facilitates the jet mixing with the ambient flow, and causes the entrainment of warmer and irrotational fluid into the jet. In the density gradient fields, a series of finger or thread-like entities emerge from the jet surface and dissolve gradually into the ambience. Similar structures were observed in the experiments by Chehroudi et al. (2002a and 2002b) under the same flow conditions.
Owing to the strong initial density stratification between the injected fluid and surroundings, a string of large density-gradient region forms around the jet core. Strong anisotropy of turbulence occurs close to this density interface, where large eddies of integral-length scales become flattened, and the vertical component of the TKE is transferred to its horizontal quantity (Hannoun et al., 1988; Atsavapranee, 1997; Zong et al., 2004). Such a TKE redistribution among its spatial components considerably modifies the amount of energy available for fluid mixing in the shear layer. The strong density stratification effectively suppresses radial velocity fluctuations in the flowfield and inhibits the development of instability waves. Compared with incompressible turbulent jets, both vortex roll-up and paring are delayed, leading to a longer potential core, around $8D_{inj}$ for Case 1. The length of the potential core for an incompressible turbulent jet is approximately 3-5 times the injector diameter (Ho and Huerre, 1984). The influence of density stratification decreases with increasing pressure. The location of vortex roll-up shifts upstream from $x/D_{inj} \approx 5$ in Case 1 to $x/D_{inj} \approx 3$ in Case 2. In addition, the jet spreads wider and the length of the potential core reduces to $6 \sim 7D_{inj}$ in the latter case.

To identify the formation of the density-stratification layer near the jet boundary, conditional-averaged temperatures over regions where the density-gradient magnitudes exceed pre-specified cutoff values are determined. The result is given in Table 5.2. The maximum density gradients ($|\nabla \rho|_{max}$) in the entire field are around $1.17 \times 10^7$ and $1.15 \times 10^7$ kg/m$^4$ for Cases 1 and 2, respectively. The conditional temperature decreases with increasing cutoff density gradient, and approaches the value at the inflection point on the isobaric $\rho-T$ curve (see Fig. 5.2). The overall trend is identical to that observed in the previous axisymmetric simulation (Zong et al., 2004). Table 5.3 summarizes the inflection temperatures for the two different ambient pressures considered herein. It is noteworthy that fluid properties usually undergo rapid variations across this point, where the specific heat reaches its local maximum and the thermal
diffusivity becomes minimum in an isobaric process, as evidenced in Fig. 5.2. When the fluid temperature transits through the inflection point, the enhanced volume dilatation and reduced thermal diffusivity hinder small-scale mixing and diffusion. The fluid layers at that temperature behave like a boundary separating the cold injected fluid from the warm ambience, and further facilitate the formation of steep density gradients.

Table 5.2: Conditional averaged temperatures (K) in regions with $|\nabla \rho| >$ cutoff value.

| Cutoff | $0.1 \cdot |\nabla \rho|_{\text{max}}$ | $0.2 \cdot |\nabla \rho|_{\text{max}}$ | $0.3 \cdot |\nabla \rho|_{\text{max}}$ |
|--------|-----------------|-----------------|-----------------|
| Case 1 | 151.0           | 148.0           | 145.5           |
| Case 2 | 158.0           | 154.0           | 151.3           |

Table 5.3: Temperatures at inflection points on isobaric $\rho - T$ curves at different pressures

<table>
<thead>
<tr>
<th>$p_\infty$ (MPa)</th>
<th>Case 1</th>
<th>Case 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.9</td>
<td>142.1</td>
<td>148.6</td>
</tr>
<tr>
<td>9.3</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 5.3 shows snapshots of the constant-pressure specific heat ($C_p$), thermal diffusivity ($\alpha$), kinematic viscosity ($\nu$), and compressibility factor ($Z$) fields. All properties are normalized with respect to the values of the injected fluid. The specific heat exhibits a steep variation across the jet boundary. It increases rapidly and reaches a peak as the fluid temperature transits through the inflection point on the isobaric curve. The thermal diffusivity and kinematic viscosity also exercise large excursions of variations across the jet mixing layer. The compressibility factor, which measures the departure from ideal-gas behavior, has values of 0.34 and 0.42 in the jet core region for Cases 1 and 2, respectively. As the injected fluid mixes with the ambient gases, its temperature changes rapidly and volume dilates. The compressibility factor
increases expeditiously and approaches unity at an axial location of $x / D_{inj} = 20$ on the centerline for Case 1, where the fluid behaves almost ideally.

The near-field flow structures can be further explored in the volume-dilation field because the flow evolution is inherently coupled with this quantity. Figure 5.4 shows snapshots of the iso-surface of volume-dilation magnitude at $1.2 \times 10^4 \text{ } 1/s$, corresponding to 15% of the maximum value in the entire domain. Large-scale helical structures and discrete vortex rings form intermittently in the near field. The phenomena are consistent with the predictions from inviscid stability theories for ideal gas jets (Michalke and Hermann, 1984), in that the first helical and axisymmetric instability modes are equally unstable. The frequencies associated with these two modes are fairly close to each other, and have values of 34.8 kHz for Case 1 and 37.2 kHz for Case 2, corresponding to the frequencies of the most amplified modes of the initial shear-layer instability waves. As the pressure increases, the stabilizing effect of density stratification reduces and the instability wave amplifies rapidly. Although the vortex ring and helical structure still can be identified in Case 2, they become more transient and irregular.

The disintegration of the injected fluid is visualized by the temporal evolution of the density field shown in Fig. 5.5, in which three snapshots of iso-surfaces of different densities are given. The outer boundary of the jet is indicated by the density level of $80 \text{ kg/m}^3$ close to the ambient value of $77 \text{ kg/m}^3$ and the dense fluid core is emphasized by the density level of $580 \text{ kg/m}^3$. The jet surface measured by the density level of $80 \text{ kg/m}^3$ is relatively smooth downstream of the injector, which is then twisted by vortical waves and becomes irregular in all three spatial directions. As the injected fluid is convected downstream, the jet core reduces. A series of dense fluid parcels shed from the core region after the large-scale vortices pinch the centerline. Since the effect of interfacial thermodynamics disappears under supercritical conditions, the dense-fluid parcels dissolve into the environment in a diffusion/convection
controlled mode due to intensive turbulent mixing and rapid heat transfer from the surroundings. The frequency spectral of the density variations at the three different centerline locations downstream of the potential core \((x/D_{inj} = 10, 12, 14)\) indicates a disintegration frequency of approximately 14.5 kHz. The value is slightly lower than the jet preferred mode frequency of 17.4 kHz measured at \(x/D_{inj} = 9\) and \(r/D_{inj} = 0.5\). The discrepancy of the two frequencies mainly results from the different locations of measurement.

Accompanying with intensive mixing and severe fluid property variations, strong volume dilatation occurs in the transition region \((9 \leq x/D_{inj} \leq 25)\) and the shear-layers surrounding the jet. Such fluid expansion gives rise to a slightly decrease of pressure inside the dense fluid parcel. Consequently, a distribution of negative gauge pressure, defined as the deviation between the local static pressure and the chamber pressure, appears in those regions as shown in the top plot of Fig. 5.5.

### 5.2.2 Vortical Dynamics

Vorticity dynamics plays an essential role in the description of turbulent flows. To identify the major mechanism responsible for vorticity production/destruction under supercritical conditions, the budget of vorticity magnitude is examined to quantify the overall vorticity variation. The transport equation for vorticity magnitude takes the form

\[
\frac{D(\omega \cdot \omega)}{Dt} = 2\omega \cdot (\omega \cdot \nabla)u - 2(\nabla \cdot u)\omega - 2\omega \cdot \nabla \left(\frac{1}{\rho}\right) \times \nabla p + 2\omega \cdot \nabla \times \left(\frac{1}{\rho} \nabla \cdot \tau\right)
\]

\((5.1)\)

where \(D/Dr\) is the substantial derivative. The first term on the right-hand side represents vortex stretching and titling. The second term describes volume-dilatation, and the third term denotes baroclinic torque produced by the misalignment between pressure and density gradients.
The last term arises from viscous dissipation. For cryogenic fluid injection under supercritical conditions, severe property variations occur when the jet is heated by the ambient gas. Both baroclinic torque and volume dilatation may play important roles in determining vorticity transport.

Figure 5.6 presents the radial distributions of the vorticity-magnitude budget, spatially averaged in the azimuthal direction, at two different axial locations. The results are normalized by the bulk velocity ($u_{inj}$) and the initial momentum thickness ($\theta_0$), estimated based on the fully developed turbulent pipe flow velocity profile specified at the injector exit, whose value is 0.011 mm for both two cases. At $x/D_{inj} = 2$, a position slightly upstream of the vortex roll-up, all terms except viscous dissipation contribute positively to the vorticity production. In Case 1, the dissipation term has the largest magnitude. The baroclinic torque rivals the vortex stretching and titling, indicating the influence of variable fluid properties on vorticity production. The influence of volume dilatation is relatively weak. In Case 2, the vortex stretching mechanism prevails, suggesting more dynamic flow activities in the upstream region due to reduced damping effect associated with density stratification at an elevated pressure. The enhanced vortical flow motion intensifies pressure variation and subsequently gives rise to a strengthened baroclinic torque in comparison with Case 1. In two cases, the activities of all terms in Eq. 5.1 are more apt to concentrate on the lighter gaseous nitrogen side and attain their maximum magnitudes in regions with strong stratification and shear. Similar observations were made by Okong’o et al. (2002) in their simulation of supercritical heptane/nitrogen mixing layer.

As the injected cold fluid is convected downstream towards the end of the potential core ($x/D_{inj} = 10$), it mixes with the entrained surrounding gas and the effect of density stratification is smoothed. Consequently, the contributions from baroclinic torque and volume dilatation reduce. Their magnitudes, on average, are one order-of-magnitude smaller than that of the
stretching and dissipation terms in both two cases. Viscous dissipation, which is negative, competes with vortex stretching over the regions where intensive mixing occurs. The dominance of vortex stretching and tilting implies that small-scale turbulent structures prevail close to the end of the potential core. The influence of pressure on the magnitude of each term appears moderate, although the radial distribution of each term becomes more irregular as a result of strengthened vortical flow motions in Case 2.

5.2.3 Shear-layer Instability and Jet Prefer Mode

Theoretically, a fluid jet has two distinct length scales: the momentum thickness ($\theta_0$) of the initial shear layer determining the near-field dynamics, and the jet diameter ($D_{nj}$) governing the flow evolution in the downstream region. The associated instability modes are the high-frequency shear-layer mode and low-frequency jet column / preferred mode.

Figure 5.7 shows the frequency spectra of pressure oscillations at different axial locations in the shear layer ($r/D_{nj}=0.5$) in Case 1. The results are normalized by the bulk injection velocity and injector diameter. A dominant frequency of 0.58 (34800 Hz) is observed close to the injector exit (probe 1), corresponding to the most amplified mode of shear layer instability. As the fluid is convected downstream (probe 2), a subharmonic with a frequency of 0.29 (17400 Hz) appears. There still exist several intermediate peaks between 0.58 and 0.29 due to the non-linear interaction of vortices. The oscillation at the frequency of 0.29 reaches its maximum at $x/D_{nj} = 9$ (Probe 3), indicating the completion of the first paring. The experimental results of gaseous mixing layers indicated that vortex paring is associated with the saturation of the first subharmonic of the most amplified frequency of the shear layer (Ho and Huang, 1982). Since the stabilization effect of density stratification abates in Case 2, both the vortex roll-up and paring shift upstream (see Fig. 5.8). The vortex passage frequency after the first paring (0.31) emerges
at an upstream location (probe 1). This harmonics becomes dominant at \(x/D_{ij} = 6\) (probe 2), with its amplitude reaching a maximum downstream of the potential core (probe 3). The spectral contents of flow oscillations are very close to those obtained from the axisymmetrical simulations (Zong et al., 2004) and linear stability theories (Liu, 2004).

The flow instabilities and vortex shedding in constant-density shear layers were reviewed by Schadow and Gutmark (1992). The initial vortex shedding frequency, \(f_i\), can be scaled with the shear-layer momentum thickness \(\theta_0\) and a characteristic velocity \(\bar{U}\), normally taken as the average bulk velocity of the two streams. The result yields a non-dimensional frequency or Strouhal number, \(St_i = f_i\theta_0 / \bar{U}\), which ranges from 0.044 to 0.048 for a planar turbulent shear layer. As the vortices move downstream, they merge together to oscillate at the sub-harmonics of the initial vortex shedding frequency, \(f_i/N(N = 2, 3, 4, \cdots)\). Although the above analysis was formulated for planar flows, it can be applied with good accuracy to mixing layers in axisymmetric configurations if the thickness of the shear layer is much smaller than the radius of the injector. In the present work, \(\bar{U} \approx 8\, m/s\) and the initial momentum thickness \(\theta_0\) estimated for a fully developed turbulent pipe flow is 0.011 mm. If the Strouhal number is chosen to be \(St_i = f_i\theta_0 / \bar{U} = 0.048\), then the most amplified frequency becomes \(f_i = 34.9\, kHz\) and the corresponding second harmonic frequency is 17.5 kHz. The result agrees reasonably well with the vortex-shedding frequencies obtained in Cases 1 and 2.

Distinct from the most amplified mode of shear layer instability, a jet flow inherently possesses a preferred (or jet-column) mode due to the presence of another second length scale - the injector diameter, \(D_{ij}\). The associated presence frequency corresponds to the vortex passage frequency at the end of the potential core. When a circular jet is excited by a monochromatic excitation at its preferred frequency, the maximum response, measured as the amplitude of the pressure oscillation at the jet centerline, are observed. The preferred frequency, normalized by
the injector diameter and bulk injection velocity, was found to vary between 0.25 and 0.5 (Gutmark and Ho, 1983). The experimental data was usually measured for incompressible turbulent jets in the region between \( x/D_\text{inj} = 3 \) and 5, corresponding to the end of the potential core. The wide range of preferred frequency was resultant from the background noise inherent in each facility (Ho and Huerre, 1984). For a supercritical fluid jet, both vortex roll-up and paring are inhibited by the effect of density stratification. The dominant frequencies of 0.29 and 0.31 for Cases 1 and 2, respectively, fall into the range of 0.25-0.5 for the jet preferred mode, as suggested by Gutmark and Ho (1983).

### 5.2.4 Mean Flow and Turbulence Characteristics

To validate the present analysis and to characterize supercritical fluid jet mixing, the mean-flow and turbulence properties are calculated and compared with experimental results of several different jet flows. There include supercritical cryogenic fluid jets (Chehroudi et al., 2002a and 2002b), incompressible but variable-density jets (Amielh et al., 1996), and constant-density turbulent jets (Wygnanski and Fiedler, 1969; Panchapakesan and Lumley, 1993; Hussein et al. 1994). The operating conditions are summarized in Table 5.4, where \( x_0 \) denotes virtual origin. The value of \( x_0 \) is directly associated with the length of the jet potential core.

Figure 5.9 shows the distributions of the normalized temperature, velocity, and density along the centerline. The density and temperature profiles remain unchanged in the potential core, whose length slightly decreases with increasing pressure. The centerline velocity decays following the \( x^{-1} \) law below in the downstream region of the potential core (Boersma et al. 1998),
where the subscript \( c \) refers to the quantity at the centerline. The decay constant, \( B_u \), ranges between 5.7 and 6.1 for constant-density jets (Wygnanski and Fiedler, 1969; Panchapakesan and Lumley, 1993; Hussein et al., 1994). For reference, the curve fit (\( x_0 = 2.7 \) and \( B_u = 5.9 \)) on the experimental data of Hussein et al. (1994) is also presented. Since the fluid jets are much denser than the surrounding gases, their centerline velocities decline relatively slower than that of constant-density turbulent jet, leading to a much greater decay constant around 8.0 and a longer virtual origin. The normalized centerline temperature bears a very similar trend to the axial velocity, but decreases slightly more rapidly. Owing to the volume dilatation, the density profile exhibits a severe drop in the region right behind the potential core (\( 9 \leq x/D_{inj} \leq 18 \)), where the mean temperature transits across the inflection point on constant-pressure \( \rho - T \) curve (see Fig. 5.2). The fluid density almost approaches ambient value at the axial location \( x/D_{inj} = 30 \). The distribution of the full-width-half-maximum (FWHM) location, defined as the radial location where the flow property of concern is one half of the centerline value (i.e. axial velocity in the present figure), is also presented in Fig. 5.9. The growth rate of FWHM (\( r_{1/2} \)) decreases at axial
locations $x / D_{nj} = 27$ and 30 for Cases 1 and 2, respectively, indicating the end of the transition region.

Figure 5.10 shows the radial distributions of the normalized mean density, $\rho^* = (\bar{\rho} - \bar{\rho}_\infty) / (\bar{\rho}_c - \bar{\rho}_\infty)$, at different axial locations. The radial coordinate is normalized by the FWHM ($r_{1/2}$) based on the density at the axial position of concern. Three distinct flow regimes, similar to incompressible turbulent jets, are identified. The potential core is manifested by the flat-hat distribution near the injector. The density profiles merge into a single distribution further downstream ($x / D_{nj} > 30$), suggesting the existence of a fully developed self-similarity region.

A transition region occurs between 10 and $30D_{nj}$. The experimental data obtained using the Raman scattering technique at the test condition of Case 1 (Chehroudi et al., 2002a) is also plotted for comparison. Good agreement between calculations and measurements was achieved with a maximum deviation of 8%.

The spatial growth rate of a jet flow is usually assessed with a visual spreading angle ($\theta$), determining by the outer most observable extent/boundary of the jet. On a shadowgraph image, $\theta$ was measured as the angle between the centerline and the ray origins from the tip of injector exit and passes the outer boundary of jet. An empirical correlation for the spreading angle of cryogenic fluid jet under both sub- and supercritical pressures was proposed by Chehroudi et al. (2002b). The equation combines the correlation for isothermal liquid spray (Reitz and Bracco, 1979), and the relationship for incompressible variable-density turbulent jet (Papamoschou and Roshko, 1988), which takes the following form.

$$\theta = 0.27[F(\rho_\infty / \rho_{nj}) + (\rho_\infty / \rho_{nj})^{1/2}]$$

$$F(\rho_\infty / \rho_{nj}) = 5.325 \rho_\infty / \rho_{nj} + 0.0288$$

$$= 0.5 \quad \rho_\infty / \rho_{nj} < 0.0885$$

$$\rho_\infty / \rho_{nj} \geq 0.0885$$
Under the present flow conditions, \( \rho_\infty / \rho_{\text{inj}} \) is greater than 0.0885 and a constant of 0.5 is adopted for the function \( F \). The jet boundary in the simulation is obtained following the suggestion of Chehroudi et al. (2002b), where it is defined as twice the FWHM(\( r_{1/2} \)) based on the density at the axial location of concern. In Fig. 5.11, the calculated jet spreading angles fall onto the predicted curve (i.e. Eq. 5.3) with a maximum derivation of 5%. Both the simulation and experimental results follow the correlation proposed by Dimostakis (1986) for incompressible variable-density mixing layers.

Figure 5.12a compares the centerline velocity with experimental data of variable-density turbulent jets at atmosphereical pressure (Amielh et al., 1996). The lighter gaseous Helium jet tends to mix more quickly with the ambience than the denser ones, where its centerline velocity fall-off is greater than those of the air and CO\textsubscript{2} jets. The deviation of velocity distributions, however, appears moderate in the region of concern \((0 \leq x / D_{\text{inj}} \leq 35)\), when density ratio \((\rho_{\text{inj}} / \rho_\infty)\) further increases from 1.4 for CO\textsubscript{2} jet to 7.8 of Case 1. Since the velocity decay of variable-density jet may also be linked to buoyancy effect, the inertial dominant region, where body force is negligible, is evaluated based on the correlation suggested by Papanicolaou and List (1988) to exclude this uncertainty. The Helium and CO\textsubscript{2} jets are momentum (inertial) dominant in the region 15 and 40\(D_{\text{inj}}\) downstream of the injector exit, respectively, and the two cryogenic jets of concern are in favor of inertial over 0 to 120\(D_{\text{inj}}\) (Chehroudi et al., 2002a). This indicates that density variation indeed exerts a crucial influence on the jet evolution in the near-field.

Based on the similarity law proposed by Chen and Rodi (1980), the velocity decays of constant and variable-density jets could be described by a single correlation, in which the effect of initial density ratio is taken into account by introducing an effective diameter \((D_{\text{eff}} = D_{\text{inj}}(\rho_{\text{inj}} / \rho_\infty)^{1/2})\). The virtual origin \((x_o)\), which is directly associated with the potential...
core length and has a greater value for a denser jet, is also employed to correlate data. In the experiments of Amielh et al. (1996), $x_0$ equals to $-0.2$, $-2.6$, and $-2.9D_{\text{inj}}$ for the helium, air, and CO$_2$ jets, respectively, as summarized in Table 5.4. For the supercritical jets considered herein, the values of $-3.0$ and $-4.0D_{\text{inj}}$ are chosen for Cases 1 and 2, respectively. It should be noted that a low-velocity co-flow surrounding the jet was employed in the experiments of Amielh et al. (1996). The influence of such co-flow on the centerline velocity distribution can be filtered out by subtracting it from the mean flow \( \frac{\bar{\tau}_{\text{inj}}}{\bar{\tau}_{\infty}} = \frac{\bar{\tau}_{\text{inj}}}{(\bar{\tau}_e^2 - \bar{\tau}_e^2)^{1/2}} \). Figure 5.12b presents the centerline velocity distributions over the inertial dominant region, where the correlation of Chen and Rodi (1980) is valid. The axial coordinate is normalized by the effective diameter, $D_{\text{eff}}$. After transformation, the velocity decays of the three variable-density jets collapse together, whereas, the profiles of the two supercritical jets exhibit totally different trends. To investigate the influence of the virtual origin, $x_0$ was intentionally increased to $-6.0$ and $-5.0D_{\text{inj}}$ for Cases 1 and 2, respectively. The large deviations between low- and high-pressure jets still exist (not shown). Compared with incompressible variable-density jets, the density of the cryogenic fluid jets decrease severely in the transition region (see Fig. 5.9). This effect, however, is not included in the Chen and Rodi’s correlation. To accurately model velocity distributions of cryogenic fluid jets, the intense fluid property variations in the near-field should be fully taken into account.

Figure 5.13 shows the comparison of turbulence intensities along the centerline with those of variable density jets (Amielh et al., 1996). Compared with incompressible variable-density jets, the turbulent kinetic energy in a supercritical jet remains basically unchanged in the potential core, and starts to increase rapidly in a relatively downstream region due to the stabilizing effect of density stratification. It reaches a peak value of 32% around the axial location of $x/D_{\text{inj}} = 18$ and then decreases and approaches a constant level close to that of its low-pressure counterpart. A similar phenomenon was observed by Zhou et al. (2001) in their
numerical simulation of turbulent buoyant jets, in which the TKE peak off was attributed to the secondary instability induced by buoyancy force. In the present work, the injected fluid is much heavier than the surrounding gas and no body-force effect should be considered. Furthermore, the velocity decay is slower in the transition region than the constant density or lighter gaseous jets (as shown in Fig. 5.12a). In other hand, the regions of higher turbulence intensity and severe density variation (see Fig. 5.9) are highly correlated. The evidence obtained, so far, suggests that the volume dilatation significantly enhances the turbulent flow motions in the transition region.

Figure 5.14 shows the radial distribution of the normalized mean axial velocity \( \bar{u} = (\bar{u} - \bar{u}_\infty) / (\bar{u}_\infty - \bar{u}_w) \) in a universal self-similarity coordinate \( \eta = r / (x - x_0) \). The data was obtained by averaging the profiles in the fully developed self-similar region \( 30 \leq x / D_{inj} \leq 35 \). Also included are experimental results for constant-density turbulent jets measured by Panchapakesan and Lumley (1993), Hussein et al. (1993), and Wygnanski and Fiedler (1967) in the further downstream regimes. The five data sets collapse together. Figure 5.15 shows the radial distributions of normalized Reynolds stresses. The calculated profiles are obtained by the same way as the mean velocity. All Reynolds stress components of Cases 1 and 2 fall into the ranges of constant-density turbulent jet.

Richards and Pitts (1993) noted, based on experimental observations of gaseous helium, methane, and propane injected into quiescent air at room conditions, that due to the entrainment and mixing, the density difference between the injected and environmental flows diminishes in the far field, where a variable-density jet behaves like a constant-density jet. The effects of initial density ratio and velocity profile can be taken into account in the description of the far field flow development by properly choosing a virtual origin. The same observation appears to be valid even for supercritical fluid jets. In spite of the strong density stratification and steep property
variations in the upstream region, the intensive turbulent mixing, augmented by volume dilatation in the transition region, renders the jet behave like its low-pressure counterpart in the far field.

5.3 Summary

A three-dimensional large-eddy-simulation has been conducted to investigate cryogenic fluid jets dynamics under supercritical conditions. The near-field dynamics is well captured and the influences of the real-fluid thermodynamics on the jet evolutions are identified in terms of mean and turbulence properties. The major results are summarized below.

1. The jet dynamics is largely dictated by the local thermodynamic state through its influence on the fluid properties. Owing to the different fluid state and flow conditions between the injected fluid and the ambience, a string of large density-gradient regions forms surrounding the jet. This layer exerts a stabilization effect on the jet evolution, which inhibits the initial instability-wave growth and vortex rolling up and paring.

2. The underlying mechanism of hydrodynamic instability is analyzed by examining the vorticity and vorticity magnitude transport equations. The vortex stretching and viscous dissipation are dominant in the vorticity production/destruction. Baroclinic torque rivals in magnitude with stretching term at the upstream. Its influence decays as the decreases of the density stratification.

3. A local volume dilatation occurs in the transition region as the injected fluid is heated by the hot ambience. The severe fluid property variations have considerable influence on jet evolution in terms of the mean and turbulence properties. Thereby, treating the supercritical fluid jet simply as a variable-density incompressible jet without considering the near field properties variations could lead to fatal deviation.
4. The density stratification and volume expansion decay as the fluid is convected downstream. In the downstream region \((30 < x/D_{aj} < 35)\), both the velocity and Reynolds stress components match that of the incompressible turbulent jets.
Figure 5.1: Effect of pressure on vorticity magnitude, $|\omega|$, temperature, $T$, and density gradient, $|\nabla \rho|$, fields ($T_\infty = 300$ K, $u_{\text{inj}} = 15$ m/s, $T_{\text{inj}} = 120$ K, $D_{\text{inj}} = 254$ µm, $t^* = 80$).
Figure 5.2: Thermo-physical properties of nitrogen as functions of pressure and temperature.
Figure 5.3: Effect of pressure on specific heat, $C_p$, thermal diffusivity, $\alpha$, kinematic viscosity, $\nu$, and compressibility factor, $Z$, fields ($T_\infty = 300$ K, $u_{\text{inj}} = 15$ m/s, $T_{\text{inj}} = 120$ K, $D_{\text{inj}} = 254$ $\mu$m, $t^* = 88$).
Figure 5.4: Large coherent structures visualized by iso-surfaces of dilatation magnitude, $|\nabla \cdot \vec{u}|$, at $1.2 \times 10^4$, corresponding to 15% of the maxima, a) Case 1: $p_\infty = 6.9$ MPa, $T_\infty = 300$ K, $u_{inj} = 15$ m/s, $T_{inj} = 120$ K, $D_{inj} = 254$ µm; b) Case 2: $p_\infty = 9.3$ MPa, $T_\infty = 300$ K, $u_{inj} = 15$ m/s, $T_{inj} = 120$ K, $D_{inj} = 254$ µm.
Figure 5.5: Time averaged pressure field and the time evolution of the density field showing the dense fluid jet disintegration process, Case 1: $p_\infty = 6.9$ MPa, $T_\infty = 300$K, $u_{inj} = 15$ m/s, $T_{inj} = 120$ K, $D_{inj} = 254$ $\mu$m.
Figure 5.6: Effect of pressure on the spatial averaged vorticity magnitude budgets at different axial locations ($T_\infty = 300$ K, $u_{inj} = 15$ m/s, $T_{inj} = 120$ K, $D_{inj} = 254$ µm, $t^* = 88$).
Figure 5.7: Power spectral densities of pressure fluctuations at different axial locations with $r/D_{inj} = 0.5$, Case 1: $p_a = 6.9$ MPa, $T_a = 300$ K, $u_{inj} = 15$ m/s, $T_{inj} = 120$ K, $D_{inj} = 254 \mu$m.
Figure 5.8: Power spectral densities of pressure fluctuations at different axial locations with $r/D_{inj} = 0.5$, Case 2: $p_\infty = 9.3$ MPa, $T_\infty = 300$ K, $u_{inj} = 15$ m/s, $T_{inj} = 120$ K, $D_{inj} = 254$ µm.
Figure 5.9: Effect of pressure on the normalized temperature, velocity, density along jet centerline, and the FWHM distributions ($T_\infty = 300$ K, $u_{inj} = 15$ m/s, $T_{inj} = 120$ K, $D_{inj} = 254$ µm).

Figure 5.10: The normalized density distributions in radial direction at different axial locations ($T_\infty = 300$ K, $u_{inj} = 15$ m/s, $T_{inj} = 120$ K, $D_{inj} = 254$ µm).
Figure 5.11: Tangent of the jet visual spreading angle versus the ambience to injectant density ratio.
Figure 5.12: Effect of initial density ratio on velocity decay, a) velocity decay, b) velocity decay normalized using the pseudo-similarity laws suggested by Chen and Rodi (1980).
Figure 5.13: The normalized turbulence intensity distributions along jet centerline ($T_\infty = 300 K$, $u_{inj} = 15 m/s$, $T_{inj} = 120 K$, $D_{inj} = 254 \mu m$).

Figure 5.14: The normalized velocity distributions in radial direction averaged among the region $30 < x/D_{inj} < 35$ ($T_\infty = 300 K$, $u_{inj} = 15 m/s$, $T_{inj} = 120 K$, $D_{inj} = 254 \mu m$).
Figure 5.15: The normalized Reynolds stress components distributions in radial direction averaged among the region $30 < x/D_{inj} < 35$ ($T_\infty = 300$ K, $u_{inj} = 15$ m/s, $T_{inj} = 120$ K, $D_{inj} = 254$ µm).
Chapter 6

High-pressure LOX and Methane Mixing Process

6.1 Problem Description

Extensive experimental and theoretical studies have been conducted to provide detailed understanding of cryogenic propellant mixing and combustion under both trans- and supercritical conditions. Most of those studies were focused on the LOX/GH2 system. For future development of high-performance reusable liquid rocket engines, the mixing and combustion of LOX and methane have recently attracted considerable interest. The key issues of concern include injector performance, combustion efficiency, stability, and soot formation.

In this chapter, the numerical model developed and validated above is employed to explore various fundamental physiochemical mechanisms associated with injection and mixing of LOX and methane under supercritical pressure. Results not only enhance the basic understanding of the subject problem, but also provide a quantitative basis to identify the key design parameters and flow variables that exert strong influence on this process.

A schematic diagram of the model injector employed in the study is illustrated in Fig. 6.1. Co-flowing methane (outer) and oxygen (inner) streams are injected at the inlet and separated by a 0.3 mm thick LOX post. The inner diameter of the LOX post is 1.2 mm, and that of the methane duct is 2.4 mm. The injector is the same as that employed by Gurliat et al. (2003) to study LOX/GH2 combustion. To simplify the problem, the computational domain starts from the faceplate of the injector and includes only part of the combustion chamber. Fully developed turbulent pipe flow velocity profiles are assumed for the injected streams at the injector outlet.
In the cases considered, the combustion chamber is preconditioned with gaseous methane at 300 K and a reference pressure of 100 atmospheres. The injection temperature and velocity of the streams are varied to obtain a representative and comparable set of thermophysical and fluid dynamic characteristics. Case 1 provides subcritical conditions within the two streams, where the methane and oxygen injection temperatures of $T_1 = T_2 = 150K$ are specified. In Case 2, the temperature of the methane stream is set at a supercritical value $T_2 = 220K$, and that of oxygen is fixed at $T_1 = 150K$. As a result, the two streams are mixing in a transcritical state. For reference, the critical points of the propellants are listed in Table 6.1. Since thermo-physical properties play a significant role in determining the flow evolution at high-pressure, their variations are plotted over the fluid state of concern in Fig. 6.2 and Fig. 6.3 for methane and oxygen, respectively.

Table 6.1: The critical points of methane and oxygen.

<table>
<thead>
<tr>
<th></th>
<th>$P_c$ (atm)</th>
<th>$T_c$ (K)</th>
<th>$V_c$ (L/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>46</td>
<td>190</td>
<td>0.099</td>
</tr>
<tr>
<td>Oxygen</td>
<td>50</td>
<td>154</td>
<td>0.076</td>
</tr>
</tbody>
</table>

Figure 6.1: Schematic of shear co-axial injector employed in the simulation.
Figure 6.2: Thermo-physical properties of methane as functions of pressure and temperature.

Figure 6.3: Thermo-physical properties of oxygen as functions of pressure and temperature.
Three factors should be considered when selecting the injection velocities of methane and oxygen: 1) it is desirable to specify mass flow rates typically employed in practical systems; 2) it is desirable to minimize respective Reynolds numbers due to the stringent requirement to resolve the characteristic turbulence scales; and 3) it is desirable to maximize the velocity ratio of the streams. Presently, the injection velocities of the two streams are chosen to match the mass ratio of the experiments conducted by Singla et al. (2004). The relevant parameters associated with simulation conditions are summarized in Table 6.2.

Table 6.2: Simulation conditions for the analysis of high-pressure LOX/methane injection and mixing process. Subscript 1 denotes the oxygen stream, and subscript 2 denotes the methane stream.

<table>
<thead>
<tr>
<th></th>
<th>Case 1</th>
<th>Case 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>p (atm)</td>
<td>100 atm</td>
<td>100 atm</td>
</tr>
<tr>
<td>$T_1$ (K)</td>
<td>150</td>
<td>150</td>
</tr>
<tr>
<td>$T_2$ (K)</td>
<td>150</td>
<td>220</td>
</tr>
<tr>
<td>$T_\infty$ (K)</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>$\rho_1$ (kg/m$^3$)</td>
<td>800</td>
<td>800</td>
</tr>
<tr>
<td>$\rho_2$ (kg/m$^3$)</td>
<td>360</td>
<td>180</td>
</tr>
<tr>
<td>$\rho_\infty$ (kg/m$^3$)</td>
<td>75</td>
<td>75</td>
</tr>
<tr>
<td>$\rho_1/\rho_2$, $\rho_1/\rho_\infty$</td>
<td>2.2, 10.6</td>
<td>4.4, 10.6</td>
</tr>
<tr>
<td>$u_1$ (m/s)</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>$u_2$ (m/s)</td>
<td>30</td>
<td>60</td>
</tr>
<tr>
<td>$u_1/u_2$</td>
<td>0.33</td>
<td>0.17</td>
</tr>
<tr>
<td>$\rho_1u_1/\rho_2u_2$</td>
<td>0.74</td>
<td>0.74</td>
</tr>
<tr>
<td>$a_1$ (m/s)</td>
<td>461</td>
<td>461</td>
</tr>
<tr>
<td>$a_2$ (m/s)</td>
<td>1070</td>
<td>390</td>
</tr>
<tr>
<td>$M_1$</td>
<td>0.022</td>
<td>0.022</td>
</tr>
<tr>
<td>$M_2$</td>
<td>0.028</td>
<td>0.154</td>
</tr>
<tr>
<td>Re$_1$</td>
<td>$14.6\times10^4$</td>
<td>$14.6\times10^4$</td>
</tr>
<tr>
<td>Re$_2$</td>
<td>$4.9\times10^4$</td>
<td>$16.4\times10^4$</td>
</tr>
</tbody>
</table>
The computational domain downstream of the injector measures a length of $40\delta$ and a radius of $12\delta$, where $\delta$ is the thickness of the LOX post. The dimensions are sufficient to minimize the effect of the far-field boundary conditions on the near-injector flow evolution. Because of the enormous computational efforts required for calculating the three-dimensional flowfield, only a cylindrical sector with period boundary conditions specified in the azimuthal direction is treated herein. The entire grid system consists $360 \times 200$ points along the axial and radial directions, respectively. The grid size falls in the inertial sub-range of the turbulent kinetic energy spectrum estimated based on the inlet Reynolds number of the LOX stream. To resolve the wake region and the vortical structures which shed off the LOX post tip, 40 radial points are used to cover the splitter. The grids are clustered in the shear-layers and near the solid walls to resolve the predominant processes and large property gradient. For clarity, a grid system at one-fourth of the original grid density is presented in Fig. 6.4. The computational domain is divided into 36 blocks, with each calculated on a single processor of a distributed-memory parallel computer. The physical time step is $0.5 \times 10^{-3}$ ms, and the maximum CFL number for the inner-loop pseudo-time integration is 0.7. For each case, simulation is conducted for 12 flow-through times (i.e., 10 ms) to obtain statistically meaningful data.

Fully developed turbulent pipe flow velocity profiles are assumed for the injected streams. Turbulence properties at the inlet are specified by superimposing broadband disturbances onto the mean velocities. The disturbances are generated by a Gaussian-random number generator with an intensity of 10% of the mean quantity. The temperature and species distributions are specified with top-hat profiles. The extrapolate boundary condition with a fixed back pressure is imposed at the outlet and the radial boundaries. The no-slip adiabatic condition is employed for the solid wall connected to the injector.
6.2 Presentation of Results

6.2.1 Instantaneous Flow Dynamics

We first considered the mixing of oxygen and methane under conditions without the occurrence of combustion. Figure 6.5 presents the vorticity and oxygen mass-fraction fields near the injector faceplate. Three shear layers are observed. The inner one forms around the oxygen jet, and the other two emerge from the inner and outer boundaries of the annular methane stream. A series of large-scale vortices shed from the outer rim of the LOX post. As those vortices grow up, the two shear layers separated by the LOX post merge together. The dominance of the inner vortex string in the near field contradicts the experimental observation of coaxial injection of
water without a splitter between two streams, where the evolution of the outer shear layer is dominant over the inner one because of the greater velocity difference between the high-speed outer stream and the ambience (Rehab et al., 1997).

The relatively higher speed of the methane stream in Case 2 has substantial influence on the flow evolution. The vortices formed downstream of the LOX post are stronger and have longer length scales. They spread the oxygen much wider and pinch the central line earlier. The outer-shear layer becomes more unstable, and the instability waves associated with it roll up into at an upstream location. The interactions among vortices give rise to a much more complicated field with the emergence of small structures.

Figure 6.6 presents the methane mass-fraction, density, normalized vorticity, and velocity vector fields immediately downstream of the LOX post. A string of large vortices shed from the outer rim of the LOX in a manner analogous to that produced at a backward facing step. Although those energy containing eddies concentrate in the lighter fluid side due to the density stratification, they entrain the denser oxygen much deeper into the methane stream and facilitate the mixing process. Mixing of the two propellant streams occurs immediately behind the LOX post. In Case 2, since the density of methane decreases at a supercritical temperature, the vortices are more apt to be confined in the lighter fluid. Therefore, severe velocity variation occurs between the inner and outer streams and large strain rate emerge around the oxygen jet boundary.

The near-field flow evolution is further examined in the vorticity and velocity-vector fields, in which the large-scale vortices and the wake region are manifested. Those structures play a crucial flame-holding role in hot-fire conditions, which will be addressed in the subsequent study.

Since mass diffusion is inhibited under supercritical conditions, the mixing of the two streams mainly results from the entrainment effect of large eddies, which occurs during both their initial growth and interactions (Ho and Huerre, 1984). The evolution of the vorticity field over one cycle of vortex paring in Case 1 is shown in Fig. 6.7. At the beginning, the vortices emerge...
from the LOX post tip and are displaced to different radial locations due to their phase difference. Owing to the radial velocity gradient, the two vortices acquire different speeds and the later vortex could catch the earlier one. Two vortices finally merge into a single structure by kinematic induction. During the paring process, the outer shear layer is engulfed into the center. The interaction between the vortices and the outer shear layer causes the layer break into a series of fine structures. Large strain rates occur, and the interface between the two streams is enhanced. Because a greater interfacial area could provide more space for the short-range molecular diffusion, the total yield of mixing increases.

6.2.2 Spectral Characteristics

In order to check whether the outer and inner shear-layers evolve according to the Kelvin-Helmholtz instability mechanism, the power spectral densities of the radial velocity oscillations at different axial locations are calculated.

Figure 6.8 presents the results of Case 1. The vortex shedding from the LOX post tip switches between two different modes intermittently. In the first mode, a string of discrete vortex sheds from the LOX post tip at the dominant frequency of 18.4 KHz. Those vortices tend to keep the same length scale until they merge or interact with the outer shear-layer. In the second mode (see Fig. 6.7), a strong vortex forms at 18.4 kHz and is immediately followed by a weaker vortex. The oscillation of 11.9 kHz, which appears at the probe location 2 and reaches its maximum at probe 3, is resultant from the paring of those two vortices. Compared with inner vortex string, the outer shear layer is relatively stable upstream. Sinusoidal wave structures appear at the probe 5, where both the initial vortex shedding frequency of the inner layer (18.4 kHz) and an oscillation close to 11.9 kHz are dominant.
Because the methane stream moves faster in Case 2, the inner vortex shedding frequency increases to 22.1 kHz (see Fig. 6.9). The second mode of vortex shedding observed in Case 1 is inhibited. Only discrete vortices shed from the LOX post tip. Since vortex paring occurs relatively upstream, the initial shedding oscillation decays rapidly. Its first subharmonic becomes the dominant one at the probe location 3. The oscillation from the inner mixing layer still acts as a forcing on the outer shear layer.

The flow characteristics of the coaxial water jet without a splitter between two streams were studied by Rehab et al. (1997) and Carlos et al. (2003). They reported that the outer shear-layer dynamics are dominant over the inner one, and its most amplified frequency can be predicted by the correlation proposed by Schadow and Gutmark (1992). Based on the same correlation, the most unstable frequencies of each shear layer in Cases 1 and 2 are estimated and presented in Table 6.3. The momentum thickness used in the correlation is estimated using the one-seventh power law for the velocity distribution. None of those predictions match the present simulation results. The existence of the second length scale (i.e. LOX post thickness) significantly changes the near field flow dynamics. The vortices shed from the LOX post tip in a manner analogous to the vortex generated behind a backward facing step, where the eddy-formation frequency is of order $O(0.1)$ in terms of the Strouhal number defined based on the bulk velocity of the outer stream and the step thickness (Wee et al., 2004). The obtained information, so far, indicates that the flow dynamics of high-pressure coaxial injection of oxygen and methane is different from its counterpart at low-pressure.

Table 6.3: The predicted initial vortex shedding frequency of each shear layer in Cases 1 and 2.

<table>
<thead>
<tr>
<th></th>
<th>outer layer</th>
<th>intermediate layer</th>
<th>inner layer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>45 kHz</td>
<td>45 kHz</td>
<td>3.7 kHz</td>
</tr>
<tr>
<td>Case 2</td>
<td>105 kHz</td>
<td>105 kHz</td>
<td>3.7 kHz</td>
</tr>
</tbody>
</table>
6.2.3 Mean Flowfields

The time-mean data is obtained by averaging the instantaneous quantity over 10 ms (about 12 flow-through times) after the calculated flowfield has reached its stationary state. Figure 6.10 presents the time-averaged axial velocity, turbulent kinetic energy (TKE), and oxygen mass-fraction fields of the two cases. For comparison purpose, the axial velocity and TKE are non-dimensionalized by the bulk velocity of the oxygen stream (10 m/s).

Since the outer stream is faster, it is dominant in the velocity field and spreads both outward and inward. A wake with negative axial velocity is generated behind the LOX post. It has been reported that if the velocity ratio between the inner and outer streams is greater than a critical value, the wake may extend to the central region to form a recirculation zone (Carlos et al., 2003). Although no recirculation is observed, the velocity of the oxygen stream decays rapidly due to the influence from the stronger wake in Case 2. TKE is low in the core region of the oxygen stream and readily increases along the centerline. The intensive vortical flow motions in the inner and outer shear layers give rise to two TKE concentration regions. Those regions merge downstream after the outer layer is engulfed into the center. The vigorous turbulent motion in Case 2 enhances the mixing process. Thus, the core of the LOX stream is reduced, and the oxygen is distributed wider as reflected in the mass-fraction field.

Figure 6.11 shows the radial distributions of the mean oxygen mass-fraction, density, axial velocity, and turbulent kinetic energy at various axial locations. The top-hat mass fraction profile close to the injector faceplate indicates the presence of a potential core of the oxygen stream. A similar core in the annular methane stream is manifested by the staged density distribution. The lengths of the inner and outer cores are reduced in Case 2. In addition, the relatively flatter oxygen mass-fraction distributions imply a better mixing downstream.
The high speed annular stream and the wake with negative axial velocity are indicated in the axial velocity distribution at $x/\delta = 2$. As the wake extends into the center, the centerline velocity decays ($x/\delta = 6$). The inner and outer shear layers are revealed by the peaks of the TKE distributions. They merge together at the axial locations $x/\delta = 10$ and 6 for Cases 1 and 2, respectively.

Figure 6.12 shows the time-averaged velocity vector fields downstream of the LOX post. For clarity, the vectors are specified with uniform length. A recirculation zone forms right behind the LOX post and extends $2\delta$ downstream in Case 1. Its end is roughly indicated by the circular mark in the flowfield. As the outer stream velocity increases in Case 2, two counter rotating bubbles are generated in the wake, and the length of the recirculation zone is elongated to $4\delta$. The effects of those structures on the flame-stabilization mechanisms will be studied in the subsequent research.

The axial distributions of time-average density, mass-fraction, velocity, and turbulent kinetic energy along the centerline are presented in Fig. 6.13. The density and mass fraction distributions remain unchanged until $x/\delta = 9$ and 6 for Cases 1 and 2, respectively, corresponding to the ends of the potential cores. The density and oxygen mass fraction then decrease rapidly downstream of the potential core and finally reach a constant. The centerline velocity first decreases due to the extension of the wake flow into the core region, and almost reaches a stagnation point at $x/\delta = 9$ in Case 2. The axial velocity then increases after the outer stream penetrates the centerline.

Villermaux and Rehab (2000) studied the co-axial injection of water over a wide range of velocity ratios. They proposed that the length of the inner potential core is inversely proportional to the velocity ratio

$$L/D = A \cdot (u_z / u_t)^{-1}$$  \hspace{1cm} (6.1)
where \( D \) stands for the inner jet diameter, and the constant \( A \) ranges from 6 to 8. To take into account the density difference between two streams, the velocity ratio in Eq. 6.1 could be replaced by the square root of the momentum ratio \( M^{1/2} = (u_2 / u_1)(\rho_2 / \rho_1)^{1/2} \) (Villermaux and Rehab, 2000). The resultant correlation takes the form

\[
L / D = A \cdot M^{-1/2}
\]

Based on this equation, the potential core lengths are estimated to be \( 12\delta \) and \( 9\delta \) for Cases 1 and 2, respectively. The values are greater than those obtained in the present simulation. It should be noted that the Eq. 6.2 does not consider the influence of the wake behind the LOX post, because the thickness of the splitter is small and thus be neglected in their experiments (Villermaux and Rehab, 2000). In the present study, the thickness of the LOX post and the diameters of the jets are on the same order of magnitude. The wake flow significantly influences the entire flow evolution. The energetic eddies shedding from the LOX post tip and their subsequent interactions facilitate the entrainment of the annular stream and give rise to a shorter inner potential core.

Based on the results discussed above, the near-injector flowfield could be characterized below. The two shear layers generated from the inner and outer rims of the LOX post merge after the wake and form the inner mixing layer. The oscillations generated from this layer play as force on the outer shear layer. The vortex shedding from the LOX post tip does not follow the fundamental Kelvin-Helmholtz mechanism, but rather in a manner analogous to that produced at a backward facing step. The oscillations generated from the vortex shedding serve as a forcing on the outer mixing layer.

In contrast to Case 1, methane is injected at a supercritical temperature in Case 2. To keep the same mass ratio, the outer stream velocity is increased. With the increase of the momentum flux ratio, turbulent mixing between the two streams is enhanced, and the potential
core of the LOX jet is reduced. This agrees with the experimental observations of Singla et al. (2004).

6.3 Summary

Various fundamental physiochemical mechanisms associated with injection and mixing of oxygen and methane of a shear coaxial injector operating at supercritical pressures have been investigated numerically. The effects of momentum flux ratio and injection fluid state on the near field flow evolution are studied systematically. The major results are summarized below.

1. The key phenomena associated with shear coaxial injection and mixing of oxygen and methane are identified. The near field dynamics can be characterized by the evolution of the inner and outer mixing layers.

2. Owing to the strong density stratification between the two streams, the formation of the large scale vortices at the LOX post tip does not follow the fundamental Kelvin-Helmholtz instability mechanism, but occurs in a manner analogous to that produced at a backward facing step.

3. The effects of momentum flux ratio on the flow evolution are demonstrated. As the injection velocity of the methane stream increases, turbulent mixing is enhanced. The cores of the inner and outer streams are reduced.
Figure 6.5: Snapshots of oxygen mass fraction and vorticity fields of shear coaxial injection of LOX and methane for Cases 1 and 2.
Figure 6.6: Mass fraction, density, vorticity, and velocity vector fields in the region near the LOX post for Cases 1 and 2 in Table 6.2.
Figure 6.7: Time evolution of vorticity field over one cycle of vortex pairing of Case 1 in Table 6.2.
Figure 6.8: Frequency spectra of the radial velocity oscillations along the inner and outer shear-layers, Case 1 in Table 6.2
Figure 6.9: Frequency spectra of the radial velocity oscillations along the inner and outer shear-layers, Case 2 in Table 6.2.
Figure 6.10: Time averaged axial velocity, turbulent kinetic energy (TKE), and oxygen mass fraction fields of Cases 1 and 2 in Table 6.2.
Figure 6.11: Comparison of the radial distributions of the time averaged density, oxygen mass fraction, axial velocity, and turbulent kinetic energy at the different axial locations for Cases 1 and 2 in Table 6.2.
Figure 6.12: Time-averaged velocity vector distributions near the LOX post of Cases 1 and 2 in Table 6.2.
Figure 6.13: Axial distributions of time-averaged density, oxygen mass fraction, axial velocity, and turbulent kinetic energy along the centerline.
Chapter 7

High-Pressure Cryogenic Propellant Swirl Injection

7.1 Problem Description

Compared with a shear coaxial injector, an injector with central LOX swirling (see Fig. 1.6) distinguishes itself in many aspects (Bazarov, et al. 2005). First, for the same pressure drop and liquid flowrate, the swirl injector could produce finer droplets, whose median diameter is 2.2 to 2.5-fold smaller than that of the shear injector. Second, a swirl injector is not sensitive to manufacturing errors, such as deviation from prescribed diameter and surface misalignment. In addition, its flow passage area is much larger than that of the shear ones with the same mass flowrate and consequently, the swirl injector is less susceptible to choking or cavitation. Although swirl coaxial injectors have been widely applied in liquid rocket propulsion systems, systematic investigations into their injection and combustion dynamics are lacking.

This chapter presents a series of simulations on the swirl injection of cryogenic fluid under supercritical pressures. Both the internal flow dynamics and the external mixing process of a swirl injector are investigated. Emphasis is placed on the effects of various scaling parameters on the injector performance. To help understand the physical phenomena involved, a theoretical model is established. Its predictions are consistent with the simulation results.

As a beginning, only the central LOX post of a coaxial injector is considered. It can be referred to as a simplex swirl injector, which includes three major parts: a tangential inlet, a vortex chamber, and a discharge nozzle, as shown in Fig. 7.1. The geometrical parameters of the studied injector are listed in Table 7.1. Presently, the diameters of the swirl chamber and the discharge nozzle are set identically. The geometrical characteristic constant \( K \) is defined as
\[ K = \frac{A_n R_n}{A_{in} R_{in}} \]

where \( R_n \) is the nozzle radius, \( R_{in} \) is the radial location of the inlet passage center, \( A_n \) is the nozzle area, and \( A_{in} \) is the total area of the inlet passages. A swirl injector with the same mass flowrate (0.15 kg/s) and similar geometry has been successfully applied to the RD-0110 liquid rocket engine.

![Swirl Injector Diagram](image)

Figure 7.1: Schematic of simplex swirl injector employed in the present study, 1-injector casing; 2-vortex chamber; 3-discharge nozzle, 4-tangential passages.

<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 7.1: Geometric parameters of the studied swirl injector.

The computation domain includes the swirl injector and a portion of the combustion chamber connected to it, as shown in Fig. 7.2. Because of the enormous computational effort required for simulating the flowfield in the entire three-dimensional region, only a cylindrical sector with periodic boundaries specified in the azimuthal direction is treated herein. For a typical simulation, a two-dimensional grid system is generated. A 50×100 grid is employed.
inside the injector, and a $150 \times 200$ grid is located outside. The grids are clustered near the wall to resolve the boundary layer and the rapid flow property variations. The mean grid size within the injector is around $50 \ \mu m$, which can roughly resolve the turbulence length scales in the inertial sub-range of the turbulent energy spectrum. The computational domain is divided into 13 blocks, with each calculated on a single processor of a distributed-memory parallel computer. The physical time step is $1 \times 10^{-2} \ ms$, and the maximum CFL number for the inner-loop pseudo-time integration is 0.7. For each case, simulation is conducted for 10 flow-through times (i.e., 0.1 s) to obtain statistically meaningful data.

Figure 7.2: Schematic of 2D axi-symmetric grid system at one-third of the original grid density.

Since it is impossible to simulate a round hole on the surface of the LOX post in an axi-symmetric space, the tangential passage is modified as a slit. At the inlet boundary, the mass flowrate and temperature are specified. The pressure is extrapolated from the inner flowfield. The radial and azimuthal velocities are determined from the tangential inlet injection angle. Turbulence properties at the inlet are specified by superimposing broad-band disturbances with an
intensity of 3% of the mean quantity onto the mean velocity profiles. The nonreflecting boundary conditions are applied at the exit boundary, along with the specification of a back-pressure. At the radial direction, a second order extrapolation with a fixed pressure is adopted. Finally, the non-slip adiabatic conditions are enforced to the inner surface of the injector and the solid wall connected to it.

7.2 Limitations of Quasi-Three-Dimensional Simulation

Since this work should ultimately be part of an engineering design process, a quasi-three-dimensional simulation is the reasonable choice as a good compromise between accuracy and computation cost. The quasi-three-dimensional implies that the full three-dimensional equations are employed with an axi-symmetric approximation. As a result, although the swirling effect could be considered, the variations and gradients in the azimuthal direction are neglected. Presently, this concept is implemented by treating a cylindrical sector of the domain (see Fig. 7.2) with period boundary conditions specified in the azimuthal direction. Assuming axi-symmetric flow configuration introduces several limitations (Menon, 2004):

1) The geometry of the studied injector is modified. The tangential inlets, which are six small round tubes connected to the swirl injector, are simplified as a thin slit on the surface of LOX post. The radial and azimuthal velocities are determined from the original inlet injection angle and the mass flowrate.

2) The variations and gradients in the azimuthal direction are neglected owing to the axi-symmetric assumption. Consequently, the interactions of flow structures in azimuthal direction and the azimuthal instability, which is important in swirling flow (Wang, 2002), cannot be taken into account. In addition, since vortex stretching and tilting is a three-dimensional process, it is neglected owing the limitation of quasi-three-dimensional simulation.
7.3 Simulation Results

Since surface tension vanishes and no droplet is formed at supercritical conditions, the parameters that can characterize the LOX swirling jets are the liquid film thickness \( h \) and the spray cone angle \( \alpha \) at the injector exit. Other physical variables needed to describe the flow evolution include the injector geometric constant \( K \), the injector length \( L \) and diameter \( D \), the axial and azimuthal velocities of the swirling flow, and the thermodynamic properties of the injected and ambient fluids. Based on the Buckingham Pi theorem, two dimensionless equations can be obtained:

\[
\frac{h}{D} = g\left(\frac{\rho_{\text{inj}}}{\rho_{\infty}}, \frac{\mu_{\text{inj}}}{\mu_{\infty}}, \text{Re}_L, K\right) \tag{7.1}
\]
\[
\tan \alpha / 2 = \tan^{-1} \frac{u_n}{w_n} = g\left(\frac{\rho_{\text{inj}}}{\rho_{\infty}}, \frac{\mu_{\text{inj}}}{\mu_{\infty}}, \text{Re}_L, K\right) \tag{7.2}
\]

The tangent of spreading angle \( \alpha \) can be calculated as the ratio of the axial velocity \( u_n \) to the azimuthal velocity \( w_n \) at the injector exit. \( \rho \) and \( \mu \) are the density and viscosity of the fluid, respectively. The subscript \( \text{inj} \) and \( \infty \) denote the injected and ambient conditions, respectively. The Reynolds number is defined as \( \text{Re}_L = \frac{\rho_{\text{inj}} u L}{\mu_{\text{inj}}} \). Among those parameters, density and viscosity ratios are determined by the operating conditions. Other parameters are related to the geometry of a swirl injector. Their influences on the injector performance will be studied in detail.

Liquid oxygen at a temperature of 120 K is injected into the swirl injector through the tangential passage. The temperature and pressure of the ambient gaseous oxygen remain at 100 atm and 300K, respectively. The pressure is below the combustion chamber pressure (200 atm) of the Space Shuttle Main Engine (SSME) but much higher than the critical pressure of oxygen (50.4 atm). The important scaling parameters studied are oxygen mass flowrate, LOX post length, tangential passage position, and swirl strength. The detail simulation conditions are
presented in Table 7.2, where ΔL is the distance between the inlet center and the injector head end.

Table 7.2: Test Conditions*

<table>
<thead>
<tr>
<th>Cases</th>
<th>Re_L (kg/s)</th>
<th>L (mm)</th>
<th>K (mm)</th>
<th>ΔL (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5.4×10^6</td>
<td>0.15</td>
<td>3.2</td>
<td>8.3</td>
</tr>
<tr>
<td>2</td>
<td>3.8×10^6</td>
<td>0.10</td>
<td>3.2</td>
<td>8.3</td>
</tr>
<tr>
<td>3</td>
<td>7.6×10^6</td>
<td>0.20</td>
<td>3.2</td>
<td>8.3</td>
</tr>
<tr>
<td>4</td>
<td>5.7×10^6</td>
<td>0.15</td>
<td>3.2</td>
<td>8.3</td>
</tr>
<tr>
<td>5</td>
<td>4.9×10^6</td>
<td>0.15</td>
<td>3.2</td>
<td>8.3</td>
</tr>
<tr>
<td>6</td>
<td>1.1×10^7</td>
<td>0.15</td>
<td>3.2</td>
<td>8.3</td>
</tr>
<tr>
<td>7</td>
<td>1.6×10^7</td>
<td>0.15</td>
<td>3.2</td>
<td>8.3</td>
</tr>
<tr>
<td>8</td>
<td>2.2×10^7</td>
<td>0.15</td>
<td>3.2</td>
<td>8.3</td>
</tr>
<tr>
<td>9</td>
<td>5.8×10^6</td>
<td>0.15</td>
<td>3.2</td>
<td>8.3</td>
</tr>
</tbody>
</table>

*p_∞=10MPa, \rho_{inj}/\rho_∞=7.6

Two important definitions should be clarified before we present the simulation results and compare them with the theoretical predictions.

Unlike most of the cold flow experiments that were conducted at standard pressure using water as oxidizer simulant, the chamber pressure of the present simulation is chosen close to the operating pressure of the SSME, which is well above the critical point of oxygen. Although the injected dense fluid still possesses liquid-like density and characteristics, there is no distinction between the injected fluid and the ambience due to the vanishment of surface tension and enthalpy of vaporization. This leaves us freedom to define the injected fluid boundary. In the early works regarding convective high-pressure droplet vaporization, Meng et al. (2005) argued that the critical temperature and critical mass fraction of oxygen-hydrogen mixture are not located at the same position without phase equilibrium, rendering the critical mixing state meaningless. Only the droplet boundary defined at the critical temperature of oxygen is physically meaningful and unique state. However, because part of the injected fluid is heated and the temperature could exceed the critical value, this definition becomes inaccurate in characterizing the liquid film.
thickness. Then, another definition based on mass conservation is introduced. The dense fluid boundary is defined at the radial position, where mass flowrate equals the initial value at the inlet.

In the classical inviscid theory, the spray cone angle is defined as twice the apex angle of the asymptotic cone to the hyperboloid of revolution corresponding to the profile of the spray (Tanasawa and Kobayasi, 1955). It can be calculated as the ratio of the circumferential to the axial velocities \( \tan \alpha / 2 = w_r / u_a \) at the exit. In the experiments, the spray cone has curved boundaries because the ambience gas was entrained into the injected fluid, which imposes a major difficulty in its measurement. The cone angle is generally quoted as the angle formed by two straight lines drawn from the discharge orifice to cut the spray contours at some specified distance from the injector exit (Ortman and Lefebvre, 1985). Presently, the angle is computed directly from its definition.

### 7.3.1 Flow Structures

The characteristics of a typical swirl injector flowfield are presented in Fig. 7.3. Cold liquid oxygen is introduced tangentially into the injector through circular holes or slots. Since the injected fluid has only the azimuthal velocity, a swirling liquid film forms and moves downstream along the inner wall. The strong radial pressure gradient resultant from centrifugal force prevents the injected fluid from penetrating into the central region, where a whirling air core, called cavity, is formed. Because the chamber pressure (100 atm) is higher than the critical pressure of oxygen (50.4 atm), no obvious boundary between the injected fluid and the air core is observed. The solid line on the density field is the critical isothermal \( T = 154.6 \) K, which roughly represents the boundary between the injected fluid and the ambience. As the cold oxygen fluid discharges into the combustion chamber, the swirling fluid film spreads away from the exit. Since the hot ambience is entrained into the injected fluid, the fluid density decreases during the
mixing and heating process, and its value exhibits a sudden drop across the critical isothermal. The azimuthal velocity and centrifugal force decrease simultaneously. Then, the flow passage shrinks toward the centerline. Near the injector exit, a slowly swirling gaseous region forms. The adverse pressure gradient in this region gives rise to recirculation flow and finally produces a central tornado recirculation zone (CTRZ). Presently, the recirculation flow even penetrates into the LOX post. The extension of the recirculation region (wake region) into the discharge nozzle was also observed by Panda and McLaughlin (1994) in the experimental study on swirling jet instabilities at high swirl and large Reynolds numbers. They attributed it to the earlier burst of vortices. In the combustion chamber, the CTRZ could serve as a flame stabilization region, where the hot products are mixed with the incoming fuel and oxidizer mixture.

Figure 7.4 presents the mean velocity components, temperature, density, and compressibility distributions in radial direction at various axial locations. Based on the different evolution patterns observed, the flow motions inside the LOX post could be divided into three stages. At the developing stage ($0 \leq x \leq 6\, \text{mm}$), the injected fluid with strong swirling fills more than half of the tube, and the azimuthal velocity reaches the maximum magnitude at the dense fluid boundary. Compared with it, the axial velocity is smaller. The injected fluid shrinks to the wall promptly due to the centrifugal force. Meanwhile, the momentum transfers from its azimuthal component to the axial one. A balance is reached in the stable region ($6 \leq x \leq 23\, \text{mm}$), where the radial distributions of flow properties (i.e., velocity, film thickness, and thermophysical properties) vary slowly along the axial direction. For example, only slightly variations of the axial velocity profiles can be observed at the axial positions $x = 10\, \text{mm}$ and $18\, \text{mm}$. Inside the fluid layer, a thin boundary layer is generated, where the velocity components increase quickly from zero at the wall to a relative flat profile in the film. Since the length to diameter ratio ($L/D$) of the injector is much greater than that of the conventional swirl atomizer, viscous loss, which has been ignored in the classical theory, influences the axial and azimuthal velocity
distributions, and should be included in an improved analytical model. Because the static pressure at the outlet equals the ambient pressure, the overpressure resultant from centrifugal force is transformed into the momentum flux, which gives rise to an acceleration of axial velocity with a decreasing in the film thickness near the injector ($23 \leq x \leq 25mm$).

The injected fluid discharges into the chamber as a hollow-cone sheet. After it interacts and mixes with the ambient gaseous oxygen, both the axial and the azimuthal velocities decay. At the axial position $x = 40mm$, the velocity distributions become flat with a recirculation region appearing in the chamber center, as indicated in Fig. 7.3.

In those profiles, no distinct boundary between the injected fluid and the ambient gas is observed. The thermo-physical properties of oxygen, including density, temperature, and compressibility factor, vary continuously in radial direction. The axial and azimuthal velocities change smoothly, too. In classical theory, the interaction between liquid and gas is neglected, and a solid body rotation with zero axial velocity is assumed for the core. To accurately model the swirl injector behavior at high-pressure, the transient fluid property variations and the interaction between the dense fluid and gaseous environment should be considered.

The existence of the three different flow patterns, again, is illustrated in Fig. 7.5, in which the liquid film thickness along the wall is presented. Close to the head end, the flow motion in the azimuthal direction is dominant. The dense fluid with strong swirling penetrates deeply into the center. The film thickness reaches the maximum right at the head end. The fluid shrinks to the wall until a minimum thickness is achieved at $x=6mm$. After that, the film thickness starts a monotonic increase with the boundary layer development. It drops promptly at the injector exit because the centrifugal over pressure transfers to the dynamic pressure, and the axial velocity is accelerated.

The differences between the critical isothermal and the injected fluid boundary based on the mass conservation are also manifested in Fig. 7.5. Because the cold fluid is heated by the hot
ambience and its temperature could exceed the critical value (154.6 K), the critical isothermal always tends to move toward the inner wall of the LOX post, whereas, the film thickness increases along the wall. The critical isothermal could not accurately represent the injected fluid boundary. To fully take into account the transient fluid property variations and the viscous loss, only the thickness defined based on mass conservation is proper. The predictions from the viscous correction discussed hereafter, obviously, are smaller than the numerical simulation results since the model does not accommodate the transient fluid property variations in the radial direction.

The temporal evolution of the temperature fields within one cycle of the vortex shedding is plotted in Fig. 7.6. Excited by the initial turbulence input at the tangential inlet, a succession of wavy structures with small amplitude forms and is convected downstream around the dense fluid boundary. In a rocket system, those waves are generated due to the presence of intense oscillation inside the combustion chamber or propellant feed-line (Bazarov and Yang, 1998). As the cold oxygen is discharged into the chamber, a sinuous spanwise Kelvin-Helmholtz billows develop along the outer boundary of the fluid cone. As these billows are carried downstream, a hairpin vortice appears and grows up. This vortice then interacts and merges together with other vortices. The flow oscillations are transferred back to the upstream location through the central recirculation zone and provide the feedback necessary for the onset of the next series of instability waves. A self-sustained instability phenomenon exists. Its frequency is locked by the characteristic length and velocity of the recirculation zone. In Case 3, the length scale of the CTRZ is around 10 mm, and its characteristic velocity is order of tenth. The frequency is approximated as \( f = \frac{10}{0.01} \approx 1.0 \times 10^3 \text{Hz} \). Figure 7.7 presents the power spectral densities of the pressure fluctuations at six different locations for Case 3. A pressure oscillation at 836 Hz, which is the same order as the value estimated, is observed both outside and inside the injector.
7.3.2 Effects of Important Design Parameters on the Swirl Injector Performance

7.3.2.1 Mass Flowrate

Figure 7.8 shows the effect of mass flowrate on the axial distribution of the film thickness. The trends are almost the same. At the beginning, the injected fluid fills more than half of the tube. It, then, shrinks to the wall until reaching a minimum. With the development of the boundary layer, the thickness increases as the fluid moves downstream. It suddenly drops near the exit. Based on the classical inviscid theory (Bazarov et al., 2005), the liquid film thickness at the injector exit is independent of the mass flowrate. This assumption has been re-examined by several researchers in the cold flow experiments at standard pressure. It is reported that mass flowrate has only moderate influence on the film thickness. The differences among three cases are small in the present simulation. The liquid film thickness at the injector exit decreases with the increasing of mass flowrate, a trend consistent with boundary layer theory.

The thicknesses and the spray cone angles at the injector exit are list in Table 7.3. The subscripts vis and inv represent the prediction using classical inviscid theory and that of the viscous correction model derived in the next section, respectively. All the three liquid film thicknesses are greater than the predictions with viscous correction because present model does not take into account the transient density variations. In the classical inviscid theory, the cone angle is only a function of the injector geometry. Our simulation results indicate that it is weakly dependent on mass flowrate. The calculated angles are much smaller than those predicted by inviscid theory. This discrepancy was also noted by Rahman et al. (1995) and Dombrowski and Hasson (1969) in the cold flow experiments at low pressure, which was attributed to the more rapid decay of the tangential velocity than the axial one due to the viscous loss along the wall.
Table 7.3: Effect of mass flowrate on dense fluid film thickness and spray cone angle.

<table>
<thead>
<tr>
<th>Case</th>
<th>$m$ (kg/s)</th>
<th>$h$ (mm)</th>
<th>$h_{nv}$ (mm)</th>
<th>$h_{inv}$ (mm)</th>
<th>$\tan \alpha / 2$</th>
<th>$(\tan \alpha / 2)_{inv}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>0.10</td>
<td>0.686</td>
<td>0.56</td>
<td>0.631</td>
<td>0.752</td>
<td>1.04</td>
</tr>
<tr>
<td>Case 2</td>
<td>0.15</td>
<td>0.660</td>
<td>0.56</td>
<td>0.627</td>
<td>0.749</td>
<td>1.04</td>
</tr>
<tr>
<td>Case 3</td>
<td>0.20</td>
<td>0.632</td>
<td>0.56</td>
<td>0.625</td>
<td>0.744</td>
<td>1.04</td>
</tr>
</tbody>
</table>

Figure 7.9 presents the snapshots of temperature fields of Cases 1 to 3. As the mass flowrate increases, the vortex rolls up relatively later, and the flow pattern becomes more complicated downstream. Figure 7.10 shows the power spectral density of the pressure oscillations at two axial locations for three cases. Since vortex shedding frequency at the injector exit is locked by the length of the recirculation zone, which is enlarged with enhanced mass flowrate, the characteristic frequency is slightly reduced.

### 7.3.2.2 Slit Position

Figure 7.11 presents the effect of the tangential slit position on the dense fluid boundary. The film thickness slightly increases as the distance between the tangential slit and the head end increases. It is contradictory to boundary layer theory. Basically, as the slit position moves downstream, the displacement thickness decreases at the injector exit, and so does the film thickness. The reason is examined in Fig. 7.12, where the streamline patterns near the head end are presented. In Case 5, part of the injected fluid moves upstream to fill the volume between the tangential slit and the head end. This filling process causes an extra momentum loss and renders the film thickness thicker at the upstream than that of Case 4. In both two cases, a portion of streamlines originating from the dense fluid passes across the critical isothermal, which illustrates that the cold fluid is heated and its temperature exceeds the critical value.
In Table 7.4, the maximum spray cone angle is obtained when the slit is placed very close to the head end. Since the film thickness also reaches the minimal value at this position, an optimal injector performance could be obtained. However, a constant mass flowrate is specified at the inlet in the present simulation. In the application, if the tangential inlet is placed very close to the head end, a greater pressure drop between the feed line and the combustion chamber should be employed to overcome the viscous loss at the head end and to maintain the same mass flowrate. The inlet location should be chosen based on the following rules: 1) stable flow motion at the injector exit; 2) a minimal momentum loss; 3) wide spreading angle and thin liquid film.

Table 7.4: Effect of slit position on film thickness and spray cone angle.

<table>
<thead>
<tr>
<th>Case</th>
<th>( \Delta L ) (mm)</th>
<th>( h ) (mm)</th>
<th>( h_{inv} ) (mm)</th>
<th>( h_{vis} ) (mm)</th>
<th>( \tan \alpha / 2 )</th>
<th>( (\tan \alpha / 2)_{inv} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 4</td>
<td>0.5</td>
<td>0.660</td>
<td>0.56</td>
<td>0.63</td>
<td>0.781</td>
<td>1.04</td>
</tr>
<tr>
<td>Case 2</td>
<td>1.5</td>
<td>0.660</td>
<td>0.56</td>
<td>0.627</td>
<td>0.749</td>
<td>1.04</td>
</tr>
<tr>
<td>Case 5</td>
<td>4.5</td>
<td>0.672</td>
<td>0.56</td>
<td>0.62</td>
<td>0.760</td>
<td>1.04</td>
</tr>
</tbody>
</table>

7.3.2.3 LOX Post Length

Owing to the propellant supply manifolding considerations, the length to diameter ratio of the liquid rocket swirl injector is much greater than that of the conventional swirl atomizer. As a result, the viscous loss along the wall affects the injection process and hence alters the spray distribution and atomization efficiency. Inamura et al. (2003) investigated the effect of viscous loss on the liquid fluid film thickness at the standard pressure. A two-dimensional theoretical model was constructed based on the flat plate boundary layer theory. Figure 7.13 compares their results with the viscous corrections given in section 7.4. The present model, which is derived for a circular duct, gives more accurate result than Inamura’s theory does. However, the predictions are still smaller than those obtained from numerical simulation since only the viscous loss is
taken into account in our model. To include the density variations in the radial direction, a reasonable density profile is needed in the mass and momentum conservation integrations. This requires tremendous numerical or experimental efforts, which is beyond the scope of this work. The spray cone angles are listed in Table 7.5. They reduce as the injector length increases. Since the friction force along the wall retards both the axial and azimuthal velocities, the obtained information indicated that the axial momentum decays relatively slower than does the swirling motion. The elongation of injector damages its performance in two aspects: (1) momentum loss along the wall with the growth of film thickness; (2) decrease of the spreading angle and the reduction in the spatial distribution of the injected fluid.

Table 7.5: Effect of LOX post length on the dense fluid film thickness and spray cone angle.

<table>
<thead>
<tr>
<th>Case</th>
<th>L (mm)</th>
<th>h (mm)</th>
<th>h_{inv} (mm)</th>
<th>h_{vis} (mm)</th>
<th>\tan \alpha / 2</th>
<th>\left(\tan \alpha / 2\right)_{inv}</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>25</td>
<td>0.660</td>
<td>0.56</td>
<td>0.627</td>
<td>0.749</td>
<td>1.04</td>
</tr>
<tr>
<td>6</td>
<td>50</td>
<td>0.709</td>
<td>0.56</td>
<td>0.681</td>
<td>0.747</td>
<td>1.04</td>
</tr>
<tr>
<td>7</td>
<td>75</td>
<td>0.738</td>
<td>0.56</td>
<td>0.717</td>
<td>0.727</td>
<td>1.04</td>
</tr>
<tr>
<td>8</td>
<td>100</td>
<td>0.796</td>
<td>0.56</td>
<td>0.744</td>
<td>0.698</td>
<td>1.04</td>
</tr>
</tbody>
</table>

7.3.2.4 Geometric Characteristic Number

The characteristic number “K” of a swirl injector is defined as \( K = \frac{A_n R_{in}}{A_{in} R_n} \). A large “K” is obtained when the tangential inlet area is small and the discharge nozzle is wide. Such a swirl injector could produce stronger swirling motion, which finally gives rise to the thinner liquid film thickness and the wider spray cone angle. Corresponding to the increase of \( K \), either the inlet area or discharge nozzle should be modified. In the present simulation, this is achieved by changing the radial to azimuthal velocity ratio at the inlet.
Figure 7.14 presents the variations of the film thickness along the injector wall. The strong swirling motion in Case 9 results in a greater radial pressure gradient, which pushes the dense fluid film closer to the wall. Due to the increase in the azimuthal velocity, the spray cone angle \( \tan \alpha / 2 \) enlarges from 0.75 to 0.95 (see Table 7.6). Since a thinner film determines the finer spray droplet and a wider spray cone angle enhances the intrainjector mixing efficiency, a better injector performance could be achieved by increasing \( K \).

Table 7.6: Effect of swirl strength on the dense fluid film thickness and spray cone angle.

<table>
<thead>
<tr>
<th>Case</th>
<th>( K )</th>
<th>( h ) (mm)</th>
<th>( h_{inv} ) (mm)</th>
<th>( h_{vis} ) (mm)</th>
<th>( \tan \alpha / 2 )</th>
<th>( \tan \alpha / 2 )_{av}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 2</td>
<td>3.2</td>
<td>0.660</td>
<td>0.56</td>
<td>0.627</td>
<td>0.749</td>
<td>1.04</td>
</tr>
<tr>
<td>Case 9</td>
<td>4.2</td>
<td>0.595</td>
<td>0.5</td>
<td>0.564</td>
<td>0.950</td>
<td>1.27</td>
</tr>
</tbody>
</table>

Enhancing the swirl strength has enormous effects on the flow dynamics both inside and outside the injector. Figure 7.15 compares the mean streamline patterns between Cases 2 and 9. As the characteristic number increases, the central recirculation zone elongates in both the radial and axial directions. The recirculation flow penetrates into the swirl injector. The flow passage of injected fluid is partly blocked by the recirculation flow, which makes the dense fluid distribute wider. Fig. 7.16 presents the power spectral density of pressure oscillation of Case 9 at Probes 1 and 5. Though the length scale of the recirculation zone is longer than that of Case 1, the characteristic velocity associated with this case is also enhanced. Therefore, the dominant vortex shedding frequency increases. Furthermore, appearing of broad-band spectral both up and downstream implies that more small scale vortices are generated.
7.4 A Viscous Correction on Classical Swirl Injector Theory

The fundamentals of swirl injector theory were established more than 60 years ago by Abramovich in 1944 and independently by Taylor in 1947. The up to date discussion of the classical theory, which is particularly easy of implementation, was presented by Bazarov et al. (2005) and Bayvel and Orzechowski (1993).

Although the classical theory is straightforward, it has two intrinsic limitations (Yule and Chinn, 1994). First, it ignores axial momentum conservation. If axial momentum balance is combined with mass and energy conservation, a more rigorous approach could be derived. Second, viscous effect is totally neglected. Compared with a conventional swirl atomizer, a liquid rocket swirl injector is featured for its large length to diameter ratio. Then, the viscous loss along the wall could result in considerable deviation.

Inamura et al. (2003) investigated the effect of viscous loss on the liquid film development at standard pressure. A two-dimensional theoretical model was constructed based on the flat-plate boundary layer theory. In the present work, their method is extended to accommodate axisymmetric injector configuration. The displacement effect of the boundary layer in a swirl injector is indicated in Fig. 7.17.

If only flow motion in the axial direction is considered, the mass conservation for the boundary layer inside the liquid film is

\[ 2\pi \int_{R - \delta(x)}^{R} \rho u(r) rdr = 2\pi \int_{R - \delta(x)}^{R} \rho u(r) rdr \]  \hspace{1cm} (7.3)

where \( \delta(x) \) is the displacement thickness and \( h'_0 \) is the thickness of the fluid where the first streamline out of the shear layer started. This equation can be rearranged as

\[ 2\pi \int_{R - h'_0}^{R} \rho u^2(r) rdr = 2\pi \int_{R - \delta(x)}^{R} \rho u u(r)rdr \]  \hspace{1cm} (7.4)

Momentum conservation is
where $D$ is the friction force along the wall. Substitute Eq. 7.4 into Eq. 7.5

$$D = 2\pi \int_{R_s - \delta(x)}^{R_s} \rho u^2(r)(u_s - u(r))rdr$$

(7.6)

Following the boundary layer theory, a momentum thickness, $\theta$, is defined for the liquid film inside the circular injector

$$D = 2\pi R_s \rho u_s^2 \theta$$

(7.7)

Equating Eq. 7.6 and Eq. 7.7, then, $\theta$ can be written as

$$\theta = \frac{1}{R_s} \int_{R_s - \delta(x)}^{R_s} \rho \frac{u(r)}{u_s}(1 - \frac{u(r)}{u_s})rdr$$

(7.8)

The friction force along the wall also can be expressed as

$$D = 2\pi R_s \int_{0}^{x} \tau_w(x)dx \quad \text{or} \quad \frac{dD}{dx} = 2\pi R_s \tau_w(x)$$

(7.9)

Equating Eq. 7.7 to Eq. 7.9, the relation of $\theta$ and $\tau_w$ is established

$$\frac{d\theta}{dx} = \frac{\tau_w(x)}{\rho u_s^2} = \frac{1}{2}c_f$$

(7.10)

where $c_f$ is the skin friction coefficient. For high-pressure supercritical fluid, the fluid Reynolds number is much higher than its counterpart at low pressure. As a result, turbulent boundary layer starts at a short distance (around 1-2 mm) away from the tangential inlet. Based on Prandtl’s power law suggestion for turbulent flow, we have $c_f = 0.02 Re_\delta^{1/2}$. The one-seventh power law velocity profile is adopted for the axial velocity distribution.

$$\frac{u}{u_s} = \left(\frac{R_s - r}{\delta(x)}\right)^{1/7} \quad (R_s - r \geq \delta(x))$$

(7.11)

Substituting Eq. 7.11 into Eq. 7.8, the momentum thickness $\theta$ can be integrated, which is
Inserting Eq. 7.12 into Eq. 7.10, a formulation related displacement thickness $\delta(x)$ and the injector length $x$ is obtained

$$d\delta \over dx = \frac{0.02 \text{Re}_{\delta}^{-1/6}}{(72 - \frac{7}{120} \frac{\delta}{R_n})}$$

(7.13)

Since $\delta = 0$ at $x = 0$, Eq. 7.13 can be integrated from 0 to $x$. If $\delta(x)$ is known, the liquid film thickness can be solved based on the mass conservation. However, if the tube is long enough, the displacement thickness $\delta(x)$ may exceed the liquid film thickness $h(x)$. In order to accommodate this situation, the axial position $x_i$, where $\delta(x) = h(x)$, can be calculated based on the momentum conservation.

$$2\pi \int_{R_n-h_0}^{R_n} \rho u_r^2 r dr - 2\pi \int_{R_n-\delta(x)}^{R_n} \rho u_r^2 r dr = 2\pi r_i \int_0^{x_i} \tau_w(x) dx$$

(7.14)

Because $\delta(x)$ and $\tau_w(x)$ are only function of $x$, $x_i$ can be solved iteratively from Eq. 7.14.

Finally, when $L \geq x_i$

$$r_{mn} = \sqrt{(R_n - \delta)^2 + 2\left[\frac{7}{8} R_n \delta - \frac{7}{15} \delta^2\right] - \frac{Q}{\pi u_s}}$$

(7.15)

When $L < x_i$, $r_{mn}$ can be iteratively solved by the Newton-Raphson method through Eq. 7.16

$$\left[R_n^2 - (R_n - h_0)^2\right] - 2\delta^{-1/7} \left[\frac{7}{8} R_n r_{mn}^{6/7} - \frac{7}{15} r_{mn}^{15/7}\right] = 0$$

(7.16)

The original liquid film thickness $h_0$ and velocity $u_s$ are evaluated by the classical inviscid theory.
7.5 Summary

The flow evolution inside and outside a swirl injector is investigated numerically. The effects of mass flowrate, tangential slit position, injector length, and geometrical characteristic number on the injector performance are studied. The major results are summarized below:

1. The present analysis allows for a detailed investigation into the temporal and spatial evolution of the flowfield both inside and outside the swirl injector under supercritical conditions. The features which distinct high-pressure swirling injection from its counterpart at low-pressure are noted.

2. The parametric study illustrates that both the dense fluid film thickness and the spray cone angle weakly depend on the mass flowrate. Therefore, a larger oxidizer swirl element with greater mass flowrate than that of the shear coaxial injector still can obtain the required intraelement mixing efficiency.

3. The tangential inlet position has significant influence on the flow evolution. If the slit is located away from the head end, part of the injected fluid will move upstream to fill the gap between the slit and the end wall, which impairs the injector performance.

4. Increasing the geometric characteristic number of the injector results in a thinner film thickness and a wider spray cone angle. This suggests that a better injector performance could be achieved by enlarging the discharge nozzle exit or reducing the tangential inlet area.
Figure 7.3: Mean density and velocity components fields ($p_\infty = 10 \, MPa$, $T_{\text{pay}} = 120 \, K$, $T_\infty = 300 \, K$, $\dot{m} = 0.2 \, kg/s$, $K = 3.2$).
Figure 7.4: Radial distributions of mean velocity components, temperature, density, and compressibility factor at various axial locations ($\dot{m} = 0.2 \text{ kg/s} \ , \ K = 3.2$).
Figure 7.5: The dense fluid film thickness along the injector inner wall ($p_w = 10 \, MPa$, $T_{w} = 120 \, K$, $T_{c} = 300 \, K$, $m = 0.2 \, kg/s$, $K = 3.2$).
Figure 7.6: Temporal evolution of temperature field over one cycle of the dominant vortex shedding process ($p_n = 10 \text{ MPa}$, $T_{inj} = 120 \text{ K}$, $T_o = 300 \text{ K}$, $m = 0.2 \text{ kg/s}$, $K = 3.2$).
Figure 7.7: Power spectral densities of the pressure fluctuations at six different axial locations ($P_e = 10\, MPa$, $T_{inj} = 120\, K$, $T_0 = 300\, K$, $\dot{m} = 0.2\, kg/s$, $K = 3.2$).
Figure 7.8: Effect of mass flowrate on the film thickness.
Figure 7.9: Effect of mass flowrate on the temperature fields.
Figure 7.10: Effect of mass flowrate on the power spectral density of the pressure oscillations.
Figure 7.11: Effect of slit position on the film thickness.
Figure 7.12: Effect of slit position on the pseudo streamline patterns near the head end.
Figure 7.13: Comparison of liquid film thickness predicted from different theoretical models and the simulation results.

Figure 7.14: Effect of the swirl strength on the film thickness.
Figure 7.15: Effect of swirl strength on the pseudo streamline patterns.

Figure 7.16: The power spectral density of pressure oscillations at different axial locations ($p_o = 10\, MPa$, $T_{inj} = 120\, K$, $T_o = 300\, K$, $m = 0.2\, kg/s$, $K = 4.2$).
Figure 7.17: Schematic of displacement effect in a swirl injector.
Chapter 8

Conclusions and Recommendations

8.1 Conclusions

This research addresses a wide variety of basic and practical issues related to modeling high-pressure cryogenic propellants mixing and combustion processes. In particular, a comprehensive numerical analysis has been established to investigate the dynamics of high-pressure fluid mixing and combustion based on a large-eddy-simulation technique. The model accommodates full conservation laws and real-fluid thermodynamics and transport phenomena. All of the thermophysical properties are determined directly from fundamental thermodynamics theories, along with the use of the corresponding state principles. In addition, a unified treatment of general fluid thermodynamics is developed and implemented into an all-Mach number preconditioning scheme, which rendering a robust and self-consistent numerical method valid for fluid flows at all speeds and at all thermodynamic states. The theoretical and numerical framework described above is validated against a wide range of flow problems in order to establish its creditability and accuracy.

The dynamics of a nitrogen fluid jet is studied systematically over a broad range of ambient pressure. Both the two- and three-dimensional simulations are conducted. The simulation conditions match the experiments of Chehroudi et al. (2002). A good agreement is obtained between the numerical and experimental results in terms of the mean fluid density and the jet visual spreading angle. The jet dynamics is largely dictated by the local thermodynamic state through its influence on the fluid thermophysical properties. When the fluid temperature transits across the inflection point on an isobaric density-temperature curve, the resultant rapid
property variations may qualitatively modify the jet behavior. Owing to the differences of fluid states and flow conditions between the jet and surroundings, a string of strong density-gradient regimes is generated around the jet surface and exerts a stabilizing effect on the flow development. It acts like a solid wall that transfers the turbulent kinetic energy from its axial to radial component. The spatial growth rate of the surface instability wave is inhibited by the density stratification. The frequency of the most unstable mode exhibits a weak pressure dependence at high pressures. It, however, decreases significantly in the near-critical regime due to the enhanced effect of density stratification and increased mixing-layer momentum thickness. The result agrees well with the linear stability analysis. A suddenly volume expansion occurs in the transition region as the injected fluid is heated by the hot ambience, which significantly affects both the mean and turbulence properties. The supercritical fluid jet could be characterized into three regimes: a potential core with strong density stratification, a transition region accompanying with severe volume expansion, and a variable density gaseous jet downstream. Simply treating it as a variable-density incompressible jet could cause unexpected error in the near-field.

The validated model is applied to examine key phenomena associated with shear co-axial injection of LOX and methane. Based on the results obtained, the near field dynamics could be characterized as the evolution of the inner and outer mixing layers, because the two shear layers generated from the upper and lower tips of the LOX post merge together immediately after the wake and form an inner vortex string. This layer is dominant in the flowfield. The oscillations associated with the vortex shedding from it sever as a forcing on the outer mixing layer. The formation of those vortices does not follow the hydrodynamic instability mechanism, but is in manner is analogous to that produced at a backward facing step. The dominating effects of the velocity ratio on the near field flow evolution are also demonstrated. As the injection velocity of the methane stream increases, turbulent mixing is enhanced and the potential core of the LOX jet
is reduced. This agrees with the experimental observations of Singla et al. (2004). If the velocity ratio between the outer and inner streams further increases, the wake region may extend to the centerline and generate a recirculation zone.

The last part of the thesis presents a parametric study on the swirl injection of cryogenic oxygen under supercritical pressure. The influences of various geometric parameters and operation conditions, including mass flow rate, tangential slit position, injector post length, and swirl strength on the injector dynamics and performance were investigated systematically. Mass flow rate plays a minor role in dictating the swirl injector performance in terms of the liquid film thickness and spray cone angle. The slit position, which has tiny effect on the spray cone angle, could strongly affect the liquid film thickness. The film thickness increases as the distance between the tangential slit and the head wall increases. Elongation of injector causes a great momentum loss in the azimuthal direction and a reduction in spray cone angle. Increasing the swirl strength, which could be achieved by changing the injector geometrical constant (K), results in a decrease in the liquid film thickness and an increase in the spray cone angle. To help understand the physical phenomena involved, a theoretical model is also established. Its predictions are consistent with the simulation results.

8.2 Recommendations for Future work

The focus of the present study is placed on the development of a comprehensive numerical model, which could be applied to the entire fluid state of concern. However, the real fluid equation of state can not be solved in a completely non-iterative manner in the context of compressible Navier-Stokes simulations using the mass and energy conservation equations. The intensive iterations at each grid point and time step are overly taxing for three-dimensional simulation and prohibit it from engineering application. In order to overcome this difficulty, a
completely explicit solution technique is needed. The best approach is an accurate curve fit methodology in the state space which could provides the density explicitly as a function of the temperature, pressure, and mass fractions. The method was recently tested and will be implemented.

Although the non-equilibrium thermodynamic effects from which species concentrations diffuse due to temperature gradients (Soret effect, or “thermal-diffusion”) and thermal energy diffuse due to concentration gradients (Dufour effect, or “diffusion-thermal”) has unnoticeable influence on the large energy containing flow motions, it could be very important for the transport processes in the subgrid scale level. However, the sgs model adopted in the present work is a static Smagorinsky model established for compressible turbulence investigation, in which the cross diffusion effect is neglected. Developing and implementation of a subgrid scale model that could accommodate general fluid mixture under supercritical pressure is challenging.

The resolved-scale chemical source terms have been approximated only using resolved field quantities in the present combustion model, while the effects of the subgrid-scale fluctuations are neglected. Such an assumption is valid only for cases in which reactions are slow relative to the time scales associated with the decay of the species fluctuations, which is rarely the case in contemporary combustors, and becomes decreasingly valid with increasing pressure. The use of gradient diffusion terms to model turbulence species transport is also questionable due to the effect of heat release on the subgrid-scale turbulence field. A state-of-art turbulent combustion model, such as linear-eddy-model (LEM), filtered-density-functions (FDF), or conditional-moment-closure (CMC), should be implemented in the future work.
Bibliography

Abramovich, G. N., *Applied Gas Dynamics*, Nauka, Moscow, Russia, 1976


Appendix A

Properties of the Favre Average (Based on Reynolds Average)

The Favre average is defined as

$$\tilde{f} = \frac{\rho f}{\rho}$$  \hspace{1cm} (A.1)

then,

$$\rho f = \rho(\tilde{f} + f') = \rho \tilde{f} + \rho f' = \frac{\rho f + \rho f'}{\rho + \rho f'} = \rho \tilde{f} + \rho f'$$

thus,

$$\frac{\rho f'}{\rho} = 0$$  \hspace{1cm} (A.2)

in the mean time,

$$\tilde{f} = \frac{\rho f}{\rho} = \frac{(\rho + \rho')(\tilde{f} + f')}{\rho + f'} = \frac{\rho \tilde{f} + \rho f'}{\rho} = \tilde{f} + \frac{\rho f'}{\rho}$$  \hspace{1cm} (A.3)

on the other hand, \(\frac{\rho f}{\rho} = \tilde{f} + f'\), then

$$\rho f' = \tilde{f}$$  \hspace{1cm} (A.4)

by definition, we have, \(\rho f = \tilde{f} = \tilde{f} \),

$$\tilde{f} = f$$  \hspace{1cm} (A.5)

another important relation is:

$$\frac{\rho fg}{\rho} = \rho(\tilde{f} + f')(\tilde{g} + g') = \tilde{f}g + \tilde{f}g' + f'\tilde{g} + f'g' = \frac{\rho f'g + \rho f'g'}{\rho}$$  \hspace{1cm} (A.6)
Appendix B

Thermodynamic Relationships

Based on the Soave-Redlich-Kwong equation of state, the following derivative expressions, which are used extensively in property evaluations and numerical Jacobians, can be directly written as

\[
\left( \frac{\partial p}{\partial T} \right)_{\rho_j} = \frac{\rho R_u}{(M_w - b \rho)} - \frac{1}{M_w} \left[ \frac{\partial}{\partial T} \left( a \alpha \right) \right]_{\rho, Y_j} \left( M_w + b \rho \right)
\] (B.1)

\[
\left( \frac{\partial p}{\partial \rho} \right)_{T, Y_j} = \frac{M_w R_u T}{(M_w - b \rho)^2} - \frac{a \alpha}{M_w} \frac{\rho (2M_w + b \rho)}{(M_w + b \rho)^2}
\] (B.2)

\[
\left( \frac{\partial p}{\partial \rho_i} \right)_{T, \rho_{j \neq i}} = \frac{M_w R_u T}{M_w (M_w - b \rho)^2} \left[ M_w + \rho (b_i - b) \right] - 2 \rho \sum_j x_j a_{ij} \alpha_{ij} \frac{\rho}{M_w (M_w + b \rho)} + \frac{a \alpha b_i \rho^2}{M_w (M_w + b \rho)^2}
\] (B.3)

where the indexes \( i, j = 1 \cdots N \), and the derivative \( \frac{\partial}{\partial T} \left( a \alpha \right) \) is given in Appendix C.

It should be noted that these derivatives could be derived based on any equation of state following the fundamental thermodynamics.

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

\[
e(T, \rho) = e_0(T) + \int_0^\rho \left[ \frac{P}{\rho^2} - \frac{T}{\rho^2} \left( \frac{\partial p}{\partial T} \right)_T \right] d\rho
\] (B.4)
where the subscript 0 indicates a reference ideal state at a low pressure.

Utilizing SRK equation of state and the partial derivative relation Eq. B.1, Eq. B.4 is integrated, which leads to the following relationship

\[
e(T, \rho) = e_0(T) + \frac{T^2}{bM_w} \left( \partial a \alpha / \partial T \right)_{\rho, Y_j} \ln \left( 1 + \frac{b \rho}{M_w} \right) \tag{B.5}
\]

where the partial derivative \( \partial a \alpha / \partial T \) is presented in Appendix C.

According to the definition for the partial density property, the partial density internal energy (\( \bar{\varepsilon}_j \)) can be expressed as

\[
\bar{\varepsilon}_i = e_{i,0} + \frac{2}{bM_{wi}} \left[ \sum_j T \frac{\partial}{\partial T} (a_{ij} \alpha_{ij}) - a_{ij} \alpha_{ij} \right] \ln \left( 1 + \frac{b \rho}{M_w} \right) + \frac{b_i}{bM_{wi}} \left[ T \frac{\partial}{\partial T} (a \alpha) - a \alpha \right] \frac{\rho}{M_w + b \rho} - \frac{1}{b} \ln \left( 1 + \frac{b \rho}{M_w} \right) \tag{B.6}
\]

In addition, utilizing Eq. B.6, the internal energy of a mixture can be related to the partial density internal energy as

\[
e = \sum_i Y_i \bar{\varepsilon}_i - \frac{1}{M_w} \left[ T \frac{\partial}{\partial T} (a \alpha) - a \alpha \right] \frac{\rho}{M_w + b \rho} \tag{B.7}
\]

Based on thermodynamics,

\[
\rho h = \rho e + p \tag{B.8}
\]

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.8, and keeping temperature and all the other partial densities constant

\[
\left( \frac{\partial \rho h}{\partial \rho_i} \right)_{T, \rho j \neq i} = \left( \frac{\partial \rho e}{\partial \rho_i} \right)_{T, \rho j \neq i} + \left( \frac{\partial p}{\partial \rho_i} \right)_{T, \rho j \neq i} \tag{B.9}
\]
It is equivalent to Eq. B.10

\[ \tilde{h}_i = \tilde{e}_i + \left( \frac{\partial p}{\partial \rho_i} \right)_{T, \rho_j \neq i} \]  

(B.10)

The following thermodynamic expression exists, which relates a partial density property to a partial mass property

\[ \tilde{\phi}_i = \tilde{\phi}_i + \rho \left( \frac{\partial \phi}{\partial p} \right)_{T, \rho_j \neq i} \left( \frac{\partial p}{\partial \rho_i} \right)_{T, \rho_j \neq i} \]  

(B.11)

where the parameter \( \phi \) refers to any proper intensive thermodynamic property, such as enthalpy, and internal energy.

Substituting Eq. B.10 into Eq. B.11, and taking use of the fundamental enthalpy expression, which can be found in any thermodynamics textbook, the following relation concerning the partial mass enthalpy (\( \tilde{h}_i \)) can be established

\[ \tilde{h}_i = \tilde{e}_i + \frac{T}{\rho} \left( \frac{\partial p}{\partial T} \right)_{\rho_j} \left( \frac{\partial p}{\partial \rho_i} \right)_{T, \rho_j \neq i} \]  

(B.12)

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

\[ C_v = \left( \frac{\partial e}{\partial T} \right)_{\rho, \rho_j} \]  

(B.13)

Utilizing Eq. B.5, it is straightforward to find

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

(B.14)
where the derivative $\frac{\partial^2}{\partial T^2}(a\alpha)$ is given in Appendix C.

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

$$C_p = C_v + \frac{T}{\rho^2} \left( \frac{\partial p}{\partial T} \right)^2 \rho_j \left( \frac{\partial p}{\partial \rho} \right)_{T,Y}$$  \hspace{1cm} (B.15)

In order to find the thermodynamic relationships regarding chemical potential, the partial density and partial mass entropy have to be derived first

$$s(T, \rho) = s_0(T, \rho_0) - \int_{\rho_0}^{\rho} \left[ \frac{1}{\rho^2} \left( \frac{\partial p}{\partial T} \right) \rho \right]_{T} d\rho$$  \hspace{1cm} (B.16)

Based on the definition of partial density entropy, it is found

$$\tilde{S}_i = \int_{\text{ref}}^{T} C_{\rho,0} \frac{dT}{T} - \frac{R_u}{M_{wi}} (1 + \ln x_j) - \frac{R_u}{M_{wi}} \frac{\rho}{p_{\text{ref}}} \frac{R_u}{M_w} T$$

$$+ \frac{R_u}{M_{wi}} \ln \left(1 - \frac{b\rho}{M_w}\right) - \frac{R_u}{M_{wi}} \frac{b_i}{M_w} \frac{\rho}{M_w - b\rho} + \frac{b_i}{M_w} b^2 \frac{\partial (a\alpha)}{\partial T} \left| \frac{b\rho}{M_w + b\rho} \right|$$

$$- \ln \left(1 + \frac{b\rho}{M_w}\right) + \frac{2}{bM_{wi}} \sum_j x_j \frac{\partial (a_j \alpha_j)}{\partial T} \ln \left(1 + \frac{b\rho}{M_w}\right)$$  \hspace{1cm} (B.17)

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

$$\bar{S}_i = \tilde{S}_i + \left( \frac{\partial p}{\partial T} \right)_{\rho,Y_i} \bar{V}_i$$  \hspace{1cm} (B.18)

where the partial mass volume is

$$\bar{V}_i = \frac{1}{\rho} \left( \frac{\partial p}{\partial \rho_i} \right)_{T,\rho_j \neq i} \left\langle \frac{\partial p}{\partial \rho} \right\rangle_{T,Y_j}$$  \hspace{1cm} (B.19)
The chemical potential of species \( i \) can be calculated as

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

(B.20)

Finally, the partial derivatives regarding chemical potential can be expressed as

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

(B.21)

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

(B.22)
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 $\alpha_y\alpha_y$ are functions of temperature. The derivative of $a\alpha$ to temperature is given as

$$\frac{\partial a\alpha}{\partial T} = \sum_{i=1}^{N} \sum_{j=1}^{N} x_i x_j \sqrt{a_i a_j} \frac{\partial}{\partial T} \sqrt{\alpha_i \alpha_j}$$  \hspace{1cm} (C.1a)

where

$$\frac{\partial}{\partial T} \sqrt{\alpha_i \alpha_j} = \frac{1}{2} \left( \frac{\alpha_i}{\alpha_j} \right)^{\frac{1}{2}} \frac{\partial}{\partial T} \alpha_j + \frac{1}{2} \left( \frac{\alpha_j}{\alpha_i} \right)^{\frac{1}{2}} \frac{\partial}{\partial T} \alpha_i$$  \hspace{1cm} (C.1b)

$$\frac{\partial}{\partial T} \alpha_i = -\frac{S_i}{\sqrt{T T_{c,i}}} \left[ 1 + S_i \left( 1 - \sqrt{T T_{c,i}} \right) \right]$$  \hspace{1cm} (C.1c)

$$\frac{\partial}{\partial T} a_{ij} \alpha_{ij} = \sqrt{a_i a_j} \frac{\partial}{\partial T} \sqrt{\alpha_i \alpha_j}$$  \hspace{1cm} (C.2)

The second derivative of parameter $a\alpha$ to temperature is

$$\frac{\partial^2 a\alpha}{\partial T^2} = \sum_{i=1}^{N} \sum_{j=1}^{N} x_i x_j \sqrt{a_i a_j} \frac{\partial^2}{\partial T^2} \sqrt{\alpha_i \alpha_j}$$  \hspace{1cm} (C.3a)

where
The variable $\alpha_i$ for species H$_2$ ($\alpha_{H_2}$), is treated differently since hydrogen is a quantum gas. The derivative of this variable is

$$\frac{\partial^2 \sqrt{\alpha_i \alpha_j}}{\partial T^2} = \frac{1}{2} \left( \frac{1}{\alpha_i \alpha_j} \right)^{\frac{3}{2}} \frac{\partial \alpha_i}{\partial T} \frac{\partial \alpha_j}{\partial T} - \frac{1}{4} \left( \frac{\alpha_j}{\alpha_i} \right)^{\frac{3}{2}} \left( \frac{\partial \alpha_j}{\partial T} \right)^2$$

(C.3b)

$$- \frac{1}{4} \left( \frac{\alpha_j}{\alpha_i} \right)^{\frac{3}{2}} \left( \frac{\partial \alpha_i}{\partial T} \right)^2 + \frac{1}{2} \left( \frac{\alpha_j}{\alpha_i} \right)^{\frac{3}{2}} \frac{\partial^2 \alpha_j}{\partial T^2} + \frac{1}{2} \left( \frac{\alpha_j}{\alpha_i} \right)^{\frac{3}{2}} \frac{\partial^2 \alpha_i}{\partial T^2}$$

$$\frac{\partial^2 \alpha_i}{\partial T^2} = \frac{1}{2} \frac{S_i^2}{T_{c,i}} + \frac{1}{2} \frac{S_i}{\sqrt{T^3 T_{c,i}}} \left[ 1 + S_j \left( 1 - \frac{T}{T_{c,j}} \right) \right]$$

(C.3c)

The variable $\alpha_i$ for species H$_2$ ($\alpha_{H_2}$), is treated differently since hydrogen is a quantum gas. The derivative of this variable is

$$\frac{\partial \alpha_{H_2}}{\partial T} = -\alpha_{H_2} \left[ 0.30228 \frac{1}{T_{c,i}} \right]$$

(C.4)

$$\frac{\partial^2 \alpha_{H_2}}{\partial T^2} = \alpha_{H_2} \left[ 0.30228 \frac{1}{T_{c,i}} \right]^2$$

(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

$$T = \begin{pmatrix} (\frac{\partial \rho}{\partial p})_{r,x} & 0 & 0 & 0 & -\frac{A_T}{A_p} & -\frac{A_Y}{A_p} & \cdots & -\frac{A_{e_{q-1}}}{A_p} \\ \tilde{u}(\frac{\partial \rho}{\partial p})_{r,x} & \bar{p} & 0 & 0 & -\frac{A_T}{A_p} & -\frac{A_Y}{A_p} & \cdots & -\frac{A_{e_{q-1}}}{A_p} \\ \tilde{v}(\frac{\partial \rho}{\partial p})_{r,x} & 0 & \bar{p} & 0 & -\frac{A_T}{A_p} & -\frac{A_Y}{A_p} & \cdots & -\frac{A_{e_{q-1}}}{A_p} \\ \tilde{w}(\frac{\partial \rho}{\partial p})_{r,x} & 0 & 0 & \bar{p} & -\frac{A_T}{A_p} & -\frac{A_Y}{A_p} & \cdots & -\frac{A_{e_{q-1}}}{A_p} \\ \tilde{h} + \left[ \tilde{h} \right]_{v} - e - \frac{P}{\rho} [\tilde{e}_{r,x}] & \bar{p} \tilde{u} & \bar{p} \tilde{v} & \bar{p} \tilde{w} & \bar{p} B_T - \frac{A_T}{A_p} & \bar{p} B_{e_{q-1}} - \frac{A_{e_{q-1}}}{A_p} & \cdots & \bar{p} B_{e_{q-1}} - \frac{A_{e_{q-1}}}{A_p} \\ \tilde{h}_{r,x} (\frac{\partial \rho}{\partial p})_{r,x} & 0 & 0 & 0 & -\frac{A_T}{A_p} & -\frac{A_Y}{A_p} & \cdots & -\frac{A_{e_{q-1}}}{A_p} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \tilde{h}_{r,x} \left(\frac{\partial \rho}{\partial p}\right)_{r,x} & 0 & 0 & 0 & -\frac{A_T}{A_p} & -\frac{A_Y}{A_p} & \cdots & -\frac{A_{e_{q-1}}}{A_p} \\ \end{pmatrix}$$

(D.1)

where the coefficients $A_p, A_T, A_Y, B_T, B_{e_{q-1}}$, and $B_{e_{q-1}}$ are defined in the Chapter 2. The terms $e_i$ and $h_i$ denote total energy and total enthalpy, respectively.

$$e_i = e + \frac{1}{2}(\tilde{u}^2 + \tilde{v}^2 + \tilde{w}^2)$$

$$h_i = e_i + \frac{P}{\rho}$$
D.2 Convective Flux Jacobians

The Jacobian matrix \( A = \partial E / \partial Z \) is given by

\[
A = \begin{bmatrix}
\tilde{u} \left( \frac{\partial \rho}{\partial \rho} \right)_{r, \gamma} & \rho & 0 & 0 & -\tilde{u} \frac{A_e}{A_p} \\
1 + \tilde{u}^2 \left( \frac{\partial \rho}{\partial \rho} \right)_{r, \gamma} & 2 \rho \tilde{u} & 0 & 0 & -\tilde{u}^2 \frac{A_e}{A_p} \\
\tilde{u} \tilde{v} \left( \frac{\partial \rho}{\partial \rho} \right)_{r, \gamma} & \rho \tilde{v} & \rho \tilde{u} & 0 & -\tilde{u} \tilde{v} \frac{A_e}{A_p} \\
\tilde{u} \tilde{w} \left( \frac{\partial \rho}{\partial \rho} \right)_{r, \gamma} & \rho \tilde{w} & 0 & \rho \tilde{u} & -\tilde{u} \tilde{w} \frac{A_e}{A_p} \\
\tilde{u} \left[ \tilde{h} + \left( \sum_{i=1}^N \tilde{Y}_i \tilde{e}_i - \frac{p}{\rho} \right) + 1 \right] \left( \frac{\partial \rho}{\partial \rho} \right)_{r, \gamma} \tilde{h} + \rho \tilde{u}^2 & \rho \tilde{v} \tilde{v} & \rho \tilde{w} \tilde{v} & \tilde{u} \tilde{w} \left( \frac{\rho B_r - A_e \tilde{e}_i}{A_p} \right) & -\tilde{u} \frac{A_e \tilde{Y}_i}{A_p} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\tilde{u} \tilde{Y}_{N-1} \left( \frac{\partial \rho}{\partial \rho} \right)_{r, \gamma} & \rho \tilde{Y}_{N-1} & 0 & 0 & -\tilde{u} \frac{A_e \tilde{Y}_{N-1}}{A_p}
\end{bmatrix}
\]
The Jacobian matrix \( B = \partial F / \partial Z \) is given by

\[
B = \begin{pmatrix}
\tilde{v}(\frac{\partial \rho}{\partial \tilde{v}})_{r,x} & 0 & \tilde{p} & 0 & -\tilde{v}\frac{A_e}{A_p} \\
\tilde{u}\tilde{v}(\frac{\partial \rho}{\partial \tilde{v}})_{r,x} & 0 & \tilde{p}\tilde{u} & 0 & -\tilde{u}\frac{A_e}{A_p} \\
1 + \tilde{v}^2(\frac{\partial \rho}{\partial \tilde{v}})_{r,x} & 0 & 2\tilde{p}\tilde{v} & 0 & -\tilde{v}^2\frac{A_e}{A_p} \\
\tilde{v}\tilde{w}(\frac{\partial \rho}{\partial \tilde{v}})_{r,x} & 0 & \tilde{p}\tilde{w} & \tilde{p}\tilde{w} & -\tilde{v}\frac{A_e}{A_p} \\
\tilde{v}\tilde{h} + (\sum_{i=1}^{N} \tilde{Y}_i - \frac{p}{\rho} + 1)(\frac{\partial \rho}{\partial \tilde{v}})_{r,x} & \tilde{p}\tilde{u}\tilde{v} & \tilde{h} + \tilde{p}\tilde{v}^2 & \tilde{p}\tilde{w}\tilde{v} & \tilde{v}(\tilde{p}\tilde{B}_e - \frac{A_e e}{A_p}) \\
\tilde{v}\tilde{Y}_1(\frac{\partial \rho}{\partial \tilde{v}})_{r,x} & 0 & \tilde{p}\tilde{Y}_1 & 0 & -\tilde{v}\frac{A_e \tilde{Y}_1}{A_p} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\tilde{v}\tilde{Y}_{N-1}(\frac{\partial \rho}{\partial \tilde{v}})_{r,x} & 0 & \tilde{p}\tilde{Y}_{N-1} & 0 & -\tilde{v}\frac{A_e \tilde{Y}_{N-1}}{A_p}
\end{pmatrix}
\]
The Jacobian matrix \( C = \partial G / \partial Z \) is given by

\[
C = \begin{pmatrix}
\bar{w} \frac{\partial \rho}{\partial \rho} & 0 & 0 & \bar{p} & -\bar{w} \frac{A_r}{A_p} \\
\bar{w} \frac{\partial \rho}{\partial \rho} & \bar{p} \bar{w} & 0 & \bar{p} \bar{u} & -\bar{u} \frac{A_r}{A_p} \\
\bar{v} \frac{\partial \rho}{\partial \rho} & 0 & \bar{p} \bar{v} & \bar{v} \bar{v} & -\bar{v} \frac{A_r}{A_p} \\
1 + \bar{w}^2 & 0 & 0 & 2 \bar{p} \bar{w} & -\bar{w}^2 \frac{A_r}{A_p} \\
\bar{w} \bar{Y}_1 \frac{\partial \rho}{\partial \rho} & 0 & 0 & \bar{p} \bar{Y}_1 & -\bar{w} \frac{A_r \bar{Y}_1}{A_p} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\bar{w} \bar{Y}_{N-1} \frac{\partial \rho}{\partial \rho} & 0 & 0 & \bar{p} \bar{Y}_{N-1} & -\bar{w} \frac{A_r \bar{Y}_{N-1}}{A_p}
\end{pmatrix}
\]

(D.4)
D.3 Chemical Source Jacobian

The Jacobian matrix associated with the chemical reaction source term \( D = \partial H / \partial Z \) is

\[
D = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
\end{pmatrix}
\]

where

\[
\frac{\partial \omega_j}{\partial p} = \frac{W_j}{p} \sum_{j=1}^{N} \left( v_{j}^\sigma - v_{j}^\sigma \right) k_{f_j} \left( \sum_{l=1}^{N} \varepsilon_{j} n_{l} \right) \left( \sum_{l=1}^{N} v_{j}^\sigma \prod_{l=1}^{N} n_{l}^\sigma - \frac{1}{k_{c_j}} \left( \sum_{l=1}^{N} v_{j}^\sigma \prod_{l=1}^{N} n_{l}^\sigma \right) \right) 
\]

(D.6)

\[
\frac{\partial \omega_j}{\partial T} = \frac{W_j}{T} \sum_{j=1}^{N} \left( v_{j}^\sigma - v_{j}^\sigma \right) k_{f_j} \left( \sum_{l=1}^{N} \varepsilon_{j} n_{l} \right) \left( m_{f_j} - \sum_{l=1}^{N} v_{j}^\sigma \right) + \frac{E_{j}}{R_a T} \prod_{l=1}^{N} n_{l}^\sigma 
- \frac{1}{k_{c_j}} \left( m_{f_j} - \sum_{l=1}^{N} v_{j}^\sigma \right) + \frac{E_{j}}{R_a T} \prod_{l=1}^{N} n_{l}^\sigma \right) 
\]

(D.7)

\[
\frac{\partial \omega_j}{\partial Y_k} = \frac{W_j}{T} \sum_{j=1}^{N} \left( v_{j}^\sigma - v_{j}^\sigma \right) k_{f_j} \left( \sum_{l=1}^{N} \varepsilon_{j} n_{l} \right) \left( \frac{v_{j}^\sigma}{Y_k} - \frac{v_{j}^\sigma}{Y_N} \right) - \left( \sum_{l=1}^{N} v_{j}^\sigma \right) R_{k} \prod_{l=1}^{N} n_{l}^\sigma 
- \frac{1}{k_{c_j}} \left( \frac{v_{j}^\sigma}{Y_k} - \frac{v_{j}^\sigma}{Y_N} \right) - \left( \sum_{l=1}^{N} v_{j}^\sigma \right) R_{k} \prod_{l=1}^{N} n_{l}^\sigma \right) 
\]

(D.8)

and \( R_k = W \left( \frac{1}{W_k} - \frac{1}{W_N} \right) \).
VITA

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