AERODYNAMIC DESIGN OF LOW NOₓ OIL DIFFUSION FLAMES

USING THE RADIALY STRATIFIED FLAME CORE BURNER

by

Joel M. Haynes

B.S., Mechanical Engineering, Stanford University, 1990
M.S., Mechanical Engineering, Massachusetts Institute of Technology, 1993

Submitted to the Department of Mechanical Engineering
in Partial Fulfillment of the Requirements for the
Degree of

DOCTOR OF PHILOSOPHY
in Mechanical Engineering

at the

Massachusetts Institute of Technology
February 1996

© Massachusetts Institute of Technology, 1996.
All rights reserved.

Signature of Author

Department of Mechanical Engineering
January 19, 1995

Certified by

Professor Janos M. Beér
Thesis Supervisor

Department of Chemical Engineering

Certified by

Professor Ahmed F. Ghoniem
Thesis Committee Chairman

Department of Mechanical Engineering

Certified by

Professor Douglas Hart
Department of Mechanical Engineering

Approved by

Professor Ain A. Sonin
Chairman, Department Graduate Committee

Department of Mechanical Engineering

MAR 19 1996
AERODYNAMIC DESIGN OF LOW NO\textsubscript{x} OIL DIFFUSION FLAMES

USING THE RADIALLIY STRATIFIED FLAME CORE BURNER

by

JOEL M. HAYNES

Submitted to the Department of Mechanical Engineering
on January 19, 1995 in Partial Fulfillment of the
Requirements for the Degree of Doctor of Philosophy in
Mechanical Engineering

ABSTRACT

The aerodynamics of a patented, low NO\textsubscript{x}, triple-annular, swirl burner have been studied computationally. The Radially Stratified Flame Core burner utilizes multiple recirculation zones and radial density stratification in a swirling flow field to form a fuel rich core and increase fuel residence time in the core allowing for more thorough conversion of fuel-N to N\textsubscript{2}. Atomized No. 6 oil with high fuel-nitrogen content was the fuel for both the experimental and computational investigations.

Computational studies have been performed which reveal the flow field's sensitivity to the RSFC burner's operating parameters and design parameters. Insights from these studies together with experimental measurements and observations reveal the effect of burner operating parameters on NO\textsubscript{x} and CO emissions. The flow field characterizing the burner's optimal low NO\textsubscript{x} and CO performance has also been reproduced in a computational model.

A novel criteria for scaling-up the RSFC burner to higher firing rates is proposed. The principle is based upon the flow field's sensitivity to changes in the jets' angular momentum. The relevance of the scaling criteria is demonstrated computationally in relation to other similarity criteria.

The influence of density stratification on the RSFC burner's flow field has also been studied. A CFD code for incompressible flows has been modified to account for density fluctuations in the flow field; the modified code is used to study the influence of density stratification. The effect of swirl and radial density stratification on the turbulent characteristics of a jet have been demonstrated experimentally for isothermal flows by Beér et. al. These experiments have been modeled, and the modified CFD code has been evaluated based on its ability to characterize the stratification effects. The code was then applied to flow field calculations for the RSFC burner to demonstrate the significance of stratification in the establishment of the flow field associated with optimal burner performance.

Thesis Supervisor: Janos M. Beér

Title: Professor of Chemical Engineering,
Director, MIT Combustion Research Facility

2
Acknowledgments

I would like to thank my advisor, Professor Janos Beér, for being a wonderful intellectual and professional mentor. I greatly appreciate the time you’ve taken to help me grow intellectually, and I appreciate the example you have set in overseeing the CRF’s “research family.” I sense that by working with you my horizons have been stretched in more ways than I can fully appreciate at this time. I am grateful that I could be one of your last graduate students at MIT. The rest of my thesis committee I want to thank for their guidance and positive support throughout my doctoral program.

Financial support for this project from the Empire State Electric Energy Research Corporation, Eseerco, and from ABB-CE is gratefully acknowledged.

Great appreciation is also extended to Laszlo Barta for teaching me FLUENT and so many other things. The encouragement you have given me is greatly appreciated, and your excitement for combustion research has made working at the CRF a rewarding experience. I would also like to thank Paul Lewis for his dedication to the CRF team and for the ways in which he has served the whole group. Much thanks is extended to Robert Murang for his support in developing and setting up experiments. Thank you also for communicating your insights and experiences regarding the purpose of a Ph.D. The technical staff, Don Bash, Billy Mason, and Mark James, I would like to thank for their dedication to the research team and the excellent work they did in maintaining the CRF.

Thank you Bonnie for keeping everything running smoothly around the lab.

Thanks are due to members of ABB’s Power Plant Laboratories, especially Mr. Richard Borio, Dr. Majed Toqan, Mrs. Julie Nicholson, Mr. Tom Duby, and Dr. Dave Thornock. Your dedication to the RSFC project and your technical gifts have made this research project exciting and a great educational experience. I particularly want to thank Dr. Majed Toqan for working so closely with me throughout the course of this research project and entering into so many insightful discussions with me about the burner.

I would like to thank the guys who have worked with me as fellow students in the lab. Thank you Wole for making this such a nice place to work and for being an encouraging example of godly steadfastness as we’ve gone through turbulent funding situations together. Thank you also for proof reading some of this thesis. I also want to thank Alan and Jose for their enthusiastic support in all kinds of things and for helping to make this a pleasant place to work. Thank you Vigan and Dereck for livening things up around the office area and for being encouragers.

I want to give special thanks to the UROP’s who have worked with me. Mike Park, it was a lot of fun to have you around. I learned all kinds of things from you - and not just technical stuff. Thanks for your diligence and enthusiasm. Tim your help was so timely; you know I never would have finished this thesis on time if you hadn’t been there. Thanks for your dedication as a friend to do more than what could be expected of a UROP.

I want the thank the LORD God who has gone before me as He promised when I came from Stanford and traveled to the “far side of the sea” (Ps. 139:9-10) Through funding problems, computer, printer, and other equipment failures, and times of apparent futility the LORD has been my strength and provider. The scripture promises that “those
who trust in the LORD will renew their strength. They will soar on wings like eagles; they
will run and not grow weary, they will walk and not be faint.” (Isaiah 40:31) His glory,
once revealed, convinces a soul that “Jehovah is God.” When attempting to recourt what
the Lord God has meant to me with respect to this thesis I am reminded of the words of
the timeless hymn by Isaac Watts:

When I survey the wondrous cross on which the Prince of Glory died, my richest
gain I count but loss, and pour contempt on all my pride. Forbid it Lord that I should boast
save in the death of Christ, my God. All the vain things that charm me most, I sacrifice
them to His blood. See from His head, His hands, His feet sorrow and love flow mingled
down. Did ever such love and sorrow meet, or thorns compose so rich a crown? Were
the whole realm of nature mine, that were a present far too small. Love so amazing, so
divine, demands my soul, my life, my all.

The grace and support shown to me in the process of completing this thesis is
beyond what could be covered here but I would like to mention some of the wonderful
ways in which I was provided for during this arduous process. Thank you Rob for
making that lasagna for me. It was great. Thank you also for printing out graphics
drawings for me. Shoveling my car out of the snow was more than I could ever have
asked for and ne "r deserved - thank you. Jim, thank you for proof reading several
chapters and working on some of the drawings. You have been a dedicated friend - what
other person would stay up until 3AM while on the brink of being sick to help a friend on
his thesis. Kevin, thank you for working on the data for the plots and for your many acts
of kindness. Thanks for living out a set of priorities that makes the rest of the world seem
backward. “When is the thesis of a friend more important than your own?,” I now ask
myself. Jonathan thanks for bearing the load with me in these last few days when there
have been more things to deal with than I could think about. Thanks for getting me to
school, for printing things out, and with dealing with so many little things that had to be
done. You and Ien put together a mighty fine reception too. It was better than anything I
could have done myself. What can I say when you’ve blessed me with more than I could
have asked for and gone out of your way so purposefully?

Lastly I want to thank all of those special people in my life that have consistently
been there for me through thick and thin. First, I want to thank my parents for their
dedication to one another and to me and my sisters. Thank you for being there for me
from day 1 until now. I also want to thank my housemates, Andrew, Rob, John, and
Mark for putting up with me in so many ways and for cooking so many great meals.
Daniel and Tim, thanks for consistently praying with/for me. I also want to thank
Stephanie and Dean for making life anything but dull. Thank you all for celebrating with
me at this momentous time in my life, and may our hearts be filled with the single purpose
for which we may celebrate every moment of our lives.
# Table of Contents

Abstract ............................................................................................................. 2
Acknowledgments .............................................................................................. 3
List of Figures .................................................................................................... 7
List of Tables ...................................................................................................... 10
Nomenclature ..................................................................................................... 11

1 Introduction ..................................................................................................... 15
   1.1 Motivation for Low NOx Research ........................................................... 15
      1.1.1 Environmental Concerns ................................................................... 15
      1.1.2 Legal Restraints on NOx Emissions .................................................... 15
   1.2 NOx Reduction Strategies ........................................................................ 16
      1.2.1 NOx Formation Mechanisms ............................................................... 16
      1.2.2 Reduction Strategies .......................................................................... 20
   1.3 Development of the RSFC Burner ............................................................. 20

2 Scope of Burner Design Research .................................................................. 23
   2.1 Burner and Flame Design Goals ............................................................... 23
   2.2 Ideal RSFC Burner Performance ............................................................... 24
   2.3 Design Criteria ......................................................................................... 24
      2.3.1 Operating Parameters ........................................................................ 27
      2.3.2 Design Parameters ............................................................................ 27
   2.4 Scaling ...................................................................................................... 27
   2.5 Modeling Density Stratification ................................................................. 28

3 Flow Modeling .................................................................................................. 29
   3.1 Incompressible Laminar Reacting Flows .................................................. 29
   3.2 Time Averaged Turbulent Flow Equations with Density Fluctuations .... 31
   3.3 Modeling of Turbulence Correlations ...................................................... 33
   3.4 Turbulence Models with Density Fluctuations ......................................... 38
   3.5 Density Stratification in Axisymmetric Swirling Flows ............................ 40

4 Burner Configurations and Methodology for Studying Burner Design Criteria .. 43
   4.1 CFD Tools ............................................................................................... 44
      4.1.1 FLUENT Code .................................................................................. 44
      4.1.2 Two-Phase Flow Modeling .................................................................. 45
      4.1.3 Turbulence Model .............................................................................. 48
      4.1.4 Radiation Model ................................................................................ 48
      4.1.5 Discretization Scheme ........................................................................ 49
      4.1.6 Physical Properties ............................................................................ 49
   4.2 Parametric Oil Burner Performance Studies .......................................... 51
      4.2.1 ISBF Experimental Setup and Component Modeling ....................... 52
      4.2.2 Effect of Burner Operating Parameters on Performance .................. 68
      4.2.3 Effect of Burner Design Parameters on Performance ....................... 69
   4.3 Oil Burner Scaling .................................................................................... 69
4.4 Density Stratification Studies

4.4.1 Isothermal Density Stratification

4.4.2 Density Stratification in the RSFC Burner

5 Computation Results and Experimental Data

5.1 Computational Results and Experimental Data for Parametric Oil Burner Study

5.1.1 Operating Parameter Sensitivity

5.1.1.1 Primary Air Reynolds Number

5.1.1.2 Primary Air Swirl

5.1.1.3 Tertiary Air Reynolds Number

5.1.1.4 Tertiary Air Swirl

5.1.1.5 Air Distribution

5.1.1.6 Fuel Droplet Size

5.1.1.7 Atomizer Spray Angle

5.1.2 Design Parameter Sensitivity

5.1.2.1 Quarl Length

5.1.2.2 Quarl Divergence Angle

5.1.2.3 Tertiary Air Radial Spacing

5.1.2.4 Quarl Exit Area

5.2 Burner Scaling Computational Results

5.3 Experimental Data and Computational Results for Density Stratification Studies

5.3.1 Isothermal Density Stratification

5.3.2 Density Stratification in the RSFC Burner

5.3.2.1 Stratification and Flame Shape

5.3.2.2 CFD Model Modification

6 Discussion and Analysis of Results

6.1 Operating Parameter Sensitivity Analysis for NOx and CO

6.1.1 Primary Air Reynolds Number

6.1.2 Primary Air Swirl

6.1.3 Tertiary Air Reynolds Number

6.1.4 Tertiary Air Swirl

6.1.5 Air Distribution

6.1.6 Fuel Droplet Size

6.1.7 Atomizer Spray Angle

6.2 Design Parameter Analysis

6.3 RSFC Burner Scaling Criteria

6.4 Significance of Modeling Density Stratification

6.4.1 Stratified Isothermal Jet

6.4.2 RSFC Burner Density Stratification

7 Summary, Conclusions, and Recommendations

7.1 Summary

7.2 Conclusions

7.3 Recommendations for Future Work

References
List of Figures

1.1 Formation and Reduction of NO in Combustion Chemical Pathways .................. 17
2.1 Independent Variables for Burner Design .............................................. 25
2.2 Dependent Variables Indicating Burner Performance .................................. 26
4.1 Industrial Scale Burner Facility (ISBF) Geometry ...................................... 53
4.2 Industrial Scale Burner Facility Model .................................................... 55
4.3 Radially Stratified Flame Core Burner Exit and Quarter Geometry ............... 56
4.4 Characteristic Computational Grid for RSFC Burner and Furnace .................. 59
4.5 Y-Jet Atomizer Design ........................................................................... 61
4.6 Model of Atomized Oil ............................................................................ 63
4.7 Experimental Setup for Co-axial Jet Experiment ....................................... 73
4.8 Characteristic Computational Grid for Co-axial Helium (or Air) Jet ............. 74
5.1 High Re_p, Flame Shape A (Case 1) ....................................................... 77
5.2 Low Re_p, Flame Shape C (Case 2) ......................................................... 80
5.3 Critical Re_p, Flame Shape B (Between Case 1 & 2) ................................... 83
5.4 Percent Mass Flow Penetration vs. Re_p from Computational Study ............. 84
5.5 Percent Mass Flow Penetration vs. Primary Air Swirl from Computational Study .................................................................................................................. 85
5.6 High Sp, Flame Shape A (Case 1) ............................................................ 87
5.7 Low Sp, Flame Shape C (Case 1 with low Sp) .......................................... 89
5.8 High Re_T, Flame Shape A (Case 1) ....................................................... 92
5.9 Lower St_T, Flame Shape B ................................................................. 94
5.10 Flame Length vs. St_T ........................................................................... 97
5.11 Lower Re_p, High Re_T, Flame Shape BC ............................................. 98
5.12 Higher Re_S, Lower Re_p, High Re_T, Flame Shape C ............................ 101
5.13 High Re_p, Flame Shape A (Case 1) ....................................................... 103
5.14 $d_{droplet} = 35\mu$, Flame Shape B (Case 1 with high $St$) ........................................ 106
5.15 $d_{droplet} = 55\mu$, Flame Shape C (Case 1 with high $St$) ........................................ 107
5.16 Downstream Fuel Concentration (@x/d = 3.5) vs. Oil Droplet Size ................................. 109
5.17 Downstream Fuel Concentration (@x/d = 3.5) vs. Spray Angle ................................. 109
5.18 $\alpha = 0^\circ$, Flame Shape C (Case 1 with high $St$) ........................................ 110
5.19 $\alpha = 10^\circ$, Flame Shape B (Case 1 with high $St$) ........................................ 111
5.20 IRZ$_0$ Position vs. Quarl Length ................................................................. 113
5.21 Low A$qurt/A_l$, Flame Shape BC (Between Case 1 & 2) ......................................... 115
5.22 High A$qurt/A_l$, Flame Shape BC (Between Case 1 & 2) ......................................... 117
5.23 15 MW Burner, Scaled Down Using Thermal Similarity ........................................... 120
5.24 15 MW Burner Scaled Down Using Chemical Similarity ......................................... 123
5.25 15 MW Burner Scaled Down Using Kinematic Scaling ........................................... 127
5.26a Axial Velocity Decay for Air Jets with and without Flow Rotation ....................... 131
5.26b Axial Velocity Decay for Helium Jets with and without Flow Rotation ....................... 132
5.26c Decay of Axial Concentration for Helium Jets with and without Flow Rotation .................... 132
5.27 Non-swirling Co-axial He Jet ............................................................................. 135
5.28 Tangential Velocity at $x/do=4.80$ for Helium Jet in Rotating Coaxial Flow .................. 136
5.29 Normalized Density Profile at $x/de=5,10,20$ for Helium Jet in a Rotating Annular Air Stream .......................................................... 137
5.30a Axial Velocity Profile at $x/de=20$ for an Air Jet in a Non-Rotating Annular Air Stream .......................................................... 140
5.30b Turbulence Intensity at $x/de=20$ for an Air jet in a Non-Rotating Annular Air Stream .......................................................... 140
5.31a Axial Velocity Profile at $x/de=20$ for a Helium Jet in a Non-Rotating Annular Air Stream .......................................................... 141
5.31b Turbulence Intensity at $x/de=20$ for a Helium Jet in a Non-Rotating Annular Air Stream .......................................................... 141
5.32a Experimental Shear Stress Measurements at $x/de=20$ for Air Jets with Rotating and Non-Rotating Coaxial Air Streams .......................................................... 143
5.32b Computed Shear Stress at $x/de=20$ for Air Jets with Rotating and
Non-Rotating Coaxial Air Streams .................................................................143
5.33a Experimental Shear Stress Measurements at x/de=20 for Helium Jets with
Rotating and Non-Rotating Coaxial Air Streams ........................................144
5.33b Computed Shear Stress at x/de=20 for a Helium Jet with a Non-Rotating
Coaxial Air Stream..................................................................................144
5.33c Computed Shear Stress at x/de=20 for a Helium Jet with a Rotating Coaxial
Air Stream...............................................................................................145
5.34a Normalized Density Profile at x/de=20 for a Helium Jet in a Rotating
Coaxial Air Stream..................................................................................147
5.34b Computed Shear Stress at x/de=20 for a Helium Jet with a Non-Rotating
Coaxial Air Stream..................................................................................147
5.35 Modified Richardson Number, Ri* Contours for Flame Shape A ...............149
5.36 Critical Rep, Flame Shape B (Calculated using Modified Code) .................152
6.1 CO Emissions vs. Opacity for the RSFC Burner........................................158
6.2 NO vs. CO Emissions for the RSFC Burner.............................................158
6.3 Emissions vs. Rep for Phase II Experiments ...........................................161
6.4 Opacity & Emissions vs. Reh,T for Phase I Experiments...........................161
6.5 NO & CO Emissions vs. St in Phase II Experiments..................................165
6.6 Penetration vs. Primary Air Re for Scale-Down from 21 MW ....................171
6.7a Theoretical Iso-Penetration Lines for RSFC Burners...............................174
6.7b %Penetration for RSFC Burners Models with Thermal Similarity ............174
### List of Tables

3.1 Turbulence Model Constants...............................................................37
4.1 Air Composition, Turbulent Schmidt Numbers, and Formation Enthalpies........50
4.2 General Gas Properties........................................................................51
4.3 Definitions of Specific Heat as a Function of Temperature...............51
4.4 Air-Preheat and Exit O\textsubscript{2} Conditions.................................57
4.5 Atomizer Characteristics..................................................................62
4.6 Properties of Oil Fuels......................................................................64
4.7 Properties of #6 Oil Used in Modeling.............................................65
4.8 #6 Oil Reaction Kinetics Model Parameters......................................66
4.9 Baseline Operating Parameters..........................................................68
6.1 Relationship Between Flame Length and Emissions.......................156
Nomenclature

**Symbols**

A  area

A  reaction rate parameter

a, b  reaction rate concentration exponents

Bi  Biot number

C_b  vaporization rate constant

C_i  concentration of species

C_p  specific heat

C_μ  turbulent viscosity constant

D  droplet diameter

D  diffusion coefficient

D^T  thermal diffusion coefficient

d  burner diameter

dx_i; dx_j; dx_k  differential displacement vector component (tensor notation)

E  activation energy

F  force

g  gravity

ΔH_{r,288K}^o  heat of reaction

ΔH_{298}^o  formation enthalpy

h  duct height, enthalpy

h_{fy}  latent heat of vaporization for oil

\bar{h}  convection coefficient
IRZ\textsubscript{i}  
inner IRZ in the flow

IRZ\textsubscript{o}  
outer IRZ in the flow

J  
diffusive mass flux

k  
turbulent kinetic energy

k  
thermal conductivity

k  
reaction rate

k\textsubscript{c}  
mass transfer coefficient

L  
inlet duct length

L\textsubscript{flame}  
distance from the burner exit

L\textsubscript{IRZ}  
distance from the burner exit to the center of IRZ\textsubscript{o}

L\textsubscript{lip}  
quarl lip length

L\textsubscript{quar}  
quarl length

^\textsubscript{\hat{}}\text{M}  
molar mass

m  
mass flow rate

m\textsubscript{penetration}  
rate of mass flow penetration through IRZ\textsubscript{o} along the centerline

N  
Molar Flux

p  
pressure

p  
perimeter

Re  
Reynolds Number

S  
Swirl Number

S\textsubscript{c}  
Schmidt Number

S\textsubscript{h}  
enthalpy source term

S\textsubscript{m}  
mass source term

S\textsubscript{a}  
species source term

T  
temperature

t  
time

U\textsubscript{i};U\textsubscript{j};U\textsubscript{k}  
mean velocity vector component (tensor notation)
$u_i'; u_j'; u_k'$ fluctuating velocity vector component (tensor notation)

$Y$ species mass fraction

**Greek symbols**

$\alpha$ spray angle

$\beta$ spreading angle

$\theta$ quarl divergence angle

$\psi$ stream function

$\psi_0$ stream function maximum at burner exit

$\mu$ viscosity (Table 4.2)

$\rho$ density (Table 4.7)

$\tau$ stress

$\delta_{ij}$ Kronecher-delta function

**Operators, superscripts, and subscripts**

$\cdot; \cdot; \cdot_k$ tensor notation

$\cdot_t$ time average

$\cdot'$ fluctuating turbulent quantity

$\cdot^*$ at burner exit after an insert

$\cdot_{m}$ in the gas phase “far” from the surface

$\cdot_H$ based on hydraulic diameter

$\cdot_h$ hydraulic equivalent

$\cdot_i$ inner; species i

$\cdot_n$ species n

$\cdot_o$ outer; initial value

$\cdot_p$ Primary Air

$\cdot_s$ Secondary Air
\( (.)_s \)  
\( (.)_t \)  
\( (.)_i \)  

**Acronyms**

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABB</td>
<td>Asea Brown Boveri</td>
</tr>
<tr>
<td>CAA90</td>
<td>Clean Air Act of 1990</td>
</tr>
<tr>
<td>CFD</td>
<td>computational fluid dynamics</td>
</tr>
<tr>
<td>CRF</td>
<td>combustion research facility</td>
</tr>
<tr>
<td>DOE</td>
<td>Department of Energy</td>
</tr>
<tr>
<td>IRZ</td>
<td>internal recirculation zone</td>
</tr>
<tr>
<td>ISBF</td>
<td>industrial scale burner facility</td>
</tr>
<tr>
<td>LNB</td>
<td>Low NOx burners</td>
</tr>
<tr>
<td>LHS</td>
<td>left hands side</td>
</tr>
<tr>
<td>PRI</td>
<td>primary</td>
</tr>
<tr>
<td>RHS</td>
<td>right hand side</td>
</tr>
<tr>
<td>RSFC</td>
<td>radially stratified flame core</td>
</tr>
<tr>
<td>SEC</td>
<td>secondary</td>
</tr>
<tr>
<td>TER</td>
<td>tertiary</td>
</tr>
</tbody>
</table>
CHAPTER 1

Introduction

1.1 Motivation for Low NOx Research

1.1.1 Environmental Concerns

In recent decades environmental concerns over NOx emissions have risen as human understanding of its role in environmental damage and climate change have increased. NO is known to contribute to the photochemical processes that produce urban smog, and NO emissions contribute to regional acid rain problems. Because of its absorption properties, NO is classified as a greenhouse gas, linking it to recent theories about the influence of these gases in global warming and climate change. However, NO occurs in much smaller concentrations than other greenhouse gases.

1.1.2 Legal Restraints on NOx Emissions

The scientific evidence linking NO to conditions hazardous to humans has motivated a series of legal responses at all levels of government. Tort law which determines issues of local liability has been used to redress damages by companies which reduce local air quality. Federal regulation of NO is implemented through the Clean Air Act of 1990 to meet regional air quality goals; CAA90 names NO as a criteria pollutant. The Clean Air Act of 1990 establishes an ambient air quality standard of 0.053 ppm NO (annual arithmetic mean) for all regions of the country; it also gives the basis for new source performance standards for NO emissions in different industries. Some state regulations push these limits even lower and make additional requirements concerning source emissions.
1.2 NOx Reduction Strategies

An understanding of the chemical pathways for NO formation and destruction is necessary for developing a NO reduction strategy. The principle chemical processes are reviewed in the section. Multiple methods are available for regulating the interactions of the fuel, oxidant, and burned gases in order to control the degree of NO formation. Heat extraction from the system can also be a control variable. Specific strategies are not discussed in this section; rather, the necessary conditions for reducing NO emissions by combustion process modification are described. Ultimately, any modifications to the combustion system, physical or aerodynamic, must be able to influence the chemistry of nitrogen species interconversions.

1.2.1 NOx Formation Mechanisms

Figure 1.1 summarizes the principle mechanisms for NO formation and destruction. Atmospheric nitrogen, i.e. N₂, can form NO in two different ways. The most direct pathway is called “thermal NO” and occurs in a high temperature oxidizing environment. The other pathway is called “prompt NO” and involves the fixation of atmospheric nitrogen by hydrocarbon fragments in an oxygen deprived environment. The second means of NO formation involves fuel bound nitrogen. This pathway is represented in the middle of Figure 1.1; “fuel NO” is formed when heterocyclic nitrogen compounds react in a high temperature oxidizing environment. NOx is formed from NO through the interaction with other nitrogen oxides (NO + NO₂ → NOx). When the environment is oxygen deprived and fuel rich, the NOx reburn pathway is active and reduces local NOx concentrations. This is represented on the RHS of Figure 1.1. The thermodynamics and kinetics that govern these reactions are discussed by Miller et. al. [1] and Bowman [2]. A brief description of the kinetics of each mechanism is given in the following sections.
Figure 1.1 Formation and Reduction of NO in Combustion Chemical Pathways
1.2.1.1 Thermal NO

The "thermal NO" formation process is represented on the RHS of Figure 1.1. Three reactions comprise the mechanism which was first identified by Zeldovich [3]:

\[ N_2 + O \rightarrow NO + N \]  \hspace{1cm} (1.1)
\[ N + O_2 \rightarrow NO + O \]  \hspace{1cm} (1.2)
\[ N + OH \rightarrow NO + H \]  \hspace{1cm} (1.3)

The Zeldovich mechanism is the dominant mechanism for NO formation in high temperature fuel-lean systems. At 1800 K the NO formation rate becomes significant and doubles if the temperature is increased by merely 35K.

1.2.1.2 Prompt NO

The second mechanism for converting atmospheric nitrogen into NO involves the interaction of N\textsubscript{2} with hydrocarbon fragments. This process is called the Fenimore prompt-NO mechanism [4]. The terminology is used because NO formed by this process occurs early in the flame front. The reaction path is characterized in the following way:

a) molecular nitrogen, N\textsubscript{2}, reacts with hydrocarbon fragments to produce cyanide (HCN) and ammonia radicals:

\[ CH_a + N_2 \rightarrow HCN + N, NH \]  \hspace{1cm} (1.4)

b) the hydrogen abstraction reaction of HCN generates additional ammonia radicals (NH, NH\textsubscript{2}) via o xo c y a n o gen s (HNCO, NCO):

\[ HCN + OH \rightarrow HNCO, NCO + H, H_2O \]  \hspace{1cm} (1.5)
\[ HNCO, NCN + H \rightarrow NH_a + CO \]  \hspace{1cm} (1.6)

c) ammonia radicals form NO:

\[ N, NH + O, OH \rightarrow NO + H, H_2O \]  \hspace{1cm} (1.7)
The atomic nitrogen formed in the first reaction may be a low temperature source of atomic nitrogen for the last reaction.

1.2.1.3 Fuel NO

The “fuel NO” formation process is presented in the middle of Figure 1.1. Both oil and coal are composed of organically bound nitrogen compounds to varying degrees, and the “fuel NO” mechanism has a prominent role in determining the emissions associated with these fuels. When combustion occurs under high temperature fuel-rich conditions the fuel is converted to cyanogens which then form oxycyanogen radicals. These compounds lead to the formation of amines as described in Equation 1.6. In a reducing atmosphere the amines form \( \text{N}_2 \) as described in the following equation:

\[
\text{NH}_n + \text{NH}_n + \text{H} \rightarrow \text{N}_2 + \text{H}_2 \tag{1.8}
\]

Alternatively, in an oxidizing environment the nitrogen in these fuels can contribute to the formation of NOx.

NOx formed in the early part of the reaction process can later be converted to molecular nitrogen as described in Equation 1.9:

\[
\text{NO} + \text{NH}, \text{NH}_2 \rightarrow \text{N}_2 + \text{O}, \text{OH} \tag{1.9}
\]

1.2.1.4 NOx Reburn

When NOx reacts with hydrocarbon fragments, the nitrogen forms a cyanogen as described in Equation 1.10:

\[
\text{NO} + \text{CH}_n \rightarrow \text{HCN} + \text{O}, \text{OH}, \text{H}_2\text{O} \tag{1.10}
\]

This occurs most readily in a fuel-rich environment. After this step the process follows the reactions described Equations 1.5, 1.6, and 1.8 for the formation of amines and then molecular nitrogen, \( \text{N}_2 \). Wendt et. al. [5] have identified this as the “NO Reburn” process.
1.2.2 Reduction Strategies

The chemical pathways described in the previous section provide insights into how the formation and emission of NOx might be reduced. The following strategies for NOx minimization are deduced:

• *reducing the peak flame temperature* in fuel-lean flames, especially in natural gas flames. In boilers and furnaces this can be accomplished by increased heat extraction. Other methods involve the combustion products. The cooled burned gas can be reintroduced either through “in-furnace” recirculation and re-entrainment with the flame, “external” recirculation of the flue gas (FGR), or by premixing flue gas with gaseous fuel and air prior to ignition.

• *staging the combustion air* for heavy fuel oil and pulverized coal flames. The fuel-N of these fuels is converted to N\textsubscript{2} in the initial fuel rich zone, and fuel burnout it completed by the introduction of the rest of the combustion air further downstream.

• *staging the fuel* to promote NO reburn. The late introduction of the fuel facilitates the conversion of NO to N\textsubscript{2}. Equations 1.10, 1.5, 1.6, and 1.8 characterize this process. Reburning can occur without external staging by allowing combustion products to recirculate internally and be entrained into the flame.

1.3 Development of the RSFC Burner

Low NOx Burners (LNB’s) are characterized by sequential fuel-rich and fuel-lean reaction zones established by aerodynamic means; aerodynamic separation is referred to as
internal staging. This is in contrast to external staging in which air is introduced to physically separated sections of the combustion chamber.

Experimental investigations and theoretical studies by the International Flame Research Foundation [6, 7, 8, 9, 10] have focused on problems associated with burner design, modeling, and scale-up and have offered solutions to these problems. One of the most problematic issues for LNB's is associated with fuel burnout. When the flow field is internally staged, a fuel-rich pyrolysis zone is formed. However, the flame length becomes excessive, and emission of soot, CO, and hydrocarbon species reach unacceptable levels. Due to these drawbacks, the performance of LNB's was generally considered to be limited to approximately a 50% reduction in NOx emissions [11].

In an effort to push burner performance beyond the perceived limits, MIT started research in 1989 to develop an improved low NOx burner for gas, oil, and coal. The Radially Stratified Flame Core burner design (US Patent No. 5,411,394) establishes a flow field that promotes early ignition and hence early stratification of the flow. The flow field maintains a fuel-rich core and allows adequate residence time for the fuel in the core to reburn NO and form N₂ from the heterocyclic nitrogen compounds. Furthermore, the flow field has a region of vigorous mixing further downstream to promote complete burnout.

An experimental 1.5 MW RSFC burner was developed for testing the design at MIT's Combustion Research Facility. The burner could be used with natural gas, oil, or coal. The burner was designed with flexibility in mind. The swirl component of any of its three annular jets could be adjusted as well as any of the three flow rates. The burner also was equipped to recirculate fluegas. When the burner was configured with the right swirl and flow rates, NOx emissions were reduced by 70% while CO emissions were maintained at acceptable levels. In additional testing, the burner was scaled up to 21 MW
and tested with coal and fuel oil. The.reset demonstrates the effectiveness of the flow
field to reduce NOx emissions at higher firing rates and energy densities.
CHAPTER 2
Scope of Burner Design Research

2.1 Burner and Flame Design Goals

The RSFC burner is intended for application in both new and existing industrial facilities. For this reason it must meet several design and performance specifications. The foremost research goal was to reduce NOx in an oil diffusion flame using the burner’s internal staging capabilities. It is necessary to meet this goal so that customers can meet their regulatory emission requirements. Of equal importance in terms of performance is flame stability. The flame must demonstrate a robustness to instabilities in the flow. Additionally, excess air needs to be as low as possible to minimize waste gas heat losses and to minimize the tendency to convert SO_2 to SO_3 in the combustion products when using coal.

Some limitations are imposed by the configurations of existing facilities into which the burner would be added. RSFC flames can be quite long, but flame length is controlled through vigorous mixing downstream. In some cases the furnace geometry may limit flame length so that mixing must take further upstream. The pressure drop through the burner must also be minimized. Limitations on customers’ forced air capabilities and the increased energy cost associated with higher pressure drops across the burner make this condition unyielding. The burner’s swirler designs are the most important factor in controlling the pressure drop. The challenge for burner designers is to meet all of these goals when scaling up the RSFC burner for industrial use.
2.2 Ideal RSFC Burner Performance

Heavy fuel oil is selected for study because of the unique challenges associated with its atomization and its common usage in boiler systems. In light of the burner design goals stated in the previous section, it is important to outline the characteristics of the ideal oil fired diffusion flame. High flame stability is one goal; maintaining a stable recirculation zone at the burner exit will stabilize the flame if hot products are being recirculated. Another goal is early ignition of the flame to provide the hot products for radial density stratification. This is also related to the degree of air staging. Ignition should be as early as possible maximize the size of the fuel-rich combustion zone in the limited furnace space. Flame length is balanced between demands for increased fuel residence time in the fuel-rich region and limitations on furnace size. A flame length between 4.0 and 5.0 burner diameters is considered optimal. For the purposes of discussion, the flame length is defined as the distance from the burner to the farthest downstream position of the 99.9% fuel burn-out contour. Thermal NO levels are reduced by heat extraction from the flame so as to reduce the temperature in the fuel lean combustion zone below 1800K. Higher temperatures in the fuel rich zone promote more rapid reduction of the fuel bound nitrogen, so temperatures in the fuel rich zone should be as high as possible.

2.3 Design Criteria

The burner and system have many different design parameters that can be adjusted to change the burner's performance. Figure 2.1 shows several of the independent variables which can be varied in the design. The flow field can be characterized with respect to the specific flow phenomena that occur. Figure 2.2 specifies several dependent variables which help characterize the flow field. The relationship between the independent
Figure 2.1 Independent Variables for Burner Design
Figure 2.2 Dependent Variables Indicating Burner Performance
variables of the design and the dependent variables of burner performance is to be
determined.

2.3.1 Operating Parameters

The operating parameters needed to obtain the ideal RSFC burner performance
were investigated. Additionally, the sensitivity of burner performance to changes in the
operating parameters was examined both experimentally and computationally. The
influence of primary and tertiary air Reynolds number and swirl were examined
extensively. The relative air distribution between the primary, secondary, and tertiary air
ducts was also studied for its influence on establishing the ideal flow field. The role of
atomization in establishing the ideal flow field was also examined by studying the effect of
fuel droplet size and atomizer spray angle.

2.3.2 Design Parameters

The design of the burner quarl was studied to understand its influence on the flow
field. Having determined the significance of certain features, the quarl can be redesigned to
meet the minimum requirements for establishing the desired flame front. The radial
spacing of the annular jets is also important with regard to the flow field and jet
interactions, so, it was studied as well.

2.4 Scaling

After determining the design criteria which establish the ideal flow field in an
experimental burner, the changes in these criteria with burner scale-up needs to be
determined. Several different similarity criteria can be applied to a reacting system.
Determining the similarity criteria most important to reproducing the ideal flow field is of
primary interest. Discovering acceptable methods of adjusting the similarity criteria to
meet the constraints of practical burner systems is also addressed.
2.5 Modeling Density Stratification

Density stratification is known to play a crucial role in bringing about the low NOx emissions of the RSFC burner. Examination of the governing conservation equations for the flow field indicates that changes in density can play a significant role in the dynamics of a stratified system. An incompressible CFD code fails to capture these effects; so, modification of the code is undertaken to improve modeling capabilities for stratified flows and specifically for the RSFC burner. The code is tested by comparing modeling results for isothermal stratified jets with reported experimental values. The modified code is then applied to the RSFC burner to determine the influence of density stratification on the flow field.

The focus here is on the flow field and not specifically on the details of NOx chemistry. A chemical kinetics mechanism for nitrogen and hydrocarbon reactions was developed by Kee et. al. [12, 13]. It is composed of over 200 reactions. By implementing this mechanism in the numerical chemical kinetics solver, CHEMKIN, predictions can be made of the nitrogen compound interconversions in laminar plug flow or well-stirred conditions. These calculations would need to be married to the flow field solution of the CFD code in order to make a prediction of the burner's NOx emissions associated with heavy fuel oil. However, this endeavor is outside the scope of the present study. Modeling the dominant features of the flow field and determining the flow field's relationship to the burner design is of primary interest.
CHAPTER 3
Flow Modeling

3.1 Incompressible Laminar Reacting Flows

Laminar reacting flows can be described by the conservation relationships for mass, momentum, chemical species, and energy. The Reynolds transport equations give an Eulerian description of these conserved quantities by relating their local time variation and convection to their production, and dissipation. The Reynolds transport equations form a set of nonlinear equations with nonunique solutions. The laminar flow solution is the fully developed flow solution in which the velocity profile is not changing with respect to the streamwise direction.

The set of Reynolds transport equations governing the flow are given in this section. Equation 3.1 is the differential form of the Reynolds transport equation for mass.

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho U_i)}{\partial x_i} = S_m
\]  

(3.1)

Mass conversion is imposed with the assumption that mass in the system is not converted to radiative forms of energy. Mass conservation requires the net mass flux into and out of the system to be the same. However, because the different phases of matter must be treated separately, a mass generation term, \(S_m\), exists in Equation 3.1 to account for phase changes within the system. The Reynolds transport equations are used to describe the gas phase while a Lagrangian form of the conservation equations are used to model the liquid phase in the oil burner model. In Equation 3.1 the generation term is greater than zero in
regions of oil evaporation. Equation 3.2 describes the general form the mass generation term in the oil burner model.

$$S_m \geq 0 \quad (3.2)$$

In the derivation of the other governing equations, two phase interactions are modeled with the assumption that the mass of a differential volume is discrete. Therefore, in the momentum, species, and energy conservation equations the mass generation term is assumed to be zero.

Equation 3.3 is the differential form of the Reynolds transport equation for momentum. The time variation and transport of momentum is equal to the sum of the forces acting on a differential volume including pressure, shear stress, gravitational, and liquid phase interaction drag forces. The drag force, $F_i$, is computed in the solution to the Lagrangian equations governing droplet trajectories and is based on mean droplet size and a drag coefficient.

$$\frac{\partial (\rho U_i)}{\partial t} + \frac{\partial (\rho U_i U_j)}{\partial x_j} = - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i + F_i \quad (3.3)$$

Equation 3.4 is the definition of the flow shear stress, i.e. the shear stress tensor minus the normal pressure forces. The flow shear stress is computed using the local molecular viscosity. The gradient of the flow shear stress across a differential volume describes the net shear forces acting on the differential volume.

$$\tau_{ij} = \mu \left( \frac{\partial U_j}{\partial x_i} + \frac{\partial U_i}{\partial x_j} \right) \quad (3.4)$$

Molecular species are conserved in the absence of any chemical reactions. Equation 3.5 shows the Reynolds transport equation for species $n$. The time variation of species concentration in a volume and the transport of the species through the volume is balanced by the mass diffusion of the species and its formation/destruction by chemical
reactions. The species reaction source/sink term, $S_{r,s}$, is computed from species residence time in the flow volume and local reaction rates. The species phase change source/sink term, $S_{m,n}$, is based on the evaporation/condensation of the liquid phase of the species in the flow volume.

$$\frac{\partial (\rho Y_s)}{\partial t} + \frac{\partial (\rho U_i Y_s)}{\partial x_i} = \frac{\partial J_{n,i}}{\partial x_i} + S_{r,s} + S_{m,n} \quad (3.5)$$

Equation 3.6 defines the mass diffusion flux in direction $i$ according to Fick's law for molecular diffusion and the Soret effect for thermal diffusion.

$$J_{n,i} = -\rho D_{n,mix} \frac{\partial Y_n}{\partial x_i} - D_n \frac{1}{T} \frac{\partial T}{\partial x_i} \quad (3.6)$$

The last conservation relationship is the Reynolds transport equation for energy. Equation 3.7 relates the time variation of enthalpy in a differential volume and the transport of enthalpy through the volume to the flux of energy due to thermal conduction, molecular diffusion of enthalpy, pressure changes, pressure and viscous work, and chemical reaction heat release/absorption. The heat source/sink from chemical reactions is based upon the extent of the chemical reaction taking place in the volume.

$$\frac{\partial (\rho h)}{\partial t} + \frac{\partial (\rho U_i h)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \left( \sum_n h_n J_n \right) + \frac{\partial p}{\partial t}$$

$$+ U_i \frac{\partial p}{\partial x_i} + \tau_{ij} \frac{\partial U_j}{\partial x_j} + S_n \quad (3.7)$$

3.2 Time Averaged Turbulent Flow Equations with Density Fluctuations

The governing relationships for laminar flow given in Section 3.1 can be used to obtain an exact solution for the turbulent flow field. However, this requires the specification of an initial condition for the unsteady flow field, and the time resolved
solution will be nonunique. Fortunately, the mean characteristics of the turbulent flow field provide a useful description of the flow and give a unique solution which does not require specification of an initial condition. To obtain this solution, the turbulent characteristics of the flow field are specified by the sum of the ensemble averaged and fluctuating components. Equation 3.8 shows the decomposition of the turbulent velocity, \( \tilde{U}_i \), into these components.

\[
\tilde{U}_i = U_i + u'_i
\] (3.8)

When the boundary conditions are time invariant the ensemble averaged component is equivalent to a time-averaged value. The other turbulent characteristics of the flow are expressed in a similar fashion. Equation 3.9 includes the definitions for turbulent density, pressure, enthalpy, and mass fraction.

\[
\begin{align*}
\tilde{\rho} &= \rho + \rho' \\
\tilde{p} &= p + p' \\
\tilde{h} &= h + h' \\
\tilde{Y} &= Y + Y'
\end{align*}
\] (3.9)

Density fluctuations are not considered significant if the flow field has only small variations in density. In reacting flows, however, a large density gradient can exist around the reaction zone due to the temperature gradient. The effect of density fluctuations in a swirling flow field are of particular interest because they exist in the RSFC burner flow field; for this reason density fluctuations are included in this derivation.

The governing relationships in Section 3.1 are transformed into a time-averaged turbulent component form in order to solve for the time-averaged turbulent flow field. The gravitational, chemical reaction, and phase change source terms are left out to simplify the expressions. Equation 3.10 is the time-averaged turbulent form of the differential mass
conservation equation. The transport of mass includes the correlation of density and velocity fluctuations.

\[
\frac{\partial \left( \rho U_i + \rho' u_i' \right)}{\partial x_i} = 0
\]  

(3.10)

Equation 3.11 describes the turbulent transport of momentum. Here the shear stress tensor is accompanied by the Reynolds stress tensor, \(-\rho' u'_j\). Density fluctuations introduce two additional terms to the momentum transport equation.

\[
\frac{\partial \left[ (\rho U_j + \rho' u'_j) U_i \right]}{\partial x_j} = - \frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial (\rho U_j \rho' u'_j)}{\partial x_k} \frac{\partial}{\partial x_j} - \frac{\partial (\rho' u'_j U_j + \rho' u'_j u'_j)}{\partial x_j}
\]  

(3.11)

Equation 3.12 describes the turbulent transport of species in differential form. Density fluctuations change the mass diffusion flux and introduce two additional terms. The first term on the RHS is the turbulent mass diffusion flux.

\[
\frac{\partial \left[ (\rho U_i + \rho' u_i') Y_n \right]}{\partial x_i} = - \frac{\partial (\rho U_i Y_n)}{\partial x_i} + \frac{\partial \tilde{J}_{ni}}{\partial x_i} - \frac{\partial (U_i P Y_n + u_i' Y_n')}{\partial x_i}
\]  

(3.12)

Equation 3.13 is the differential form of the turbulent transport of enthalpy. The first term on the RHS is the turbulent thermal conductivity.

\[
\frac{\partial \left[ (\rho U_i + \rho' u_i') h \right]}{\partial x_i} = - \frac{\partial (\rho U_i h')}{\partial x_i} + \frac{\partial \left( k \frac{\partial T}{\partial x_i} \right)}{\partial x_i} - \frac{\partial}{\partial x_i} \left( \sum_{n} \tilde{h}_n \tilde{J}_n \right)
\]  

\[
+ \tilde{U}_i \frac{\partial \tilde{p}}{\partial x_i} + \tilde{u}_{ij} \frac{\partial \tilde{U}_i}{\partial x_j} - \frac{\partial (U_i \rho' h' + u_i' \rho' h')}{\partial x_i}
\]  

(3.13)

3.3 Modeling of Turbulence Correlations

In this section the two equation model of turbulence used in the modeling studies is formulated. The treatment of density fluctuations and other turbulence correlations are then
considered. Equation 3.11, the turbulent momentum equation, introduced the Reynolds stress (i.e. turbulent shear stress) tensor. From the turbulent momentum equation an expression for the transport of Reynolds stresses is derived, Equation 3.14. It describes the generation, pressure-strain correlation, dissipation, and diffusion of turbulent shear stress respectively.

\[
\frac{\partial (\rho U_k u'_i u'_j)}{\partial x_k} = -2\rho u'_i u'_k \frac{\partial U_i}{\partial x_k} + 2\rho' \frac{\partial u'_i}{\partial x_i} - 2\tau' \frac{\partial u'_i}{\partial x_k} \\
+ \frac{\partial \left( -2p'u'_i \delta_{ik} + 2u'_i \tau'_{ik} - u'_i u'_j \right)}{\partial x_k}
\]  

(3.14)

Three of the turbulent shear stresses are used to characterize the turbulent kinetic energy in the flow. Equation 3.15 is the definition of this quantity, \( k \).

\[
k = \frac{1}{2} \sum_i u_i'^2
\]  

(3.15)

By applying this definition to the transport of shear stress, a single expression for the transport of turbulent kinetic energy is derived.

\[
\frac{\partial (\rho U_k k)}{\partial x_k} = -\rho u'_i u'_k \frac{\partial U_i}{\partial x_k} - \tau'_{ik} \frac{\partial u'_i}{\partial x_k} \\
- \frac{\partial}{\partial x_k} \left( -p'u'_i \delta_{ik} + u'_i \tau'_{ik} - \frac{1}{2} \rho u'_i u'_j \right)
\]  

(3.16)

Kolmogorov and Prandtl were the first to propose using the transport of turbulent kinetic energy in the characterization of turbulence; it is used in the present case as well. A second turbulence quantity is needed to express the turbulent mixing length according to the characterization by Prandtl. Historically, several formulations have been tried, but each gives a very similar result. The model used in this study uses the turbulence dissipation:
\[ \varepsilon = \frac{\mu}{\rho} \left( \frac{\partial u_i'}{\partial x_k} \right)^2 \]  

(3.17)

This can be substituted into the expression for the transport of turbulent kinetic energy.

\[ \partial (\rho U_k k) = - \rho u_i' u_k' \frac{\partial U_i}{\partial x_k} - \rho \varepsilon \]

\[ + \frac{\partial}{\partial x_k} \left( -p' u_k' - \frac{1}{2} \rho u_i' u_i' + \mu \frac{\partial k}{\partial x_k} \right) \]  

(3.18)

Additionally, an expression for the transport of turbulence dissipation can be derived.

\[ \frac{\partial (\rho U_k \varepsilon)}{\partial x_k} = -2\mu \frac{\partial U_i}{\partial x_k} \left[ \frac{\partial u_i'}{\partial x_i} + \frac{\partial u_i'}{\partial x_k} \frac{\partial u_k'}{\partial x_i} \right] - 2\mu \frac{\partial u_i'}{\partial x_k} \frac{\partial u_i'}{\partial x_i} \]

\[ - \frac{\partial}{\partial x_k} \left( \rho u_i' \varepsilon' \right) - 2\nu \frac{\partial}{\partial x_i} \left( \frac{\partial p'}{\partial x_i} \frac{\partial u_i'}{\partial x_i} \right) + \frac{\partial}{\partial x_k} \left( \mu \frac{\partial \varepsilon}{\partial x_k} \right) \]

\[ - 2\rho \left( \nu \frac{\partial^2 U_i}{\partial x_k \partial x_i} \right)^2 - 2\mu \frac{\partial^2 U_i}{\partial x_k \partial x_i} u_i' \frac{\partial u_i'}{\partial x_k} \]  

(3.19)

In this two equation turbulence model the turbulent shear stresses can be described using the Boussinesque hypothesis for an incompressible flow:

\[ \rho u_i' u_j' = \frac{2}{3} \rho k \delta_{ij} - \mu_i \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \]  

(3.20)

The turbulent viscosity, \( \mu_i \), characterizes the turbulence intensity and mixing length and is defined as:

\[ \mu_i = C_{i\mu} \rho \frac{k^2}{\varepsilon} \]  

(3.21)

The turbulent viscosity is the basis for characterizing yet undefined turbulence quantities. In the transport of turbulent kinetic energy the turbulent diffusion terms are related to the diffusion of \( k \):
\[ \mu_t \frac{\partial k}{\partial x_k} = -p' u'_k - \frac{1}{2} \rho u'_k u'_i \]  

(3.22)

With this substitution, the transport of turbulent kinetic energy is described completely by known quantities:

\[ \partial (\rho U_k k) = \mu_e \left( \frac{\partial U_i}{\partial x_k} + \frac{\partial x_k}{\partial U_i} \right) \frac{\partial U_i}{\partial x_k} - \rho \varepsilon + \frac{\partial}{\partial x_k} \left( \mu_e \frac{\partial k}{\partial x_k} \right) \]  

(3.23)

where the effective viscosity is defined as the sum of the turbulent and molecular viscosity.

\[ \mu_e = \mu_t + \mu \]  

(3.24)

The turbulence model can now be completed by making appropriate substitutions for the unknown quantities in the dissipation transport equation. The turbulent diffusion of \( \varepsilon \) is characterized in the same manner as it was for \( k \):

\[ \frac{\mu_t}{\sigma_e} \frac{\partial \varepsilon}{\partial x_k} = -\rho u'_k \varepsilon' \]  

(3.25)

The generation of \( \varepsilon \), \( S_\varepsilon \), is assumed to be proportional to the generation of \( k \), \( S_k \):

\[ S_\varepsilon \propto S_k = G_k - \rho \varepsilon \]  

(3.26)

where the first generation term, \( G_k \), has the following definition:

\[ G_k = \mu_e \left( \frac{\partial U_i}{\partial x_k} + \frac{\partial U_k}{\partial x_i} \right) \frac{\partial U_i}{\partial x_k} \]  

(3.27)

The generation of \( \varepsilon \) encompasses several terms.

\[ S_\varepsilon = -2\mu \frac{\partial U_i}{\partial x_k} \left( \frac{\partial u'_k}{\partial x_i} \frac{\partial u'_i}{\partial x_k} + \frac{\partial u'_i}{\partial x_k} \frac{\partial u'_k}{\partial x_i} \right) - 2\mu \frac{\partial u'_k}{\partial x_k} \frac{\partial u'_i}{\partial x_i} \frac{\partial u'_i}{\partial x_k} \]

\[ -2\nu \frac{\partial}{\partial x_i} \left( \frac{\partial \varepsilon'}{\partial x_i} \right) - 2\rho \left( \nu \frac{\partial^2 u'_i}{\partial x_k \partial x_k} \right)^2 - 2\mu \frac{\partial U_i}{\partial x_k} \frac{u'_k}{u'_i} \frac{\partial u'_i}{\partial x_k} \]  

(3.28)

The turbulence quantities are used to formulate the correct dimensions for the generation of turbulent diffusion, and modeling constants are introduced for proportionality to the generation and dissipation respectively.
\[ S_\varepsilon = C_{1\varepsilon} \frac{\varepsilon}{k} (G_k - C_2 \rho \varepsilon) \]  

(3.29)

After making the appropriate substitutions, the two equation turbulence model is completely characterized by known quantities. The final form of the \( \varepsilon \) transport equation is as follows:

\[ \frac{\partial (\rho U_k \varepsilon)}{\partial x_k} = C_{1\varepsilon} \frac{\varepsilon}{k} (G_k - C_2 \rho \varepsilon) + \frac{\partial}{\partial x_k} \left( \frac{\mu_\varepsilon}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_k} \right) \]  

(3.30)

Many studies have been performed to evaluate the constants in the two-equation turbulence model from experimental data. In the burner modeling studies the values in Table 3.1 were used. For \( C_\mu \) the first value was used in all of the cases presented, but the second value was also examined as suggested by Ehrhardt [31]

<table>
<thead>
<tr>
<th>( C_\mu )</th>
<th>0.09 ; 0.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_\varepsilon )</td>
<td>1.3</td>
</tr>
<tr>
<td>( C_{1\varepsilon} )</td>
<td>1.44</td>
</tr>
<tr>
<td>( C_k )</td>
<td>1.92</td>
</tr>
<tr>
<td>( C_\tau )</td>
<td>1.8</td>
</tr>
<tr>
<td>( C_4 )</td>
<td>0.6</td>
</tr>
</tbody>
</table>

Table 3.1 Turbulence Model Constants

The previous derivation provides a description of the turbulent shear stresses in the flow; however, several other fluctuating terms in the Section 3.2 governing equations for turbulent flow remain undescribed. Two alternatives exist for modeling these additional terms. Additional equations can be derived which describe the transport of the turbulent correlations, or algebraic approximations can be used to represent the turbulent correlations. Algebraic approximations are chosen primarily in the interest of saving computational time but also because they have demonstrated their usefulness. An algebraic approximation for density fluctuations was given by Bilger [32] in the following form:

\[ \overline{\rho \rho' u_i} = -\frac{\mu_i}{\sigma_\rho} \frac{\partial \rho}{\partial x_i} \]  

(3.31)
\( \sigma_p \) generally has a value around 0.9. Substitution into Equation 3.11 gives an expression for momentum transport in terms of known quantities. The third order correlation is neglected.

\[
\frac{\partial}{\partial x_j} \left( (\rho U_j + \rho' u_j) U_i \right) = - \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial (\rho u' u_j)}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{\rho \sigma_p} \frac{\partial \rho}{\partial x_i} u_j \right) (3.32)
\]

A more common algebraic substitution is for the turbulent species correlation. The turbulent viscosity is related the turbulent molecular diffusion by the turbulent Schmidt number.

\[
\rho_{u_i} \dot{Y}_n = - \frac{\mu_t}{Sc_i} \frac{\partial \dot{Y}_n}{\partial x_i} (3.33)
\]

Turbulent Schmidt numbers have been found experimentally to have values around 0.7 for most species. The turbulent enthalpy correlation has similar form to the previous expression. The turbulent Prandtl number relates the turbulent viscosity to the turbulent thermal conductivity.

\[
\rho_{u_i} \dot{h} = - \frac{\mu_t}{Pr_i} \frac{\partial \dot{h}}{\partial x_i} (3.34)
\]

The turbulent Prandtl number was also set to 0.7 based on experimental results.

### 3.4 Turbulence Models with Density Fluctuations

In the computational study of density fluctuations in stratified swirling flows, the effects on the momentum, turbulent kinetic energy, and turbulent shear stress were considered. A Reynolds Stress turbulence model was used in the study to insure modeling accuracy of anisotropic shear stresses. Equation 3.32 showed the modification that was made to the momentum equation. In the rest of this section, the modifications to the transport of turbulent kinetic energy and turbulent shear stress are presented.
In Equation 3.18 the general form of the transport of turbulent kinetic energy was presented. Here, the transport equation is modified to include the contributions of density fluctuations.

\[
\frac{\partial (\rho U_k)}{\partial x_k} = - \rho \bar{u}_i' \frac{\partial U_i}{\partial x_k} - \rho \varepsilon + \frac{\partial}{\partial x_k} \left( -p' \bar{u}_k' - \frac{1}{2} \rho \bar{u}_i'u_i' + \mu \frac{\partial k}{\partial x_k} \right) \\
- \left( \rho' \bar{u}_i U_k + \rho' \bar{u}_i'u_i' \right) \frac{\partial U_i}{\partial x_k} - \frac{\partial}{\partial x_k} \left( \frac{1}{2} U_k \rho' \bar{u}_i'u_i' + \frac{1}{2} \rho' \bar{u}_i'u_i' \right) \tag{3.35}
\]

Only the generation/damping of turbulence was modeled since this is the dominant effect. Third order correlations were neglected. Equation 3.36 shows the modified turbulent kinetic energy transport equation that was applied in the modified code. All of the quantities are defined according to the previously discussed definitions.

\[
\frac{\partial (\rho U_k)}{\partial x_k} = G_k - \rho \varepsilon + \frac{\partial}{\partial x_k} \left( \mu_e \frac{\partial k}{\partial x_k} \right) + \frac{\mu_l}{\sigma_p} \left( \frac{1}{\rho} \frac{\partial p}{\partial x_i} \right) U_k \frac{\partial U_i}{\partial x_k} \tag{3.36}
\]

In the Reynolds Stress model the shear stress is solved for using the transport equation rather than modeled algebraically. Equation 3.14 showed the transport of shear stress without density fluctuations. In the following expression the contributions of density fluctuations are introduced.

\[
\frac{\partial \left( (\rho U_k + \rho' \bar{u}_k')u_i' \right)}{\partial x_k} = - 2 \rho \bar{u}_i'u_i' \frac{\partial U_j}{\partial x_k} - 2 \tau_{ij} \frac{\partial u_j}{\partial x_k} - \frac{\partial (2p' \bar{u}_i'u_i')}{\partial x_k} \\
+ \frac{\partial \left( -\rho \bar{u}_i'u_i' + 2\tau_{ij}u_j' - U_k \rho' \bar{u}_i'u_j' \right)}{\partial x_k} \\
- 2 \left( U_k \rho' \bar{u}_i'u_i' + \bar{u}_k' \rho' \bar{u}_i'u_i' \right) \frac{\partial U_i}{\partial x_k} + 2 \rho' \frac{\partial u_i'}{\partial x_k} \delta_{ik} \tag{3.37}
\]

The Reynolds Stress turbulence model uses an exact expression, Equation 3.38, for the production of shear stress.
\[ P_i = -2\rho u_i u'_{\kappa} \frac{\partial U_j}{\partial x_k} \]  
\[ P = -\rho u_i u'_{\kappa} \frac{\partial U_j}{\partial x_k} \]  

(3.38)  
(3.39)

Modeling assumptions are made for the other terms; third order correlations and some density fluctuation dissipation terms are neglected. Equation 3.37 is modeled in the form given in Equation 3.40. It shows the expressions for shear stress production, dissipation, diffusion, production from density fluctuations, and pressure/strain dissipation respectively.

\[
\frac{\partial}{\partial x_k} \left( \rho U_k + \rho' u'_k \right) u_i u'_j = P_{ij} - \frac{2}{3} \delta_{ij} \rho \varepsilon + \frac{\partial}{\partial x_k} \left( \mu_i \frac{\partial u_i u'_j}{\partial x_k} \right) + 2 \frac{\mu_s}{\sigma_p} \left( \frac{1}{\rho} \frac{\partial}{\partial x_i} \right) \frac{\partial U_i}{\partial x_k} \\
+ \left[ -C_3 \frac{\varepsilon}{k} \left( u_i u'_j - \frac{2}{3} \delta_{ij} \rho \right) - C_4 \left( P_{ij} - \frac{2}{3} \delta_{ij} \rho \right) \right] 
\]  

(3.40)

In the RSM this transport equation is used to determine each of the Reynolds stress tensor components.

### 3.5 Density Stratification in Axisymmetric Swirling Flows

The significance of density fluctuation modeling in a swirling flow will be examined analytically in this section. The foregoing tensor expressions were given in Cartesian coordinates:

\[ x_i = < x, y, z > \]  
(3.41)

In an axisymmetric system, polar coordinates are best suited to describing the flow filed:

\[ x_i = < x, r, \theta > \]  
(3.42)

Cartesian coordinate displacements as well as the time derivatives, i.e. velocity components, can be transformed into a polar form through a simple algebraic substitution.
Taken a step further, the Cartesian differentials can be expressed in polar form as the product of two transformation matrices:

\[
\frac{\partial U_i}{\partial x_j} = \begin{bmatrix} \frac{\partial U_i}{\partial \hat{x}} & \frac{\partial \hat{U}}{\partial \hat{x}} \\
\frac{\partial \hat{U}}{\partial \hat{x}} & \frac{\partial \hat{U}}{\partial \hat{x}} \end{bmatrix}
\]

(3.43)

In the limit of very small angles, the trigonometric expressions for \( \theta \) are eliminated, and a general polar representation of the Cartesian differentials is obtained:

\[
\lim_{\theta \to 0} \frac{\partial U_i}{\partial x_j} = \begin{bmatrix} \frac{\partial \hat{U}}{\partial \hat{x}} & \frac{\partial \hat{U}}{\partial \hat{r}} & \frac{\partial \hat{U}}{\partial r \hat{\theta}} \\
\frac{\partial \hat{V}}{\partial \hat{x}} & \frac{\partial \hat{V}}{\partial \hat{r}} & \frac{\partial \hat{V}}{\partial r \hat{\theta}} \\
\frac{\partial \hat{W}}{\partial \hat{x}} & \frac{\partial \hat{W}}{\partial \hat{r}} & \frac{\partial \hat{W}}{\partial r \hat{\theta}} + \frac{\hat{V}}{r} \end{bmatrix}
\]

(3.44)

This transformation is implemented in the following analysis of axisymmetric jets.

Changes in jet entrainment are characteristic of density stratification experiments. For an axisymmetric jet the rate of entrainment is closely associated with the turbulent mixing. In the \( k-\varepsilon \) turbulence model, the magnitude of the turbulent kinetic energy is a good indicator of the degree of radial mixing. In the RSM turbulence model, the energy associated with radial fluctuations in the flow, \( \rho \hat{V}' \hat{V}' \), is indicative of the work done in radial mixing and hence entrainment. In the absence of turbulent kinetic energy, the jet would be governed by molecular shear stresses and molecular diffusion which are much smaller in magnitude than their turbulent counterparts. Henceforth, the effect of density fluctuations on the turbulent kinetic energy in a swirling axisymmetric flow are examined.

Equation 3.36 described the transport of \( k \) inclusive of the effects of density fluctuation on the generation of turbulent kinetic energy. In the cases of interest, density
stratification dampens the turbulent kinetic energy. Equation 3.45 relates the damping of turbulent kinetic energy by density stratification to its generation due to shear stress.

\[
\frac{\text{Damping of T.E.}}{\text{Generation of T.E.}} = - \frac{\mu_i \left( \frac{1}{\rho} \frac{\partial \rho}{\partial x_i} \right) U_k \frac{\partial U_i}{\partial x_k}}{\mu_e \left( \frac{\partial U_i}{\partial x_k} + \frac{\partial U_k}{\partial x_i} \right) \frac{\partial U_i}{\partial x_k}} \tag{3.45}
\]

The sign is negative because a positive ratio is chosen to be indicative of damping by density stratification.

In a stratified axisymmetric swirling jet the dominant terms in the numerator are associated with the radial density gradient, i=2, and the swirl, k=3. The dominant term in the denominator is associated with the radial gradient, k=2, and the axial jet velocity, i=1; generation of turbulence modeled in this term comes from the strong axial shear stresses acting within the jet. After transforming Equation 3.45 into polar coordinates and removing the second order terms, the ratio of damping to generation of turbulent kinetic energy can be expressed in the form of the modified Richardson number [33]:

\[
Ri^* = \frac{1}{\rho} \left( \frac{r \hat{W}}{\partial \hat{r}} \right)^2 \left( \frac{\partial \hat{U}}{\partial \hat{r}} \right)^{-2}
\]

(3.46)

When the RSM turbulence model is modified to include the effects of density fluctuations as given in Equations 3.32, 3.36, and 3.40, the modified Richardson number effects are included in the model as well as many others. The modified Richardson number gives a simple expression for the effect of density stratification in "laminarizing" a turbulent flow. According to experiments by Townsend [14] the Richardson number first begins to effect jet development at values around 0.05, and the mixing of outside fluid into the jet nearly ceases when Ri = 0.30.
CHAPTER 4

Burner Configurations and Methodology for Studying Burner Design Criteria

The burner and furnace design and operating conditions establish the boundary conditions which govern the physical phenomena occurring in the furnace. The study of the relationship between these boundary conditions and burner performance can be performed experimentally or computationally. Experimental testing can be both expensive and time consuming and is often impractical for large scale burner designs. For this reason it is desirable to use computational methods as extensively as possible to model the physical phenomena occurring in the furnace.

Experimental tests were conducted using a scaled-up version of the RSFC burner in the ABB Industrial Scale Burner Facility (ISBF). The computational design studies of the RSFC burner were conducted to gain a better understanding of the design features critical to the burners performance and to determine the design of the subsequent experimental burner. This chapter deals with the computational methods used in the modeling, the experimental facility which was the basis for the modeling work, and the strategy used in the parametric studies. This chapter also presents the guidelines that were followed for studying burner scale-up, and the approach that was taken to investigate stratification effects. Section 4.1 specifies the numerical methods used in the Computational Fluid Dynamics (CFD) code. Section 4.2 describes the experimental facility and the method of modeling the furnace; it also provides the experimental test conditions and the scope of each of the parametric studies. Section 4.3 describes the approach that was taken to investigate scale-up of the RSFC burner. Section 4.4 reviews
the boundary conditions for the density stratification experiments by Beér and Chigier, and describes the manner in which the experiments were modeled. Section 4.4 also describes the manner in which the influence of density stratification was assessed for the RSFC burner.

4.1 CFD Tools

Calculating the general features of an oil fired RSFC flame requires the simulation of a two-phase, reacting, swirling, turbulent flow. A commercial Computational Fluid Dynamics (CFD) code was selected that incorporated these features and had the capacity to model an axisymmetric domain of at least 25,000 spatial nodes.

4.1.1 FLUENT Code

FLUENT is a flexible CFD package that supports customized grid generation, applies a finite difference solver to the governing fluid dynamic equations, and handles basic data post-processing tasks. The equations governing fluid dynamic behavior are founded on the assumption that the fluid is a continuum, i.e. the fluid and its properties are continuously distributed in space. The computational framework for simulating a continuous medium is a discretized representation of the space occupied by the fluid. Using FLUENT Version 3.03 a customized 2D rectilinear grid was generated for the axisymmetric spatial domain of the burner. The grid has a one-to-one mapping to the computational domain. Each four-sided cell in the computational domain represents a control volume in space, and each cell has a unique set of fluid properties assigned to it.

The dynamics of the continuous phase fluid flow are characterized from a Eulerian frame of reference by a system of partial differential equations describing the conservation of mass, momentum (Navier-Stokes), energy, turbulence quantities, and chemical species. These equations are discretized for each cell in the computational domain according to the
finite difference method to create a system of algebraic relations describing the
interdependence of the cells. A solution is obtained through an interactive process of
setting up the system of equations and solving for the properties of each cell until the cell
properties approach an equilibrium.

The solution has multiple arrays of data which contain the computed fluid dynamic
properties for each control volume. The pressure, velocity, turbulence quantities, enthalpy,
and species concentration data arrays are computed directly using the governing partial
differential equations. Other fluid properties of interest are calculated for each control
volume using these data. Some properties are computed automatically; however, the
FLUENT post-processor can be used to compute any user defined property. An array of
data is displayed graphically using a contour plot drawn in the physical domain by the
FLUENT post-processor. Some problems exist in the algorithm for drawing streamline
contours and caused discontinuities to be drawn around wall cells that protrude into the
domain. However, this problem is not indicative of an error in the solution. Annular and
radial slices of the domain are presented in standard 2D plots.

4.1.2 Two-Phase Flow Modeling

The trajectory of the second phase in a two phase flow is evaluated from a
Lagrangian frame of reference. The equations for motion and trajectory of a particle are
solved for multiple incremental time steps for each cell through which the second phase
travels. The equations of motion include drag, virtual mass, and pressure gradient related
forces.

In the code the assumption is made that the second phase is dispersed. In the oil
burner models the second phase was comprised of liquid oil droplets. The assumption of
dispersed oil droplets means that interactions between droplets are neglected and interaction
with the gaseous phase is continuous over their whole trajectory. The validity of this assumption for the oil atomizer will be discussed in Section 4.2.1.5 The dispersed phase assumption requires that the oil be in distinct “packets”; for small droplets surface tension effects dominate so the assumption of spherical “packets” is reliable. The diameter of the droplets could be made uniform or of a Rosin-Rammler type size distribution.

Turbulence in the flow required that a stochastic particle tracking method be used to determine the effect of turbulent velocity fluctuations on the motion of the of the droplets. The fluctuating velocity components were calculated based on the kinetic energy of turbulence and the characteristic life time of the turbulent eddy. Turbulent velocity fluctuations were assumed to be constant over the characteristic life time of the eddy, and this was the basis for determining the time interval for direct integration of the equations of motion for a droplet in a cell.

When a droplet trajectory crosses a line of symmetry in the axisymmetric furnace model, the trajectory is re-computed as an elastic reflection off of the symmetry line. This represents the appearance of the droplet crossing the symmetry line from the other side of the annulus. Oil droplet trajectories terminated when the oil was completely converted into the gaseous phase.

In the furnace environment the oil droplets experience a thermal energy exchange with the gas phase and a mass transfer due to vaporization or boiling. Heat transfer between the droplet and the gas was governed by an energy balance relating the convective heat transfer at the droplet surface to the lumped-heat-capacity of droplet and the latent heat of vaporization. The lumped-heat-capacity model treats the droplet temperature as uniform and rests on the assumption that the internal thermal resistance is small in comparison to the external thermal resistance. This relationship is expressed in the Biot number:
\[ \text{Bi} = \frac{\bar{h} \text{ Volume}}{k \text{ Area}} \]  \hspace{1cm} (4.1)

The temperature at the center of the droplet will not differ from the surface temperature by more than 5% if it is true that:

\[ \text{Bi} < 0.1 \]  \hspace{1cm} (4.2)

Droplet vaporization occurs when the droplet temperature is between the vaporization temperature and the boiling point. The rate of vaporization is governed by “Fick’s Law”:

\[ N_i = D(C_{i,v} - C_{i,g}) \]  \hspace{1cm} (4.3)

The vapor concentration at the surface of the droplet, \( C_{i,v} \), is determined by assuming that the partial pressure of the vapor is equal to the vapor pressure at the droplet temperature. The partial pressure was defined as function of temperature for the oil. When the droplet temperature reaches the boiling point “Fick’s Law” no longer applies. Instead, the rate of mass transfer is governed by the rate of change in the droplet diameter:

\[ \frac{dD_{\text{droplets}}}{dt} = \frac{-C_b}{2D_{\text{droplet}}} \left[ 1 + 0.23 \text{Re}^{0.5} \right] \]  \hspace{1cm} (4.4)

The vaporization rate constant, \( C_b \), was evaluated from a quasi-steady analysis of droplet combustion [15]:

\[ C_b = \frac{8k_m}{\rho_{\text{droplet}} c_{p,m}} \left[ 1 + \frac{c_{p,m}}{h_f g} (T_m - T_{\text{droplets}}) \right] \]  \hspace{1cm} (4.5)

The heat and mass transfer from the liquid droplet to the gas phase changes the species concentration and enthalpy of the gas in the cells that lie along the droplet’s trajectory. This interaction is represented by source/sink terms in the energy and species conservation equations. The computational solution is obtained by alternating between the Eulerian gas phase calculations and the Lagrangian liquid phase calculations until equilibrium is reached. The liquid phase calculations result in new source/sink values for
effected cells based on the previously calculated gas phase conditions, and the gas phase calculations result in new gas phase conditions based on the previously calculated source/sink values.

4.1.3 Turbulence Model

The annular jets in the scaled-up RSFC burner had Reynolds numbers in the range of 124,000 to 267,000 indicating that the flow was fully turbulent. The dynamics of a turbulent flow differ from those of a laminar flow. The inclusion of the fluctuating velocity components in the mass conservation and Navier-Stokes equations demonstrates the contribution of the Reynolds stresses, \( \rho u_i' u_j' \), to the flow dynamics. A two equation, \( k-\varepsilon \), turbulence model was implemented to calculate the Reynolds stresses under the assumption that the turbulent viscosity is isotropic. In strongly swirling flows the turbulent viscosity is likely to vary with direction. The Reynolds Stress Model is able to model this but at the expense of significant computational time. In the RSFC parametric modeling the \( k-\varepsilon \) model was deemed to be adequate for capturing the general characteristics of the flow and its sensitivity to various design parameters.

4.1.4 Radiation Model

Numerical modeling of the reacting flow included an accounting of the radiation heat transfer in the system. FLUENT implements a six-flux radiation model to represent the radiation heat transfer within the gas phase and with the walls. This model assumes a conservation of radiation intensity. Each cell is treated as an emitter, and an absorption coefficient and scattering coefficient are determined for each cell based on its gas composition. Scattering is assumed to be isotropic, i.e. uniform in all directions. The governing equation is applied in each of the three coordinate directions before ascertaining the contribution of radiation heat flux to the local enthalpy.
4.1.5 Discretization Scheme

The existence of strong gradients, especially at an angle to the computational grid, can lead to numerical errors in the discrete representation of the continuous phase. Truncation errors can be introduced into the calculations due to the inability of the grid to accurately represent the strong gradients that may exist in some regions of the solution. Instead of using a power-law differencing scheme a higher order quadratic upwind interpolation scheme, QUICK, was used in the furnace models to reduce numerical errors of this sort. By using QUICK, computational time was increased but the gradients in the flow were better resolved.

4.1.6 Physical Properties

Several physical properties needed to be defined in order to calculated the reacting flow field of the RSFC oil burner. The properties of the gaseous species used in the code are noted in this section. The modeling of the oil is discussed in Section 4.2.1.5 although some of the properties of the oil vapor are listed here.

The inlet air for the burner was modeled using a standard two species representation. Dry atmospheric air is composed of 78.084% N₂, 20.946% O₂, and 0.934% Ar as well as some minor species. The two dominant species, molecular Nitrogen and molecular Oxygen, are the only ones considered in the air model; and Table 4.1 lists their corresponding concentrations. The molar weight of air is \( \dot{M}_{\text{AIR}} = 28.97 \text{ kg/kmole} \), but Table 4.2 shows that the air model gives a slightly lower value. The density of the air and other gases was calculated using the perfect gas law since the states exhibited here are far from the vapor dome.
The Schmidt Number, \( \text{Sc} = \frac{\mu}{\rho D} \), reflects the rate of momentum diffusion through the media relative to the rate of mass diffusion. The turbulent mass diffusion coefficient, \( D_t \), for the species transport equation is calculated using the turbulent Schmidt Number, \( \text{Sc}_t \). Table 4.1 shows that a nominal value of 0.7 was selected for gas species.

The formation enthalpy, \( \Delta H_{298}^f \), is the energy/molar unit required to form the chemical species from its pure elements in standard states. Molecular Nitrogen and Oxygen have a formation enthalpy of zero; this is the reference value for elements in their standard states. The other values in Table 4.1 come from a standard reference. [16,17]

<table>
<thead>
<tr>
<th>Air Composition</th>
<th>( \text{Sc}_t )</th>
<th>Formation Enthalpy</th>
</tr>
</thead>
<tbody>
<tr>
<td>N(_2)</td>
<td>79%</td>
<td>0.7</td>
</tr>
<tr>
<td>O(_2)</td>
<td>21%</td>
<td>0.7</td>
</tr>
<tr>
<td>CO(_2)</td>
<td>0%</td>
<td>0.7</td>
</tr>
<tr>
<td>H(_2)O</td>
<td>0%</td>
<td>0.7</td>
</tr>
<tr>
<td>Oil</td>
<td>0%</td>
<td>0.7</td>
</tr>
</tbody>
</table>

Table 4.1 Air Composition, Turbulent Schmidt Numbers, and Formation Enthalpies

In the turbulent reacting flow of the furnace the turbulent viscosity, \( \mu_i = \rho C_\mu \frac{k^2}{\varepsilon} \), is typically much larger than the molecular viscosity. Similarly, in a turbulent flow convective heat transfer is much larger than heat transfer by conduction. Because of this, the calculations were simplified so that a single value for molecular viscosity and conduction were used regardless of the composition of the gas mixture. The values that were used are shown in Table 4.2 and are based on the properties of air at standard conditions.
<table>
<thead>
<tr>
<th>$\dot{M}_{\text{AIR}}$</th>
<th>28.84 kg/kmole</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu$</td>
<td>2.00E-5 kg/m s</td>
</tr>
<tr>
<td>$k$</td>
<td>0.025 W/m K</td>
</tr>
</tbody>
</table>

Table 4.2 General Gas Properties

The specific heat of the gaseous species are defined accurately because they vary significantly with temperature and are very important to the calculation of the temperature profile within the furnace. Over the range of temperatures exhibited in the furnace the specific heat can vary by as much as 200%. The specific heat functions defined in Table 4.3 have a maximum error of 0.72% and an average error less than 0.34%. [18]

\[
c_p = a + bT + c T^2 + d T^3 \quad (\text{J/kg K})
\]

<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_2$</td>
<td>1032.1</td>
<td>-0.56107</td>
<td>+2.8861E-4</td>
<td>-1.0261E-7</td>
</tr>
<tr>
<td>$O_2$</td>
<td>796.25</td>
<td>+0.47500</td>
<td>-2.2359E-4</td>
<td>+4.1000E-8</td>
</tr>
<tr>
<td>$CO_2$</td>
<td>505.91</td>
<td>+1.3593</td>
<td>-7.9568E-4</td>
<td>+1.6975E-7</td>
</tr>
<tr>
<td>$H_2O$</td>
<td>1791.1</td>
<td>+10.638</td>
<td>+5.8610E-4</td>
<td>+1.9972E-7</td>
</tr>
<tr>
<td>Oil(g)</td>
<td>68.276</td>
<td>+5.4050</td>
<td>-3.1620E-3</td>
<td>+6.0345E-7</td>
</tr>
</tbody>
</table>

Table 4.3 Definitions of Specific Heat as a Function of Temperature

4.2 Parametric Oil Burner Performance Studies

The CFD tools were used to conduct a study of the design criteria critical to the performance of the RSFC burner. Components of the burner-furnace system were modeled with the goal of obtaining a meaningful representation without demanding an inordinate amount of computational time. The components of the experimental facility, the component models, and the assumptions implemented in the models are discussed in the next section. Following that, the scope of the parametric computational studies is discussed. Lastly, the scope of the experimental investigation is reviewed.
4.2.1 ISBF Experimental Setup and Component Modeling

The Industrial Scale Burner Facility (ISBF) at ABB Power Plant Labs was used to test the scaled-up Radially Stratified Flame Core (RSFC) burner. The first tests of the oil fired RSFC burner were conducted at MIT's Combustion Research Facility (CRF) by Shihadeh. [19] The promising results from those tests supported further study using a scaled-up version of the burner and a modeling investigation of the burner's aerodynamics and design criteria. Important features of the ISBF experimental setup and the way in which they were modeled are discussed in this section.

4.2.1.1 ISBF Furnace Geometry

The ISBF was designed to simulate an industrial scale, horizontal, front wall fired, single burner boiler. The combustion gases exit the back of the furnace through an array of water cooled tubes and then travel up a duct to an air quality control system. The side walls of the furnace were refractory lined in the region near the burner, the refractory and bare metal walls were all water cooled. Figure 4.1 shows the geometry of the ISBF from the front and side views.

The ISBF was modeled as an axisymmetric system in order to reduce computational time. In a 3D model the furnace corner effects and the non uniform span between walls would be included in determining the jet behavior. To minimize the differences with the 3D model, the diameter of the axisymmetric furnace model was set equal to the hydraulic diameter of the furnace, \( D_h = \frac{4A}{P} = 2.438 \text{ m} \) (8 ft). A cylinder of equivalent cross-sectional area would have a diameter larger than this but is believed to underestimate the wall boundary effects on the swirling jet. In confirmation of this, the RSFC furnace modeling by Sun [20] indicated that the radial position of the burner jet is modeled more accurately by using the hydraulic diameter rather than a cylinder of
Figure 4.1 Industrial Scale Burner Facility (ISBF) Geometry
equivalent cross-sectional area. To maintain the same volumetric heat release in the model as in the experimental facility, the length of the furnace model needed to exceed the actual furnace length. This is necessary because the hydraulic diameter gives a smaller cross-sectional area. Figure 4.2 illustrates the furnace model and its dimensions.

4.2.1.2 RSFC Burner Scaling, Geometry, and General Operating Conditions

The burner used in the ISBF was scaled-up from the one at MIT which had produced low NOx oil flames [19]. The MIT 1.5 MW scale RSFC burner tests were conducted at a firing rate of 0.9 MW (3 MBtu/hr) giving a volumetric heat release rate of 13,000 Btu/ft³/hr. The details of the burner geometry are discussed by Shihadeh [19]. In the first phase of ISBF experiments the burner was scaled-up to 21 MW (70 MBtu/hr) giving a heat release rate of 60,000 Btu/ft³/hr. In the second phase of ISBF testing, the burner was redesigned for a 15 MW (50 MBtu/hr) scale and was fired at 12 MW (40 MBtu/hr) giving a heat release rate of 32,000 Btu/ft³/hr. The 21 MW scale was used in the burner modeling, and the models, using the same fuel flow rate as in the phase one experiments and referenced heating values for the fuel [17], ref. Table 4.6, had a firing rate of 21 MW.

A general depiction of the near-exit geometry of the RSFC burner is given in Figure 4.3; the burner consists of three air annuli around a fuel gun which terminates with an oil atomizer. The dimensions of the annuli were varied as part of the parametric studies. The burner is interfaced with the furnace via a ceramic quarl with a diverging section of angle θ; the lip of the quarl extends into the furnace by an amount \( L_{\text{lip}} \). The quarl geometry was varied as part of the parametric studies as well.

The inlet air pre-heat and exit \( O_2 \) levels established in the burner model fell within the range tested in the first phase of ISBF experiments. For most of the first phase
Figure 4.2 Industrial Scale Burner Facility Model
Figure 4.3 Radially Stratified Flame Core Burner Exit and Quarl Geometry
experiments the air pre-heat was 480 °F, but a range of pre-heat temperatures between ambient conditions and 550 °F were included in the tests. In all of the burner models the primary, secondary, and tertiary air pre-heats were set to 530 °F. In all of the experiments the furnace had between 2% and 4% exit $O_2$; in the models, using a firing rate of 21 MW, the average exit $O_2$ was 2.4%. Table 4.4 summarizes these conditions. The details of the fuel properties and the fuel model are discussed in Section 4.2.1.5.

<table>
<thead>
<tr>
<th></th>
<th>Air-Preheat Temperature</th>
<th>Exit $O_2$</th>
<th>Firing Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Range Tested</td>
<td>Baseline</td>
<td>Range Tested</td>
</tr>
<tr>
<td>MIT Exp.</td>
<td>340 °F - 480 °F</td>
<td>540 °F</td>
<td>2% - 4%</td>
</tr>
<tr>
<td>Phase One Exp.</td>
<td>ambient - 550 °F</td>
<td>480 °F</td>
<td>2% - 4%</td>
</tr>
<tr>
<td>Modeling</td>
<td>530 °F</td>
<td>530 °F</td>
<td>2.4%</td>
</tr>
<tr>
<td>Phase Two Exp.</td>
<td>480 °F - 515 °F</td>
<td>500 °F</td>
<td>2% - 4%</td>
</tr>
</tbody>
</table>

Table 4.4 Air-Preheat and Exit $O_2$ Conditions

4.2.1.3 Grid Generation

Several guidelines were implemented in the process of grid generation so that numerical errors from the grid would be minimized and computational time decreased. Rapid changes in grid spacing can cause errors primarily in the calculation of diffusion terms. To minimize numerical diffusion errors changes in grid spacing between adjacent cells was not allowed to exceed 10%. This is a conservative guideline which assures that numerical diffusion was not significant. Cell widths varied at most by 4.7:1, and cell heights varied at most by 3:1. Generally, cell aspect ratios were less than 5:1 except for the third quarter of the furnace in which they were allowed to elongate within the limit of 11:1. That section tended to have relatively small axial gradients which prevented stability problems from developing from the high aspect ratio of the cells. The elimination of cells in that section helped lower the total number of cells to around 10,000. The actual number
of cells depends on the case being considered. Further decreases in the number of cells were not considered because of their impact on numerical accuracy; so, computational time was presumed to be as low as possible for the given geometry.

The experimental burner geometry was reproduced in the CFD model using rectangular cells. Initially, the grid design was based on the geometry of the scaled-up, 70 MBtu/hr, RSFC burner. The wall boundaries of the initial grid matched most of the horizontal and vertical boundaries of the experimental set-up. The exception to this was the thin wall between the primary and secondary air ducts. In some cases it was neglected and in others it was modeled to be too thick for the sake of maintaining reasonable grid sizes and grid spacing. Angled wall boundaries of the burner were carefully modeled so that they conformed closely to their intended slope. To maintain an accurate representation of the turbulent jet shear stresses and velocity profiles seven or more cells were used for primary and tertiary air inlets. These account for 95% or more of jet momentum in all cases. The secondary air inlet was represented by at least four cells. The burner exit flow fields for the primary and secondary air were represented by top-hat velocity profiles in some cases; in the rest of the cases the jet profiles of the primary and secondary air were allowed to develop in a duct of length:

$$h/L > 3.0$$

(4.6)

In Figure 4.4 the features described in this section are illustrated for the near burner zone of one of the computational grids.

4.2.1.4 Fuel Atomization

Fuel atomization has a significant influence on the flame shape and emissions, but the physics of atomizer design and the characteristics of the best atomizer for the RSFC
Figure 4.4 Characteristic Computational Grid for RSFC Burner and Furnace
burner are not completely understood. For this reason a variety of fuel atomizers were considered in the experiments, and atomization characteristics were examined in the operating parameter parametric study. The types of atomizers used in the experiments and the atomizer model are documented in this section.

Fuel atomizers that receive industrial use can generally be classified as either twin fluid shearing atomizers or pressure atomizers. In the RSFC experiments twin fluid shearing atomizers were used instead of pressure atomizers because they are more amenable to scaling, are better able to maintain their spray characteristics over turn down, and are more common in practical combustion systems. [21] The availability of pressurized steam in many combustion systems makes a steam shearing fuel atomizer an attractive option.

The RSFC oil burner tests at MIT utilized 6 hole Y-jet oil atomizers with spray angles, $\alpha$, of 0° and 5°. Figure 4.5 shows a schematic of a Y-jet atomizer. In the first phase of ISBF experiments, a study was conducted to scale up the MIT atomizer. Y-jet atomizers with 1 to 30 holes were considered with spray angles, $\alpha$, in the range of 0° to 30°. Variations in the fuel velocity, length of the fuel/steam mixing chamber, and shape of the jet exit hole were also examined. As a result of this study various 30 hole Y-jet atomizers with various spray angels between 0° and 10° were selected for the first phase experiments. Proprietary Bete Fog atomizers were also used. In the second phase of experiments a 22 hole Y-jet atomizer was used with alternating spray angles of 0° and 10°. Table 4.5 gives an overview of the atomizers used in the experiments.
Figure 4.5 Y-Jet Atomizer Design
<table>
<thead>
<tr>
<th></th>
<th>Atomizer Type</th>
<th># of Holes</th>
<th>Spray Angle, $\alpha$</th>
<th>$m_{gas,\text{total}}/m_{oil}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MIT Exp.</td>
<td>Y-Jet</td>
<td>6</td>
<td>0°, 5°</td>
<td>≈0.10</td>
</tr>
<tr>
<td>MIT Exp.</td>
<td>Sonicore</td>
<td>N/A</td>
<td>N/A</td>
<td>≈0.50</td>
</tr>
<tr>
<td>Phase I Exp.</td>
<td>Y-Jet</td>
<td>30</td>
<td>0° to 30°</td>
<td>≤0.30</td>
</tr>
<tr>
<td>Phase I Exp.</td>
<td>Bete Fog</td>
<td>x</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>Modeling</td>
<td>Y-Jet</td>
<td>-</td>
<td>0°, 5°, 10°</td>
<td>0, 0.05</td>
</tr>
<tr>
<td>Phase II Exp.</td>
<td>Y-Jet</td>
<td>22</td>
<td>Alt. 0° &amp; 10°</td>
<td>≤0.30</td>
</tr>
<tr>
<td>Phase II Exp.</td>
<td>Y-Jet</td>
<td>22</td>
<td>10°</td>
<td>≤0.30</td>
</tr>
</tbody>
</table>

Table 4.5 Atomizer Characteristics

In the computational study of the burner’s performance, the atomizer was modeled using liquid fuel injection sites into the gaseous phase. The mean droplet exit angle from the Y-jet atomizer was assumed to be the spray angle, $\alpha$. The spray from a Y-jet atomizer hole was modeled as 10 distinct droplet streams spread out evenly around the spray angle. In the model, the spreading half angle, $\beta$, is 20°; this means that 50% of the fuel is distributed within ±10° of the spray angle. Figure 4.6 illustrates these parameters for the oil droplet spray and shows the distribution pattern created by multiple holes in the Y-jet atomizer. The mass flow in each of the droplet streams is the same, and the droplet size is uniform for the spray. In the physical system the droplet size will be distributed; however, the Y-jet atomizer gives a relatively narrow distribution of droplet sizes. [21] Additionally, the effect of droplet size was of interest in the parametric study; so, uniform droplet size facilitated making a clear distinction of the effects of droplet size on flame shape. A nominal droplet size of $d_{\text{droplet}} = 35\mu$ was used in the computational models. The velocity of the droplets exiting the atomizer was assumed to be 180 m/sec based on high speed film observations of oil droplet trajectories from a twin fluid atomizer. [22] Although the atomizer in that study is different in design, the measured droplet velocities were treated as representative.
Figure 4.6 Model of Atomized Oil
4.2.1.5 Composition of #6 Oil, Properties, and Oxidation Model

Heavy (#6) fuel oil is obtained as one of the byproducts of the oil refining process. Light distillates, kerosene, light, and medium fuel oils are separated out of the crude oil and #6 oil is obtained as a residue. The various #6 oils can be distinguished by their composition and heating values. The major species of #6 oil are carbon and hydrogen. The #6 oil is distinguished from the other hydrocarbons by its low hydrogen-carbon ratio, H/C = 1.5; in contrast the ratio is H/C = 2.0 for kerosene. Sulfur, Oxygen, Nitrogen, Ash, and water are minor species in the oil. The fuel Nitrogen is of special interest because it drives the fuel NO reactions and can be the primary source of NO in a #6 oil flame. Orimulsion is composed of a bitumen, Orinoco, emulsified in water. The Orinoco has a high viscosity making it difficult to atomize and burn, but the viscosity of Orimulsion is closer to that of water because water is the continuous medium of the emulsion. The high water content of Orimulsion gives it a lower heating value. Table 4.6 shows the characteristics of fuels used in the experiments and modeling studies.

<table>
<thead>
<tr>
<th></th>
<th>Fuel Type</th>
<th>H/C</th>
<th>High $\Delta H_{r,298K}$ (MJ/kg)</th>
<th>Fuel N (% vol.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MIT Exp.</td>
<td>#6 Oil</td>
<td>1.5</td>
<td>42.6</td>
<td>0.3%</td>
</tr>
<tr>
<td>Phase I Exp.</td>
<td>#6 Oil</td>
<td>1.5</td>
<td>42.6</td>
<td>0.3% - 0.5%</td>
</tr>
<tr>
<td>Modeling</td>
<td>-</td>
<td>1.5</td>
<td>42.9</td>
<td>-</td>
</tr>
<tr>
<td>Phase II Exp.</td>
<td>#6 Oil</td>
<td>1.5</td>
<td>42.6</td>
<td>0.28% - 0.47%</td>
</tr>
<tr>
<td>Phase II Exp.</td>
<td>Orimulsion</td>
<td>1.66</td>
<td>30.4</td>
<td>0.38%</td>
</tr>
</tbody>
</table>

Table 4.6 Properties of Oil Fuels

Initially in a liquid phase, the #6 oil is heated so that it can be transported and atomized. In the model it is assumed that the oil leaving the atomizer initially has the same temperature as saturated water vapor, $T_{o,oil} = 373$ K; this is very close to the 380 K oil...
injection temperature used in the phase II experiments. After leaving the atomizer, droplet histories are modeled individually. The atomizing steam was at least 5% of the oil mass in all cases; this makes the steam at least 80 times more abundant by volume. This factor, in addition to the ability of the Y-jet atomizer to produce similarly sized droplets, supports the noninteracting oil droplet model. If the droplet size distribution were broader, droplet coalescence would be considered more significant.

The oil begins to vaporize as soon as it enters the furnace. The rate of vaporization is dependent mainly on the droplet size and on the temperature of the droplet which determines the vapor pressure and hence the partial pressure at the surface of the oil. The rate of vaporization is also controlled by the binary diffusion coefficient. In the oil droplet model this was assumed to be the same as for pentane in air. The other properties in Table 4.7 for #6 oil were based upon referenced values for heavy fuel oil. [17] In the oil model the specific heat of the #6 oil vapor, ref. Table 4.3, was modeled as n-Butane since exact data could not be obtained. The #6 oil used in the experiments had less than 0.5% ash. Due to the small ash content and the intent to simplify the oil droplet model, it was assumed that the droplets could be vaporized completely.

<table>
<thead>
<tr>
<th>#6 Oil Model Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (liquid)</td>
</tr>
<tr>
<td>Thermal Conductivity (liquid)</td>
</tr>
<tr>
<td>Specific Heat (liquid)</td>
</tr>
<tr>
<td>Heat of Vaporization</td>
</tr>
<tr>
<td>Boiling Point</td>
</tr>
<tr>
<td>Binary Molecular Diffusivity</td>
</tr>
</tbody>
</table>

Table 4.7 Properties of #6 Oil Used in Modeling
The stoichiometric coefficients for the oxidation of #6 oil were simply determined from the hydrogen-carbon ratio. Equation 4.7 includes all of the major reactants and products of the oxidation reaction.

$$C_4H_6 + 5.5 (O_2 + 3.76 N_2) \rightarrow 4CO_2 + 3H_2O$$  \hspace{1cm} (4.7)

The oxidation of #6 oil is not actually a single-step reaction but includes hundreds of other reactions as part of the reaction mechanism. Modeling the intermediate reactions requires the introduction of intermediate species to the model and increases computational time. The chemical reaction mechanism and chemical intermediates are of secondary importance in determining the flow field in the furnace. For this reason, a more complex reaction model was not introduced to the parametric modeling study of the RSFC oil burner.

Equation 4.7 describes the single-step reaction mechanism which was used to model the oxidation of the #6 oil. A single-step reaction rate, $k$, in the Arrhenius form was used to describe the global reaction rate. The reaction rate of #6 oil was assumed to be the same as for butane; data on which to make a better approximation was not available. The reaction rate parameters are based on experimental data and give excellent prediction of the flammability limits of butane. [24] Equation 4.8 shows the form of the Arrhenius equation that was implemented, and Table 4.8 lists the reference values used in the single-step reaction rate model.

$$k = A \left[ C_4H_6 \right]^a \left[ O_2 \right]^b e^{E/RT}$$  \hspace{1cm} (4.8)

| Reaction Rate Parameters | \[ \begin{array}{|c|c|}
| A & 4.161E9 (m^3/kmol)^{a+b-1}/sec \\
| E & 1.254E8 J/kmol \\
| a & 0.15 \\
| b & 1.60 \\
| \end{array} \] |
|---|---|

Table 4.8 #6 Oil Reaction Kinetics Model Parameters
The higher heating value of the #6 oil is used to calculate several important characteristics of the fuel. The value used in the modeling, ref. Table 4.6, was based upon a reference value for heavy fuel oil. [17] The formation enthalpy for the oil, ref. Table 4.1, was calculated using this value, the standard higher heating values for the other species, and the stoichiometric relationships in the global reaction. Based on this data the adiabatic flame temperature for the pre-heated air and #6 oil mixture was computed to be $T_{\text{adiabatic}} = 2570$ K (4170 °F). The formation enthalpy is used to determine the firing rate from the fuel flow rate.

4.2.1.6 ISBF Thermal Boundary Condition at the Walls

A rough estimation of the ISBF thermal boundary condition was implemented in the computational modeling. The ISBF is enveloped by a water jacket heat sink maintained at 323 K. The forward two-thirds of the furnace wall are insulated, and the last third is metal lined. Based on an experimental furnace exit gas temperature of $T_{\text{exit}} = 1640$ K (2500 °F) the heat removal by radiation and convection in the furnace is calculated to be around 8.6 MW or about 40% of the thermal input. The computational studies did not make a detailed examination of radiation effects; so wall radiation was regarded as a control variable. Wall temperatures were identical between computational cases. Variations in wall temperature depend on wall insulation, cooling fluid, and furnace gas temperatures which are strongly influenced by flame length and the impingement point of the tertiary air jet with the wall. Since gas temperature profiles varied between models, a uniform wall temperature was assumed so that no particular flame length would be favored by the wall temperature profile. Based on an average gas temperature of $T_{\text{exit}}$, it was estimated that 80% of heat removal would occur by radiation heat transfer if wall temperatures were
1460K. The gas temperatures in the region of the flame vary significantly between the wall and the flame core. The smaller radiative area of the hotter gas was not considered in the previous estimate of wall temperature, so the estimate is assumed to be high. Therefore, a uniform furnace wall temperature of $T_{\text{wall}} = 1400$ K seemed reasonable.

4.2.2 Effect of Burner Operating Parameters on Performance

Understanding how the operating parameters effect flame shape and ultimately the burner emissions is of major interest in the scale-up and refinement of the RSFC burner design for industrial use. In the field design some operating parameters will remain adjustable so that burner performance can be “tuned”, but other operating parameters will be built into the burner design. In the MIT experiments all of the operating parameters were adjustable; in the ISBF experiments the primary and secondary air swirl were inherent to the burner design.

The general operating conditions for the burner experiments have been noted in the previous sections. The specifics of the MIT burner design are given by Shihadeh [19]; the design specifications for the other tests are proprietary. Except where noted, a single operating parameter was varied with respect to baseline operating parameters. Table 4.9 lists the baseline operating parameters for the cited experimental tests and the various computational cases. The Y-jet atomizer with #6 oil is used in the experiments except where noted otherwise.

<table>
<thead>
<tr>
<th></th>
<th>%Pri</th>
<th>%Sec</th>
<th>%Ter</th>
<th>$S_p$</th>
<th>$S_S$</th>
<th>$S_T$</th>
<th>$\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MIT Exp.</td>
<td>15</td>
<td>0</td>
<td>85</td>
<td>0.2</td>
<td>0.2</td>
<td>0.6</td>
<td>5</td>
</tr>
<tr>
<td>Phase I Exp.</td>
<td>6 - 21</td>
<td>1 - 9</td>
<td>93 - 70</td>
<td>=0.9</td>
<td>-</td>
<td>1 - 1.2</td>
<td>0 - 30</td>
</tr>
<tr>
<td>Modeling: Case 1</td>
<td>20.7</td>
<td>2.3</td>
<td>77</td>
<td>0.9</td>
<td>0.9</td>
<td>1.0</td>
<td>5</td>
</tr>
<tr>
<td>Modeling: Case 2</td>
<td>13</td>
<td>2.3</td>
<td>84.7</td>
<td>0.9</td>
<td>0.9</td>
<td>1.0</td>
<td>5</td>
</tr>
<tr>
<td>Modeling: Case 3</td>
<td>15</td>
<td>10</td>
<td>75</td>
<td>1.1</td>
<td>1.1</td>
<td>1.0</td>
<td>5</td>
</tr>
<tr>
<td>Modeling: Case 4</td>
<td>15</td>
<td>3</td>
<td>82</td>
<td>1.1</td>
<td>1.1</td>
<td>1.0</td>
<td>5</td>
</tr>
<tr>
<td>Phase II Exp.</td>
<td>15</td>
<td>15</td>
<td>70</td>
<td>0.9</td>
<td>2.5</td>
<td>1.0</td>
<td>$0^\circ$&amp;$10^\circ$</td>
</tr>
</tbody>
</table>
Table 4.9 Baseline Operating Parameters

The various component models described in Section 4.2.1 were implemented in a general computational study of burner performance under various operating conditions. The component models were not altered except where specified, and only cases with similar geometry and a single variation in the operating condition are used in direct comparisons. In the operating parameter study the effect of primary air Re, primary air swirl number, tertiary air Re, tertiary air swirl number, air distribution between the ducts, atomizer spray angle, and fuel droplet size on flame shape and NOx destruction capabilities are examined. Even with differences in the scale between the computational studies and some of the experiments, parallels can drawn with regard to the influence of particular operating parameters.

4.2.3 Effect of Burner Design Parameters on Performance

A variety of burner geometries were examined in a computational burner performance study. In the study, one of the cases (1, 2, 3, or 4) was selected and subject to alterations in design while maintaining the same operating conditions. The changes in geometry usually required a change in the grid as well. The quarl length, quarl divergence angle, tertiary air radial spacing, and the quarl exit area were all examined for their influence on flame shape and potential for destroying NOx.

4.3 Oil Burner Scaling

Burner scaling was examined because it proves to be one of the most significant obstacles to applying positive laboratory results to practical systems. A model is of greatest benefit when there is a similarity, i.e. one to one correspondence, between the design and phenomena in the scaled down model and those in the full scale prototype. For
boiler systems these can not be scaled precisely because several criteria effect the burner 
performance and these criteria scale differently. A determination of the design 
relationships and phenomena of primary importance is an important insight which is 
needed to guide the scale-up of an experimental system. When more than one criteria is 
significant, the ideal scaled-up system will represent a compromise between the different 
scaling requirements.

Three scaling criteria were considered for the RSFC burner and furnace. Thermal 
similarity requires a one to one correspondence between the temperature differences of the 
prototype and the model. Both radiative and convective heat transfer can effect the 
temperature in the system. Through a similarity analysis the following scaling criteria are 
obtained:

\[
\begin{align*}
U &= \text{const} \\
\dot{Q} &\propto L^2
\end{align*}
\]

(4.9)

where \( \dot{Q} \) is the burner firing rate, \( U \) is the burner exit velocity, and \( L \) is the geometric length 
scale. The burner firing rate is proportional to both the fuel flow and air flow rates because 
the stoichiometry of the system is maintained. The burner exit swirl velocities are held 
constant because the burner swirl numbers are maintained. The conductive heat loss per 
unit furnace wall area is also to be held constant in thermal scaling. This condition was not 
imposed explicitly; but it is closely approximated by holding the furnace wall temperature 
constant. Thermal scaling conditions were only applied to the flow rates and geometry in 
the scaling study.

Chemical similarity requires the chemical species residence time in the reaction 
zone to be equal for both the prototype and model. This is obtained generally by keeping 
the flow residence time, \( \tau = \frac{L}{U} \), constant. This leads to the following scaling criteria:
\[
\begin{align*}
U & \propto L \\
\dot{Q} & \propto L^2 U
\end{align*}
\] (4.10)

As in the previous case, the stoichiometry of the system is maintained and the burner swirl numbers are held constant. Chemical similarity requires the total heat losses through the wall to be proportional to the firing rate. However, this requires much higher wall temperatures for a scaled-down model. This condition was neglected in the chemical scaling of the burner, and the furnace wall temperatures were held constant. This is presumed to be more representative of a practical scaled-down model.

Kinematic similarity is characterized by maintaining the momentum fluxes of the turbulent jets in the system at a constant value. This produces a similarity in the turbulent jet characteristics. This condition can be expressed in the following manner:

\[
\begin{align*}
UL & = \text{const} \\
\dot{Q} & \propto L^2 U
\end{align*}
\] (4.11)

The jet swirl numbers were maintained, and the stoichiometry in the system was kept the same when kinematic scaling was applied. This scaling condition has no specific implications for heat losses through the walls, and wall temperatures were simply held constant as in the previous cases.

4.4 Density Stratification Studies

Density stratification has been hypothesized to play a critical role in maintaining the fuel rich zone of low NOx RSFC flames. The capability of the FLUENT CFD code to model the effects of density stratification on jet entrainment has been questioned; the primary reason for this is that the standard turbulence model neglects the density fluctuation phenomena related to the modified Richardson number. In Chapter 3 a set of CFD model modifications which incorporate density fluctuation effects were described. To test the validity of these modifications, a modeling study of an isothermal density
stratification experiment was performed. The experimental data is compared with the
test predictions of the FLUENT CFD code and the modified CFD code. The modified
code is also applied to an RSFC burner model so that the influence of the code
enhancements can be evaluated. In this manner the significance of the density fluctuation
effects in flow stratification are evaluated.

4.4.1 Isothermal Density Stratification

In experiments by Beer et. al. [33] the influence of rotation and density stratification
on turbulence was studied. To observe the effects of rotation and stratification
independently four separate experimental cases were considered. The experimental
configuration consisted of a moveable block swirler with a long tube mounted at its exit.
On the centerline of the swirler and flush with its exit was positioned a small tube for
introducing a coaxial jet. Figure 4.7 illustrates the experimental configuration and some of
the dimensions. In each experimental case the annular flow through the swirler consisted
of air flowing at an average velocity of 1.3 m/sec. In two cases the air had an effective
swirl number of about 1.5, and in the other two cases no swirl was introduced to the flow.
In combination with these conditions, the central jet consisted of either Helium or air
exiting at an average velocity of 45 m/sec. Velocity measurements were made in the flow
using a hot-wire anemometer, and gas density measurements were made using a gas-phase
chromatograph.

These experiments were modeled using the FLUENT CFD code. An
axisymmetric model with only a fraction of the tube length was used. The annular ducts
had inner diameters consistent with the dimensions in Figure 4.7; the wall thickness of the
small tube was set to 0.5 mm. Figure 4.8 shows a segment of the computational grid.
Finer grid spacing was used in the region where the central jet is introduced to the annular
Figure 4.8 Characteristic Computational Grid for Co-axial Helium (or Air) Jet
flow and in the proximity of the central jet. Cell aspect ratios were 5:1 or better. Changes in grid spacing between adjacent cells did not exceed 10% in order to avoid numerical diffusion errors. For the non-swirling cases a top hat velocity profile was used for both the annular and central jets. For the cases with swirl a complex arrangement of injection sites and flow profiles into a radially converging inlet was used to reproduce the swirl profile generated by the block swirler. The RSM turbulence model was used, and a power law differencing scheme was implemented in the isothermal jet models.

4.4.2 Density Stratification in the RSFC Burner

The contribution of density fluctuation modeling to RSFC flames was evaluated. One measure of the significance of density fluctuations in radial stratification is the magnitude of the modified Richardson number. This was computed for selected flow fields by applying a discretized form of Equation 3.46 to the computational results. The significance of density fluctuations was also examined by applying the modified CFD code to an RSFC burner model.
CHAPTER 5

Computational Results and Experimental Data

5.1 Computational Results and Experimental Data for Parametric Oil Burner Study

5.1.1 Operating Parameter Sensitivity

The flow rates, swirl numbers, and type of oil atomization have a strong influence on the flow pattern that is established. In this section the experimental evidence and the results of the computational modeling will be presented. In the following discussion of the modeling Cases 1 and 2 from Table 4.9 will be referenced; additionally, a classification is made of characteristic flame shapes. They are called flames shapes A, B, C.

5.1.1.1 Primary Air Reynolds Number

The primary air Re was found to have a strong influence on flame length and the primary and secondary jet penetration into the internal recirculation zone. Three computational models are presented here. The first model uses the Case 1 operating parameters. This model has a relatively high primary air Reynolds number, Re_p = 267,000.

The flow characteristics are shown in Figures 5.1a, b, c, and d. Figure 5.1a illustrates the normalized stream function, Ψ/Ψ*, for the flow; the contour lines enclose a specified percentage of the total mass flow. The 0% stream line delineates the large downstream internal recirculation zone, IRZ_o, from the flow towards the furnace exit. Figure 5.1b shows the lean fuel concentration boundary of the vaporized droplets. The profiles range from 1.1% down to 0.1%. At the temperatures existing in the furnace, flame
Figure 5.1a High $Re_p$, Flame Shape A (Case 1)  
Contours of $\%$ Mass Flow

Figure 5.1b High $Re_p$, Flame Shape A (Case 1)  
Contours of Fuel Concentration
Figure 5.1c High $Re_p$, Flame Shape A (Case 1)
Contours of Temperature (Kelvin)

Figure 5.1d High $Re_p$, Flame Shape A (Case 1)
Contours of Oxygen Concentration
burnout is characterized by the 0.1% fuel concentration line; this was the basis for estimating the length of the flame. In this case the flame was relatively short, \( x/d = 2.3 \). Figure 5.1c displays the temperature contours for the flame in increments of 200 K. The contour lines are very close in the region of ignition; after complete burning of the fuel the combustion products gradually lose heat to the furnace walls. The furnace exit gas temperature is around 1610 K. Figure 5.1d gives the contours of oxygen from atmospheric levels, 21%, down to 1%. As noted earlier the exit \( O_{2} \) for the flow is 2.4%.

This flame is distinguished from others that were studied because of its short length and strong recirculation on the centerline. This is hereafter called flame shape A. Important to the formation of this type of flame is the relatively high tertiary air swirl, \( S_T \). The NOx characteristics of this type of flame will be discussed in the next chapter.

The second case of interest has a relatively low primary air Reynolds number, \( Re_p = 134,000 \); the operating parameters are those specified in Table 4.9 as Case 2. Figure 5.2a shows that this case retains the large internal recirculation zone, \( IRZ_0 \), created by the tertiary air but also has a smaller internal recirculation zone, \( IRZ_1 \), radially inside of \( IRZ_0 \). The \( IRZ_1 \) separates the jet penetrating on the centerline from the \( IRZ_0 \) created by the tertiary air. Some of the air in the central jet is entrained back into the \( IRZ_0 \). Figure 5.2b shows the fuel contours which envelope much more of the furnace volume than in the previous case; the flame length is \( x/d = 6.6 \) in this case. Figure 5.2c shows the temperature contours. The ignition zones in the primary and tertiary air are distinct in this case. Due to the longer flame length, the peek temperatures in the flame occur further downstream. Figure 5.2d shows the oxygen contours for this low \( Re_p \) flame.

This flame is distinguished by its long flame length caused by the centerline penetration of the fuel rich jet through the \( IRZ_0 \). The high temperature, fuel rich, low \( O_2 \)
Figure 5.2a Low $Re_p$, Flame Shape C (Case 2)
Contours of % Mass Flow

Figure 5.2b Low $Re_p$, Flame Shape C (Case 2)
Contours of Fuel Concentration
Figure 5.2c  Low $Re_p$, Flame Shape C (Case 2)
Contours of Temperature (Kelvin)

Figure 5.2d  Low $Re_p$, Flame Shape C (Case 2)
Contours of Oxygen Concentration
core extends far beyond the IRZ₀. This is categorized as flame shape C throughout the rest of this report. The emissions of this type of flame are discussed in the next chapter.

In between these two cases there exists a flame in which the centerline penetration of the primary air jet is small and the flame length is between the two previous extremes. Figures 5.3a, b, c, and d illustrate this flame with a critical primary air Reynolds number Reₚ = 193,000. This is called flame shape B. The operating parameters are between those of Case 1 and Case 2.

Figure 5.3a shows that the primary and secondary air jets penetrate into the IRZ₀ but reverse direction due to the greater strength of the IRZ₀ following the adverse pressure gradient created by the swirling tertiary air. The IRZ₁ is further upstream than in flame shape C. It temporarily separates the primary and secondary air jets from the tertiary air until they are entrained by the tertiary air jet further downstream. The IRZ₁ in this case greatly adds to the flame stability because of its location in the ignition zone. Figure 5.3b shows the fuel concentration contours; the flame length in this case is x/d = 4.6. Figure 5.3c illustrates the temperature contours which lie between the extremes of the two previous cases. The O₂ concentrations in Figure 5.3d complete the description of the dominant species in the flame. The O₂ < 1% region does not extend far beyond the IRZ₀ and lies within Ψ/Ψ₀ = 12.5%.

The fraction of the flow that penetrates through the IRZ₀ is related to the Reₚ of the burner. A general examination of several different burner geometries utilizing high tertiary air swirl and variable Reₚ was conducted. Figure 5.4 displays the data gathered from these calculations. Although one might expect an increase in the primary air jet axial momentum to increase the penetration of the IRZ₀, in every case the centerline mass flow penetration, m, was reduced by an increase in Reₚ. However, when Reₚ was high
Figure 5.3a Critical Re_p, Flame Shape B (Between Case 1 & 2)
Contours of % Mass Flow

Figure 5.3b Critical Re_p, Flame Shape B (Between Case 1 & 2)
Contours of Fuel Concentration
Figure 5.3c Critical $Re_p$, Flame Shape B (Between Case 1 & 2)
Contours of Temperature (Kelvin)

Figure 5.3d Critical $Re_p$, Flame Shape B (Between Case 1 & 2)
Contours of Oxygen Concentration
Figure 5.4 Percent Massflow Penetration vs $Re_p$ from Computational Study

Figure 5.5 Percent Massflow Penetration vs Primary Air Swirl from Computational Study
relative to $Re_p$ the sensitivity of the flow to changes in $Re_p$ was greatly reduced. This explains the variation in the slope of the lines. The factors governing the relationship between $Re_p$ and $m$ are discussed in Section 6.1.1.

5.1.1.2 Primary Air Swirl

Increasing the primary air swirl number, $S_p$, had the expected effect of stabilizing the flame closer to the fuel nozzle and decreasing the combustion length. Two computational models are compared here. The first one uses the Case 1 operating parameters and has a high primary air Reynolds number, $Re_p = 267,000$. Figure 5.6a shows the normalized stream function contours. Just as in Figure 5.1 the flow is characterized by a large downstream internal recirculation zone, $IRZ_0$, which penetrates to the centerline of the flow. Figure 5.6b shows the fuel concentration contours; the flame is very short, $x/d = 1.8$. Figure 5.6c gives the temperature profiles, and Figure 5.6d gives the contours of $O_2$. Clearly the data indicates that this is flame shape A.

The second model uses the Case 1 operating parameters but with reduced primary air swirl, $S_p = 0.4$; the primary air Reynolds number is identical to that of the previous case. Figure 5.7a shows the normalized stream function contours. The $IRZ_0$ still exists, but the primary and secondary air jets penetrate completely along the centerline. A thin counter-rotating $IRZ_1$ lies radially inside of the $IRZ_0$. Figure 5.7b shows that the fuel contours extend beyond the domain of the model; this means $x/d > 17$. Figure 5.7c gives the temperature contours, and Figure 5.7d shows that the contours of $O_2$ are highly stratified. The low $O_2$ zone extends beyond the end of the furnace. Because of its significant flame length and large fuel rich, high temperature zone, this can be called flame shape C.
Figure 5.6a High $S_p$, Flame Shape A (Case 1)
Contours of $\%$ Mass Flow

Figure 5.6b High $S_p$, Flame Shape A (Case 1)
Contours of Fuel Concentration
Figure 5.6c High $S_p$, Flame Shape A (Case 1)
Contours of Temperature (Kelvin)

Figure 5.6d High $S_p$, Flame Shape A (Case 1)
Contours of Oxygen Concentration
Figure 5.7a Low $S_p$, Flame Shape C (Case 1 with low $S_p$)
Contours of % Mass Flow

Figure 5.7b Low $S_p$, Flame Shape C (Case 1 with low $S_p$)
Contours of Fuel Concentration
Figure 5.7c Low $S_p$, Flame Shape C (Case 1 with low $S_p$)
Contours of Temperature (Kelvin)

Figure 5.7d Low $S_p$, Flame Shape C (Case 1 with low $S_p$)
Contours of Oxygen Concentration
These two cases are distinguished from one another only by $S_p$. This shows the significance of $S_p$ in determining flame shape. Several other geometries were examined and other values for $S_p$ were tested. Figure 5.5 shows the data for these other models. In every case the centerline mass flow penetration, $\bar{m}$, was reduced by the increase in $S_p$. The secondary influence appears to be that higher $S_p$ cases require lower swirl numbers to reach the same mass flow penetration level.

5.1.1.3 Tertiary Air Reynolds Number
A study of tertiary air Reynolds number effect was conducted by altering the geometry of the tertiary air duct of the model in Figure 5.6. The burner exit swirl number was maintained, and the operating parameters still corresponded to Case 1. Decreasing the size of the tertiary air duct decreased the tertiary air Reynolds number based upon the hydraulic diameter, $Re_{H,T}$, from 149,000 to 145,000; the tertiary air exit area decreased from 33% to 22% of the total burner area.

Figures 5.8a, b, c, and d show the computed flow field for the low $Re_{H,T}$. The flame length is $x/d = 1.6$, a decrease of 0.2 burner diameters; and the flow retains a strong IRZ$_0$ with no penetration along the centerline. This categorizes the flow as flame shape A.

5.1.1.4 Tertiary Air Swirl
The importance of the tertiary air swirl number, $S_T$, was examined in the computational study. The model which demonstrated flame shape B, Figure 5.3, was given a lower swirl number to determine the effect on the critical flame shape. The tertiary air swirl was decreased from 1.0 to 0.7; all other operating parameters remained the same. The $Re_{H,T}$ was fixed at 205,000 in both cases.

Figures 5.9a, b, c, and d illustrate the resulting change in the flow field. The flame length increases by 1.4 burner diameters to $x/d = 6.0$, although the centerline mass flow
Figure 5.8a High $Re_T$, Flame Shape A (Case 1)
Contours of % Mass Flow

Figure 5.8b High $Re_T$, Flame Shape A (Case 1)
Contours of Fuel Concentration
Figure 5.8c High Re_T, Flame Shape A (Case 1)
Contours of Temperature (Kelvin)

Figure 5.8d High Re_T, Flame Shape A (Case 1)
Contours of Oxygen Concentration
Figure 5.9a Lower $S_T$, Flame Shape B
Contours of % Mass Flow

Figure 5.9b Lower $S_T$, Flame Shape B
Contours of Fuel Concentration
Figure 5.9c  Lower $S_T$, Flame Shape B
Contours of Temperature (Kelvin)

Figure 5.9d  Lower $S_T$, Flame Shape B
Contours of Oxygen Concentration
does not change appreciably. The flame can still be described as flame shape B. The size and strength of the IRZ\(_o\) decreased significantly; this is indicated by the normalized stream function contours which show a much smaller mass in the recirculation zone. It is noteworthy that the center of the IRZ\(_o\) is 0.8 burner diameters further downstream as a result of the decrease in \(S_T\).

Additional cases were also examined. Figure 5.10 shows the relationship between flame length and \(S_T\) for different types of models. In the additional cases shown, the operating parameters, other than \(S_T\), were those of Case 1.

5.1.1.5 Air Distribution

Two additional cases are introduced here to illustrate the significance of the mass flow distribution among the three annuli. The case of reference is the one introduced in section 5.1.3, Figure 5.8; the baseline operating parameters are those of Case 1. First a redistribution of the primary air into the tertiary was examined. The swirl numbers remained the same but the mass flow in the primary air duct was decreased from 20.7% to 9.6%; the primary air Reynolds number, \(Re_p\), decreased accordingly from 267,000 to 124,000. The tertiary air Reynolds number, \(Re_{H,T}\), increased from 145,000 to 165,000. The flow field is shown in Figures 5.11a, b, c, and d. Consistent with the effects observed previously, the reduction of \(Re_p\) increases the flame length by 2.8 diameters to \(\lambda/d = 4.4\), and the centerline mass flow increases from zero to 4.1% of the flow. The increase in \(Re_{H,T}\) also contributes to the increase in flame length. The flame is changed from shape A to one with characteristics of both B and C. The flame has an intermediate length, but the flow along the centerline is above the critical value.

To examine the relevance of the secondary air jet the previous case, Figure 5.11, was modified by redistributing some of the tertiary air into the secondary air duct. The
Figure 5.10 Flame Length vs $S_t$
Figure 5.11a Lower Reₚ, High Reₜ, Flame Shape BC
Contours of % Mass Flow

Figure 5.11b Lower Reₚ, High Reₜ, Flame Shape BC
Contours of Fuel Concentration
Figure 5.11c Lower $Re_p$, High $Re_T$, Flame Shape BC
Contours of Temperature (Kelvin)

Figure 5.11d Lower $Re_p$, High $Re_T$, Flame Shape BC
Contours of Oxygen Concentration
tertiary air mass flow was decreased to 80.8% while increasing the secondary air mass flow to 9.6%. The tertiary air Reynolds number decreased to 151,000. The primary air jet had the same operating parameters as previously. The flow field is described in Figures 5.12a, b, c, and d. The flame length is $x/d = 5.6$, and 9.3% of the mass flow penetrates the $IRZ_o$ along the centerline. This is an example of flame shape C.

5.1.1.6 Fuel Droplet Size

The atomizer performance was studied by examining the oil droplet trajectories from the point of injection to the point of complete vaporization. The prior fuel concentration contour diagrams indicated the region over which the vaporized oil is distributed before reacting with the air. The following three diagrams, Figures 5.13A, B, and C show the oil droplet trajectories superimposed on the normalized stream function lines for flame shapes A, B, and C respectively. They correspond to Figures 4.1, 4.3, and 4.2. In each case the oil droplets have a spray angle of $\alpha = 5^\circ$ and a nominal droplet size of $d_{\text{droplet}} = 35\mu$. Because of the small droplet size, the droplets are strongly influenced by the flow field as evidenced in these diagrams. Flame shape B has a higher $Re_p$ and initial $U_p$ than flame shape C, but the flow decelerates quickly due to the adverse pressure gradient. The ignition zone also influences the droplet path length. In diagrams B and C the droplets that have a higher radial velocity vaporize more quickly due to the strong radial temperature gradient. Most of these droplets did not travel far beyond the 1050 K isotherm before being completely vaporized. In diagram A the flame front is away from the burner face so the droplets can travel a greater radial distance before being vaporized. The droplets in Figure 5.13B do not spread as far downstream as in Figure 5.13C, this is largely due to the differences in the velocity profiles which reposition the flame front.

Figures 5.14 and 5.15 illustrate two burner geometries with identical operating parameters but different droplet sizes. The flame in Figure 5.14 has flame shape B and a
Figure 5.12a Higher $Re_S$, Lower $Re_p$, High $Re_T$, Flame Shape C
Contours of % Mass Flow

Figure 5.12b Higher $Re_S$, Lower $Re_p$, High $Re_T$, Flame Shape C
Contours of Fuel Concentration
Figure 5.12c Higher $Re_S$, Lower $Re_p$, High $Re_T$, Flame Shape C
Contours of Temperature (Kelvin)

Figure 5.12d Higher $Re_S$, Lower $Re_p$, High $Re_T$, Flame Shape C
Contours of Oxygen Concentration
Figure 5.13A High $Re_p$, Flame Shape A (Case 1)
Figure 5.13B  Critical $Re_p$, Flame Shape B (Between Case 1 & 2)
Figure 5.13C Low $Re_p$, Flame Shape C (Case 2)
Figure 5.14 $d_{\text{droplet}} = 35\mu$, Flame Shape B (Case 1 with high $S_T$)
Figure 5.15 $d_{\text{droplet}} = 55\mu$, Flame Shape C (Case 1 with high $S_T$)
droplet size of \( d_{\text{droplet}} = 35 \mu \); when the droplet size is increased to \( d_{\text{droplet}} = 55 \mu \), shown in Figure 5.15, the flame shape changes to C. It is clear from the Figures that the larger droplets have a longer trajectory. This can be attributed to the fact that the larger droplets have a higher inertia to drag force ratio and take longer to vaporize.

Figure 5.16 shows the downstream fuel concentration in the flow at \( x/d = 3.5 \) for several computational cases. Larger droplet size is associated with higher fuel concentration downstream and longer burnout times.

5.1.1.7 Atomizer Spray Angle

Figures 5.18 and 5.19 present burner geometries with identical air flow operating parameters; these are the same as in Figures 5.14 and 5.15 also. The oil spray angle, however, varies from 0° to 10° between the cases. The droplets with a 10° spray angle are vaporized faster because they enter the steep radial temperature gradient very quickly. The droplets with the smaller spray angle travel further downstream too.

Figure 5.17 illustrates the change in downstream fuel concentration in the flow at \( x/d = 3.5 \) for three spray angle models. A smaller spray angle results in a higher fuel concentration downstream and longer burnout times for the fuel.

5.1.2 Design Parameter Sensitivity

Changes in design parameters also influence the burners performance. Changes in quarl length, divergence angle, tertiary air radial spacing, and quarl exit area are analyzed in this section. The influence of these parameters is usually less dramatic than the influence of the operating parameters on the flow field, but maintaining the design parameters within a prescribed range is important for proper RSFC burner performance.
Figure 5.16 Downstream Fuel Concentration (@x/d=3.5) vs Oil Droplet Size

Figure 5.17 Downstream Fuel Concentration (@x/d=3.5) vs Spray Angle
Figure 5.18 $\alpha = 0^\circ$, Flame Shape C (Case 1 with high $S_T$)
Figure 5.19 $\alpha = 10^\circ$, Flame Shape B (Case 1 with high $S_T$)
5.1.2.1 Quarl Length

The quarl length was found to have an influence on the position of the $\text{IRZ}_o$. Figure 5.20 shows a positive correlation between the position of the $\text{IRZ}_o$ center and the quarl length. Several computational cases with identical $S_\tau$ are compared. The positive correlation is an important consideration for designing the quarl to allow for longer flames.

5.1.2.2 Quarl Divergence Angle

The quarl divergence guides the expansion of the tertiary air jet in the near burner region. If the divergence angle is too large the tertiary air jet will separate from the wall causing early vortex breakdown. However, from the design perspective a larger divergence angle shortens the total burner length and makes retrofit easier. In the parametric studies quarl divergence angles, $\theta$, between 17 and 35 degrees were examined. The maximum allowable divergence angle for a strongly swirling flow is greater than $\theta$ for a non-swirling flow because swirl promotes jet divergence and causes the jet to adhere to the wall more strongly. When the divergence was $35^\circ$, separation was not evident. The maximum divergence angle was not determined computationally, but the range that was evaluated supports increasing the angle above the previous design limit of $25^\circ$.

5.1.2.3 Tertiary Air Radial Spacing

The influence of tertiary air radial spacing on the flow field can be observed by comparing Figures 5.1 and 5.6. The quarl diameter and location of the primary and secondary air jets is the same for both cases. However, the quarl length is shorter in Figure 5.6 in which there is greater radial separation. Increasing the radial separation of the tertiary air jet strengthens the $\text{IRZ}_o$. The case with increased radial spacing also shows that the $\text{IRZ}_o$ is drawn closer to the burner and the jet spreads more rapidly, but this is simply due
Figure 5.20  IRZ_0 Position vs. Quarl Length
to the shorter quarl length. The increase in the strength of the IRZ_o promotes more vigorous mixing and decreases the flame length.

### 5.1.2.4 Quarl Exit Area

Two extreme configurations for the quarl exit area were modeled. In Figure 5.21 a burner with quarl to burner area ratio of $A_{quarl}/A_t=1.16$ is described. It can be contrasted with the burner in Figure 5.22 in which the quarl to burner area ratio is $A_{quarl}/A_t=1.63$. The change in quarl exit area does not influence flame length, and the position of the IRZ_o remains the same. The centerline penetration of the IRZ_o is increased a small amount as a result of this large change in area; however, the strength of the IRZ_o increases with quarl area. The burner with a smaller quarl area has a larger high temperature zone downstream.

### 5.2 Burner Scaling Computational Results

Although the parametric study provided valuable insight into the influence of various design criteria on the flow field, it did not highlight the factors which are important for scaling the burner to different sizes once the parameters for flame shape B are determined. A computational study of RSFC burner scaling was conducted to determine the guidelines for reproducing the critical flame shape at different burner scales. The 21 MW burner model which demonstrated flame shape B, Figure 5.9, was chosen as the reference case for the scaling study. The thermal, chemical, and kinematic similarity criteria were applied to scale this case down to 15 MW.

The thermal scaling criteria requires the burner exit velocities to remain constant, and the length scales in the burner and furnace change according to the square root of the scaling factor, $s$:
Figure 5.21a Low $A_{\text{outlet}}/A_t$, Flame Shape BC (Between Case 1 & 2)  
Contours of % Mass Flow

Figure 5.21b Low $A_{\text{outlet}}/A_t$, Flame Shape BC (Between Case 1 & 2)  
Contours of Fuel Concentration
Figure 5.21c Low $A_{\text{quarl}}/A_t$, Flame Shape BC (Between Case 1 & 2)
Contours of Temperature (Kelvin)

Figure 5.21d Low $A_{\text{quarl}}/A_t$, Flame Shape BC (Between Case 1 & 2)
Contours of Oxygen Concentration
Figure 5.22a High $A_{\text{quar}}/A_1$, Flame Shape BC (Between Case 1& 2)
Contours of % Mass Flow

Figure 5.22b High $A_{\text{quar}}/A_1$, Flame Shape BC (Between Case 1& 2)
Contours of Fuel Concentration
Figure 5.22c High $\dot{A}_{\text{quar}}/A_t$, Flame Shape BC (Between Case 1 & 2)
Contours of Temperature (Kelvin)

Figure 5.22d High $\dot{A}_{\text{quar}}/A_t$, Flame Shape BC (Between Case 1 & 2)
Contours of Oxygen Concentration
\[ \begin{align*}
  U &= U_0 \\
  \frac{L}{L_0} &= \sqrt{s}
\end{align*} \]

(5.1)

Figures 5.23 a, b, c, d, and e show the flow field for the reference case scaled down to 15 MW using the scaling relationships in Equation 5.1. The distinguishing features of the transformation from shape B to C when the burner is scaled down in this manner are an increase in the flow penetration along the centerline and an increase in flame length. In a relative sense the oil droplets penetrate further into the flow field than in the reference case, but the absolute trajectory length for the oil droplets remains nearly the same. This similarity is related to the identical atomized droplet size for both two cases. An additional reason for the further droplet penetration is the small forward shift in the fuel gun position.

The chemical scaling criteria change the burner exit velocities and the length scales of the system in the following manner:

\[ \begin{align*}
  \frac{U}{U_0} &= \sqrt{s} \\
  \frac{L}{L_0} &= \sqrt{s}
\end{align*} \]

(5.2)

Figures 5.24 a, b, c, d, and e show the flow field for the reference case scaled down to 15 MW using the scaling relationships in Equation 5.2. The gas residence time in the furnace is the same in this case as it was in the reference case. The change in the flow field is similar to the one that occurred using the thermal scaling criteria. The flame shape changes from B to C, but the degree of penetration is higher in this case. In relative terms oil droplets penetrate farther into the flow field than in the reference case, but the actual droplet trajectory length was nearly the same as in the reference case. Implicitly, the droplets did not penetrate as far into the flow field as in the thermal scaling case.
Figure 5.23a 15MW Burner, Scaled Down Using Thermal Similarity
Contours of % Mass Flow

Figure 5.23b 15MW Burner, Scaled Down Using Thermal Similarity
Contours of Fuel Concentration
Figure 5.23c 15MW Burner, Scaled Down Using Thermal Similarity Contours of Temperature (Kelvin)

Figure 5.23d 15MW Burner, Scaled Down Using Thermal Similarity Contours of Oxygen Concentration
Figure 5.23e 15MW Burner, Scaled Down Using Thermal Similarity Droplet Trajectories
Figure 5.24a 15MW Burner Scaled Down Using Chemical Similarity
Contours of % Mass Flow

Figure 5.24b 15MW Burner Scaled Down Using Chemical Similarity
Contours of Fuel Concentration
Figure 5.24c 15MW Burner Scaled Down Using Chemical Similarity
Contours of Temperature (Kelvin)

Figure 5.24d 15MW Burner Scaled Down Using Chemical Similarity
Contours of Oxygen Concentration
Figure 5.24e 15MW Burner, Scaled Down Using Chemical Similarity
Droplet Trajectories
The kinematic scaling criteria impose more drastic changes to the gas velocities and length scales as shown in Equation 5.3:

\[
\begin{align*}
\frac{U}{U_0} &= \frac{1}{s} \\
\frac{L}{L_0} &= s
\end{align*}
\]  

(5.3)

This is the necessary condition for maintaining a jet momentum flux identical to the reference case. This scaling criteria is not useful for a practical burner system because the length scale is so strong a function of the scaling factor that the energy density becomes too small for furnaces scaled up in this way. For this reason two cases of kinematic burner scaling were considered. In the first case the furnace dimensions were scaled according the kinematic scaling criteria. In the second case the furnace dimensions were scaled according to the thermal scaling relationships while the burner size and gas velocities were scaled according to Equation 5.3. A comparison of the two cases indicated that the flow field is relatively independent of furnace size. Figures 5.25 a, b, c, d, and e show the flow field for the reference case scaled down to 15 MW in the manner specified for the second case. It is of primary interest that the critical flame shape is reproduced when the burner is scaled in this way. The flame length remains x/d = 4.6; and the flow penetration along the centerline is the same. Temperature and oxygen contours are nearly the same as well. The oil droplets penetrate further into the flow field in a relative sense, but the absolute trajectory lengths are shorter.

5.3 Experimental Data and Computational Results for Density Stratification Studies

5.3.1 Isothermal Density Stratification

The experimental data for the isothermal jet experiments is presented in this section along side the modeling results. The experiments were conducted to demonstrate the
Figure 5.25a 15MW Burner Scaled Down Using Kinematic Scaling
Contours of % Mass Flow

Figure 5.25b 15MW Burner Scaled Down Using Kinematic Scaling
Contours of Fuel Concentration
Figure 5.25c 15MW Burner Scaled Down Using Kinematic Scaling
Contours of Temperature (Kelvin)

Figure 5.25d 15MW Burner Scaled Down Using Kinematic Scaling
Contours of Oxygen Concentration
Figure 5.25e MW Burner, Scaled Down Using Kinematic Scaling
Droplet Trajectories
importance of density stratification in turbulence damping. First, the boundary conditions for the jets are described and compared with the models. Secondly, the turbulence quantities are presented and compared.

The study was performed with the intent of gaining a better understanding of stratified jets. The degree to which the experimental configuration resembles a free jet is examined first. Two conditions distinguish the experiments from a characteristic free jet. First, the inner jet is coaxial to an annular jet rather than stationary air, and secondly, entrainment by the inner jet is limited by the flow rate of the annular jet. Because the annular jet flow rate is over 20 times that of the central jet. The assumption of free jet behavior implies that the central jet’s entrainment should not be inhibited before 60 jet diameters downstream of the jet.

The modeled axial velocity profiles of the air and helium jets in swirling and non-swirling air are compared with the analytical description of free jets in stationary surroundings. Figures 5.26a and 5.26b show the reciprocal of the jet’s centerline axial velocity, 1/Um, normalized by the jet exit velocity, Uo, plotted against the axial position, x, normalized by the effective diameter, de:

\[ de = \left( \frac{\rho_o}{\rho_s} \right)^{1/2} do \] (5.4)

where \( \rho_o \) is the initial jet density and \( \rho_s \) is the density of the surrounding fluid. The analytical expression for the free jet profile is taken from the Hinze & Van der Hegge Zinjen [26]:

\[ \frac{U_o}{U_m} = \frac{1}{6.4} \left( \frac{\rho_o}{\rho_s} \right)^{1/2} \left( x + 0.6 \right) \] (5.5)

Figure 5.26a shows that the centerline velocity computed by the FLUENT code for a central jet of air inside a non-rotating annular jet decays more rapidly than the centerline
Figure 5.26a  Axial Velocity Decay for Air Jets with and without Flow Rotation
Figure 5.26b Axial Velocity Decay for Helium Jets with and without Flow Rotation

Figure 5.26c Decay of Axial Concentration for Helium Jets with and without Flow Rotation
velocity of the analytical expression for the free jet. Figure 5.26b shows a similar but weaker distinction for helium jets. For a helium jet, the profile matches the analytical expression better because the annular flow "appears" 2.7 times larger to the helium jet due to density differences. Both figures show that far downstream the profile for the contained jet begins to flatten. This is indicative of the mean flow rate associated with the contained jet. If the coaxial flow develops into a turbulent pipe flow, Uo/Um has an upper bound of 26 in contrast to the analytical expression which continues to increase. The rotating flow field is computed to have a much slower decay in its axial velocity, and this is more pronounced for the air jet. In the experiments, measurements focused on the region from the jet exit to x/de=20. While the axial velocity profiles change significantly in this region between the rotating and non-rotating cases for the air jet. The profiles for Helium jets remained quite similar.

The decay in Helium concentration on the centerline is compared with and shows good agreement with the analytical expression for a free jet in Figure 5.26c. As with the velocity profile, the similarity of the Helium jet with free jet measurements is related to the larger annular flow seen by the Helium jet. Rotation of the annular air jet has little effect on the centerline Helium concentration although the jet maintains a higher axial velocity when there is rotation.

One guideline for developing models of the isothermal jet experiments was to match the reported boundary conditions for the flow field. Having reproduced the geometry and reported flow rates, the velocity profile from the block swirler needed to be determined. The velocity profile proves to be very significant in influencing the flow pattern in the tube. Recirculation zones develop in the tube when high annular swirl restricts the entrainment by the central jet. Since a complete description of the boundary conditions was not provided some assumptions had to be made. The primary assumption
was that the flow exhibited no recirculation within the tube; this greatly limited the velocity profiles that could be used. Figure 5.27a shows the normalized stream function contours for the Helium jet in a non-swirling annular air flow; the stream function for a swirling annular flow field was required to resemble this pattern downstream of the central jet. The deflections in the contour lines reflect the entrainment by the central jet. After some investigation an annular flow was produced that maintained parallel streamlines. A general study of block swirler performance [28] provided some guidance in determining the annular jet velocity profile, but recirculation occurred in the flows scaled exactly in the manner suggested by the report. The tangential velocity profile was chosen so as to best match the reported profiles. Figures 5.28a & b show the tangential velocity profiles at x/de=4 and 80. The tangential velocity was originally matched more precisely at x/de=4, but lengthening the model domain altered the profile. The decay of swirl in the model is less than what was observed in the experiments. This discrepancy could not be compensated for by changing the velocity profiles.

Experimental measurements of radial density profiles were recorded for three axial positions for the Helium jet with rotating annular flow. The normalized density profiles predicted by the CFD code with and without the proposed modifications are compared to the experimental values in Figures 5.29a, b, and c. The experimentally reported values describe a Helium jet that has a much higher concentration of air; although the jet width is modeled fairly accurately. The Helium concentrations that were reported for the experiments seem to violate species conservation conditions if the flow velocities are at all similar to the modeled profiles at these positions. However, it is noteworthy that the centerline concentrations consistently differ from the modeled values by a factor of about 1.8. It is possible that the discrepancy is related to the improper reduction of the experimental data; this is supported by the fact that methane was also used in the
Figure 5.27a Non-swirling Co-axial He Jet
Contours of % Mass Flow

Figure 5.27b Non-swirling Co-axial He Jet
Mole Fraction of He
Figure 5.28a Tangential Velocity at $x/do=4$ for Helium Jet in Rotating Coaxial Flow

Figure 5.28b Tangential Velocity at $x/do=80$ for Helium Jet in Rotating Coaxial Flow
Figure 5.29a Normalized Density Profile at x/de=5 for Helium Jet in a Rotating Annular Air Stream

Figure 5.29b Normalized Density Profile at x/de=10 for Helium Jet in a Rotating Annular Air Stream
Figure 5.29c Normalized Density Profile at x/de=20 for Helium Jet in a Rotating Annular Air Stream
experiments and has a density 1/1.8 times that of air. The modification to the CFD code caused little difference in the computed density profile. The small changes that did occur resulted in a steepening of the density gradient so that the jet became narrower in width and maintained a higher Helium concentration on the centerline. With the modified code centerline density concentrations were reduced by 0.8% at both x/de=10 and 20.

Experimental measurements of axial velocity were made for air and Helium jets with a non-rotating annular jet. Figures 5.30a and 5.31a give a comparison between the modeled values and the experimental data. The Helium jet model follows the profile and magnitude of the experimental data; however, it does not have the off axis peak that exists in the experimental data. The air jet model has is very different from the experimental data. In comparison with the radial velocity profile for Helium, the modeled air jet has a greater width. However, the experimental data for the air jet has a narrower jet width than the Helium jet. The analytical description of a free jet’s radial velocity profile [29]:

$$\frac{U}{U_m} = \exp \left[ -K_o \left( \frac{r}{x} \right)^2 \right]$$  \hspace{1cm} (5.5)

gives a larger jet width for an air jet in comparison to a Helium jet at the equivalent axial distance, x=20 de in this case. The experimental data has similarity with the Helium jet with regard to its axial velocity. This is consistent with the predicted behavior of a free jet. However, the radial velocity profile of the experimental data seems to be in violation of the trends for free jets.

Figures 5.30b and 5.31b present the computed and experimental values of turbulence intensity for air and Helium jets in a non-rotating annular stream. Using the standard CFD code, the air jet model displays a strong radial similarity to the Helium jet model when they are scaled radially as r/Re. This is a distinctive difference from the reported experimental measurements which show a greater turbulence intensity associated
Figure 5.30a Axial Velocity Profile at x/de=20 for an Air Jet in a Non-Rotating Annular Air Stream

Figure 5.30b Turbulence Intensity at x/de=20 for an Air Jet in a Non-Rotating Annular Air Stream
Figure 5.31a Axial Velocity Profile at x/de=20 for a Helium Jet in a Non-Rotating Annular Air Stream

Figure 5.31b Turbulence Intensity at x/de=20 for a Helium Jet in a Non-Rotating Annular Air Stream
with the Helium jet. The predicted turbulence intensity for the Helium jet is closely patterned after the experimental values although lower in magnitude. In both the air and the Helium jet models the turbulence intensity boundary condition was assumed to be 10%.

The experimental and computational values of the air jet turbulence quantities are presented in Figures 5.32a and b. In each case the turbulence quantities are weighted by the local density so that they can be expressed as a shear stress. Figure 5.32a shows the experimental data reported by Beér and Chigier. It suggests that rotation in the annular flow greatly attenuates the shear stresses around the inner jet, and generates shear stresses further out in the annular jet. Air jet models did not reproduce this effect. Figure 5.32b shows that rotation in the flow field caused a small attenuation and significant narrowing of the \( \rho u'v' \) profile. The \( \rho v'w' \) profile is not shown because it was nearly negligible in magnitude. The small magnitude of \( \rho v'w' \) is consistent with the shear stress predictions made by the Bousinesque hypothesis, although the RSM turbulence model was used in these cases. The velocity gradients associated with computing \( \rho v'w' \) are small in the case of rotation and nonexistent in the non-rotating case. The profile for \( \rho u'w' \) is presented for comparison with \( \rho u'v' \). In the absence of rotation \( \rho u'w' \) is modeled to have a zero value just like the modeled values of \( \rho v'w' \). In the presence of rotation it nearly matches the computed \( \rho u'v' \) profile.

Figures 5.33a, b, and c present the experimental and computational values of the turbulence quantities associated with the Helium jet. The experimental data in Figure 5.33a shows that large stresses within the jet in the absence of rotation are attenuated in the presence of rotation. In the rotating annular flow the significant shear stresses are radially distant from the jet. The experimental values for the shear stresses are larger than those for the corresponding air jet. The Helium jet models do not reproduce this effect, but follow
Figure 5.32a  Experimental Shear Stress Measurements at x/de=20 for Air Jets with Rotating and Non-Rotating Coaxial Air Streams

Figure 5.32b  Computed Shear Stress at x/de=20 for Air Jets with Rotating and Non-Rotating Coaxial Air Streams
Figure 5.33a Experimental Shear Stress Measurements at x/de=20 for Helium Jets with Rotating and Non-Rotating Coaxial Air Streams

Figure 5.33b Computed Shear Stress at x/de=20 for a Helium Jet with a Non-Rotating Coaxial Air Stream
Figure 5.33c  Computed Shear Stress at x/de=20 for a Helium Jet with a Rotating Coaxial Air Stream
more closely the behavior of the air jet models. The zone of high shear stress is slightly
narrowed and slightly attenuated in amplitude by introducing rotation into the flow. The jet
exhibits further narrowing through the introduction of the CFD model modification. The
magnitude of $\rho \overline{v'w'}$ is very small for the same reasons as for the air jet. $\rho \overline{u'v'}$ has a zero
value in the absence of rotation, and it is significant but smaller in amplitude than $\rho \overline{u'v'}$
when the annular flow is rotated. Since, the Helium jet in a rotating annular flow can
experience the turbulence damping effects that are characterized by the Richardson number;
so, the Ri* profile is plotted along side the shear stress data for this case. The change in the
Ri* profile was negligible when the modified code was used. Significant values of Ri*, i.e.
Ri* > 0.04, only occurred at the extremities of the modeled Helium jet. This prevented the
model modifications from having a significant influence on the turbulent shear stresses in
the flow.

To more accurately assess the significance of the code modification, a second
Helium jet model was studied in which the tangential velocity was significantly higher in
the vicinity of the jet. Figures 5.34a shows that the density profile becomes noticeably
steeper when the Ri* effects are accounted for in the turbulence model. In this case the jet
"sees" Ri* values of 0.5 near its boundary. Because Ri* reached a significant level in the
interior of the jet, the shear stresses of the jet are significantly attenuated by the
incorporation of the proposed stratification effects into the computational code. Figure
5.34b displays the narrowing of the turbulent shear zone as a result of density fluctuation
effects. The velocity profiles do not change significantly in the region of the jet boundary
when the modified code is used. This means that the stratified swirling flow truly
introduces a laminarizing influence on the turbulence associated with the jet. Figure 5.34
clearly shows an attenuation of $\rho \overline{u'v'}$ within the jet. The other turbulence quantity, $\rho \overline{u'w'}$,
is attenuated in the region where Ri*>0.2, and it shows a small increase at its peak where
Figure 5.34a Normalized Density Profile at x/de=20 for a Helium Jet in a Rotating Coaxial Air Stream

Figure 5.34b Computed Shear Stress at x/de=20 for a Helium Jet with a Non-Rotating Coaxial Air Stream
$Ri^* < 0.075$. The regions of greatest turbulence attenuation correspond to regions of high $Ri^*$. These regions also have steeper density profiles when the code modification is introduced. As a secondary effect, the centerline concentration decays more slowly because of the reduced shear stresses and hence reduced jet entrainment. Further downstream this effect becomes more noticeable as a distinction between the modified and unmodified codes.

5.3.2 Density Stratification in the RSFC Burner

5.3.2.1 Stratification and Flame Shape

The three flame shapes, Figures 5.1, 2 and 3, were analyzed with regard to the magnitude of the modified Richardson number. It indicates the degree of turbulence damping due to density stratification relative to the generation of shear stress. The modified code, however, was not used in computing the flow fields, so the density fluctuation effects are not incorporated in the calculations. Rather, the $Ri^*$ contours indicate where stratification is computed to exist, and in what regions turbulence damping could be realized when using the modified code.

Figure 5.35a displays contours of $Ri^*$ for flame shape A. The zone of greatest significance is the inner part of the tertiary air jet. Here the gas temperatures drop rapidly in the radial direction in the transition from the reaction zone to the cooler feed air of the tertiary jet. In this zone oxygen concentration increases and fuel concentration decreases in the radial direction as expected in the vicinity of a flame front. Further downstream along the furnace wall there remain significant values of $Ri^*$; this reflects the fact that the walls are removing heat from the system, i.e. creating a positive radial density gradient, and that the flow is swirling.
Figure 5.35a  Modified Richardson Number, $Ri^*$ Contours for Flame Shape A

Figure 5.35b  Modified Richardson Number, $Ri^*$ Contours for Flame Shape B
Figure 5.35b shows the Ri* contours for flame shape B. In contrast to the previous case, the stratification zone begins at the burner exit. This is an indication of early ignition which is promoted by the strong IRZ₁. The Ri* contours initially have a larger axial component but then bend more rapidly toward the furnace wall. The highly stratified zone, Ri* > 1.00, is larger and more continuous than it was for flame shape A. The general relationships between the Ri* contours and oxygen and fuel concentration are consistent with the previous case.

Figure 5.35c has the Ri* contours for flame shape C. This case closely resembles flame shape B because stratification begins at the burner exit and there is a nearly continuous highly stratified zone. This case is distinguished by a more rapid divergence of the stratification zone toward the furnace wall.

5.3.2.2 CFD Model Modification

The modified computational code was applied to the RSFC burner model with the critical value of primary air Reynolds number. Figures 5.36a, b, c, and d show the flow field that develops using this code. It can be contrasted with Figure 5.3 which was computed while neglecting the contributions of density stratification to the flow dynamics. The most important distinction between the flows is the increase in the strength of the IRZ₀. Additionally, the center of the IRZ₀ is shifted slightly downstream. One consequence of the increased IRZ₀ strength is a reduction of the primary jet penetration along the centerline from 0.43% of the mass flow to 0.005% when the density stratification is modeled. This is reflected in the shift of the 0% mass flow contour zone toward the centerline. The second consequence of the increased IRZ₀ strength is more vigorous mixing in the region of the tertiary air vortex breakdown. These two consequences facilitate a reduction of flame length by half a burner diameter as shown in Figure 5.36b.
Figure 5.35c  Modified Richardson Number, Ri* Contours for Flame Shape C
Figure 5.36a Critical Re_p, Flame Shape B (Calculated using Modified Code)
Contours of % Mass Flow

Figure 5.36b Critical Re_p, Flame Shape B (Calculated using Modified Code)
Contours of Fuel Concentration
Figure 5.36c Critical $Re_p$, Flame Shape B (Calculated using Modified Code)
Contours of Temperature (Kelvin)

Figure 5.36d Critical $Re_p$, Flame Shape B (Calculated using Modified Code)
Contours of Oxygen Concentration
Figure 5.36e  Critical $\text{Re}_p$ Flame Shape B (Calculated using Modified Code)
This demonstrates the potential significance of the density stratification effects in determining the RSFC flow field.

Other changes in the flow field are of secondary importance. The oxygen and temperature contours in Figures 5.36c and d reflect the reduction in flame length. The oil droplet trajectories become shorter when the code modification is introduced as shown in Figure 5.36e. The primary air jet stagnates more rapidly as a result of increased IRZ₀ strength and increases the drag force on the oil droplets. If the oil droplet evaporation times remain constant this effect explains the shorter oil droplet trajectories.
CHAPTER 6
Discussion and Analysis of Results

6.1 Operating Parameter Sensitivity Analysis for NOx and CO
From the computational results several conclusions about the relative emission levels for the different flame shapes can be drawn which are also supported by experimental observations. First, it is inferred that opacity is proportional to the length of the fuel rich flame zone. This is due to fuel pyrolysis in the high temperature fuel rich core of the flame. This zone is evident in flame shape C in which the primary and secondary air jets punch through the IRZ_0 and the fuel rich high temperature zone is maintained far downstream of the burner. When the flame is shorter, the residence time of the fuel in the pyrolysis zone decreases. This inference is supported by experimental measurements and observations in the phase II experiments. Table 6.1 shows the observed relationship between flame length and opacity.

<table>
<thead>
<tr>
<th>Flame Length x/d</th>
<th>NOx @3% O_2 ppm</th>
<th>Opacity %</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.5</td>
<td>260</td>
<td>0</td>
</tr>
<tr>
<td>7.6</td>
<td>197</td>
<td>5</td>
</tr>
</tbody>
</table>

Table 6.1 Relationship Between Flame Length and Emissions

The second inference drawn from this data is that the flame length is inversely proportional to NOx emission levels. The reasons for this involves the application of the NOx formation mechanisms, discussed in Chapter 1, to the flames being analyzed. Thermal NO is not considered to be significant because the flame temperatures are predicted to be below 1800 K; the Zeldovich mechanism does not produce high levels of NO below this temperature. Prompt NO forms in the low temperature fuel-rich region
around the ignition zone, but it makes no significant contributions beyond this point. Fuel NO is the dominant source of NO in the oil flames studied here because of the 0.3% N content of the oil. In unmodified flames NO levels over 300 ppm have been recorded for this fuel. At these levels, fuel NO is the dominant source of NO. The NO reburn reactions convert NO back into molecular Nitrogen. Reburn occurs most rapidly in high temperature fuel rich regions; however, it is a relatively slow process so fuel residence time in the fuel rich zone is also important. Chemical kinetics modeling of the 0.3% N oil reactions has confirmed that higher fuel concentrations, higher temperatures, and longer residence times all contribute to better NO reduction by reburn [19]. Equivalence ratios around 1.5, temperatures over 1700K, and residence times of 200 ms gave an appreciable decrease of NO in the combustion products. Understanding this, the connection with flame length is more intuitive. A long RSFC flame possesses a longer high temperature fuel rich core. For flame shape C the length of the core is directly related to the length of the flame and the fuel's residence time in the core. Flame length is therefore inversely proportional to NOx emissions for this flame shape. For the critical flame shape, flame shape B, the same relationship would apply with respect to other shape B flames; however, flame shape B gives the fuel a longer residence time than a flame of shape A or C with the same combustion length because of the circuitous path followed by the fuel rich jet in flame shape B. Flame shape A has a very short fuel residence time in a fuel rich zone, so it will produce high NO flames.

The third inference is that CO emissions are directly proportional to the opacity and therefore to flame length as well. A nearly linear relationship between CO and opacity was observed in the Phase I experiments as shown in Figure 6.1. The strength of this relationship depends on the temperature and equivalence ratio in the fuel rich core. The relationship between CO emission levels and NO levels is supported by experimental
Figure 6.1 CO Emissions vs Opacity for the RSFC Burner Phase I Experiments (21 MW)

Figure 6.2 NO vs CO Emissions for the RSFC Burner Phase I Experiments (21 MW)
measurements as well; Figure 6.2 shows the measurements that were made in the Phase I experiments. Based on the conditions governing reburn, NO emissions can be lowered by increasing the temperature or the fuel equivalence ratio in the core. For flame shape B the CO emissions are lower than for flame shape C with the same $\text{IRZ}_0$ position because in flame shape B the $\text{IRZ}_0$ entrains the central jet thereby enhancing mixing. This also lowers NO by driving the transition from fuel-rich to fuel-lean more rapidly. The enhanced mixing is observable in the differences between the fuel contour plots of flame shapes B and C.

It is desirable to understand the aerodynamic influences on flame shape in order to design a flame that gives the best emissions in the available furnace space. The preceding discussion suggests that flame shape B promises to give the lowest NO and CO emissions for a given flame length requirement. Flame shape C tends to be much longer than is feasible in many furnaces and gives high opacity and CO. The influence of individual operating parameters on flame shape is discussed in the following sections.

6.1.1 Primary Air Reynolds Number

The recognition of $\text{Re}_p$ as an important burner design parameter is the first step toward creating burners that give good flame stability and low NO and CO emissions. It was demonstrated computationally that three different flame shapes can be generated simply by changing the $\text{Re}_p$. Just as important is the recognition of the influence of the secondary air on the strength of this relationship. In the three cases that were presented, the primary and secondary air jets behaved jointly. This suggests that it is the joint behavior of the swirling primary and secondary air that is significant and not simply the primary air alone. It is important to note that the changes in $\text{Re}_p$ occurred while maintaining constant swirl numbers for all of the jets. This means the angular momentum of the primary air jet was increased when $\text{Re}_p$ was increased. The higher angular momentum of the central jet
increases the strength of the adverse pressure gradient along the centerline. This is believed to be directly related to the decrease in the jet’s penetration of the $\text{IRZ}_o$. Critical to the existence of all three flame shapes is the high tertiary air swirl and angular momentum.

A simple relationship exists between $\text{Re}_p$ and CO and NO levels. Reduction of $\text{Re}_p$ increases centerline penetration and lengthens the flame. Since it was concluded that NO also has an inverse relationship with flame length, $\text{Re}_p$ is known to be proportional to NO. Likewise, $\text{Re}_p$ is inversely proportional to CO. This was verified in the phase II experiments; Figure 6.3 displays the change in the emissions when $\text{Re}_p$ was reduced below the nominal operating point.

6.1.2 Primary Air Swirl

Recognizing $S_p$ as an important flame design parameter furthers the options of the burner designer to obtain the desired flame shape. The computational data confirm the supposition that the angular momentum of the central jets determines the level of penetration through the $\text{IRZ}_o$, and adjustments in $S_p$ are just one way of changing it. Crucial to the comparisons being made is that the tertiary air retain a high swirl and angular momentum in all cases.

The relationship of $S_p$ to CO and NO emissions is readily deduced. Since decreasing $S_p$ increases flame length, an inverse relationship is expected between $S_p$ and CO emissions when the flame shape is either B and C. The same relationship applies to opacity as well. It then follows that $S_p$ is proportional to NO emissions. This conclusion has been evidenced experimentally as well. In the MIT experiments [19] the proportional relationship between $S_p$ and NO was observed: the presence of high tertiary air swirl. Additionally, the frequency of puffs of soot-related to opacity - was inversely proportional to $S_p$. 

160
Figure 6.3 Emissions vs $\text{Re}_p$ for Phase II Experiments

Figure 6.4 Opacity & Emissions vs $\text{Re}_{H,T}$ for Phase I Experiments
6.1.3 Tertiary Air Reynolds Number

The decrease in the tertiary air Reynolds number has an important effect on the
IRZ_0. While maintaining a constant swirl number and mass flow, a decrease in Re_H,T
effectively increases the angular momentum of the tertiary air jet. This creates a stronger
radial pressure gradient in the swirling flow, and strengthens the adverse pressure gradient
along the centerline. This results in more rapid vortex breakdown; the IRZ_0 moves closer
to the burner exit. Also, the IRZ_0 is stronger, the most notable change being the
downstream shift in the IRZ_0’s downstream stagnation point for flame shape A. These
changes in the flow field promote more vigorous mixing of the fuel and air in the IRZ_0;
coupled with the upstream shift in the IRZ_0 position, this results in a shorter flame. It is
important to note that the magnitude of the change was relatively small for flame shape A
with a 2.8% decrease in Re_H,T and a 55% increase in the angular momentum. However,
without maintaining a constant mass flow rate, a 31% decrease in Re_H,T and 33% increase
in the tertiary angular momentum of flame shape C caused the IRZ_0 to shift forward by
35%.

The expected changes in NO, CO, and opacity correspond to the previously
discussed relations with flame length. It is important to note that the tertiary air Reynolds
number based on hydraulic diameter, Re_H,T, decreases in magnitude when the moment
of the jet increases and the mass flow remains constant, whereas Re_T increases in such a
case. Decreasing Re_H,T is expected to increase the level of NO because it shortens the fuel
residence time in the fuel rich zone. A shorter flame has a higher volumetric heat release,
so higher temperatures are expected. This can increase NO levels through the Zeldovich
mechanism if temperatures are above 1800K, however, competing with the temperature
effect is the increase in the rate of the reburn reaction in the fuel rich zone. Overall,
residence time seems to be the deciding factor in decreasing NO. So, a lower \( Re_{at} \) is expected to reduce CO and opacity by decreasing flame length and increasing the rate of burnout of the fuel in the furnace.

In the phase I experiments the shape of the tertiary air duct was decreased by adding inserts of various sizes. The experimental geometries corresponding most closely to the models had a tertiary air exit area of 36% and 30% of the burner area. The tertiary air Reynolds number, \( Re_{HT} \), was decreased from approximately 185,000 to 160,000 by decreasing the tertiary air exit area. The effect on emissions was a 5% increase in the NO and a 47% decrease in CO in accordance with the trends predicted from the modeling; however opacity increased. Figure 6.4 shows the quantitative values for these changes. The swirl number for these cases was not known exactly, but the angular momentum of the tertiary air is known to have increased.

It is not obvious from these results whether it is precisely \( Re_{HT} \) or the angular momentum of the tertiary air that causes the changes in the emissions. Maintaining a constant \( S_T \) in the modeling blurs the distinction. An examination of effect of changing \( S_T \) while maintaining a constant \( Re_{HT} \) in the next section will isolate the influence of the tertiary angular momentum from other factors.

6.1.4 Tertiary Air Swirl

Reducing the tertiary air swirl number, \( S_T \), while maintaining the same geometry and flow rate reduces the angular momentum of the jet while keeping the axial momentum constant. The relationship existing between the tertiary air angular momentum and the flow field described in the previous section is consistent with the changes in angular momentum caused by varying \( S_T \). The IRZ \( o \) has a decreased mass when \( S_T \) is decreased, and presumably, a weaker adverse pressure gradient exists along the centerline. Likewise,
vortex breakdown occurs further downstream. These changes in the IRZ_0 caused no appreciable increase in the flow penetration along the centerline. The benefit, however, of having the IRZ_0 move downstream is increased fuel residence time in the core which means lower NO emissions. Nevertheless, it is important to recognize that S_T must be set high enough to establish the IRZ_0. Without it the flow would behave like a classical swirling diffusion flame, and density stratification would not occur, resulting in a high NO flame. It can be said that there is a critical value for S_T above which the IRZ_0 is formed and density stratification occurs. The model in Figure 5.9 appears to be just above the critical S_T; it has a value of 0.65 in this case.

Changes in the tertiary air swirl number were observed in the Phase II experiments. The tertiary air Reynolds number was Re_{HT} = 131,000 for the #6 oil experiments and Re_{HT} = 139,000 for the Orimulsion experiments. Figure 6.5 shows the effect of changing S_T on emissions. Through the computational studies it is understood that the observed transition to lower NOx with increasing S_T involves the creation the fuel rich zone through density stratification. Initially, the increase in S_T increases the size and equivalence ratio of the fuel rich zone which drives the reburn reaction. However, once that zone is established, further increases in S_T draw the IRZ_0 closer to the burner without any appreciable increase in concentration in the fuel rich zone. The increase in S_T above the critical value only serves to decrease the size and residence time of the fuel in fuel rich zone by drawing the IRZ_0 closer to the burner. This results in an increase in NOx emissions. In the Orimulsion experiments the critical tertiary air swirl appears to be around 0.6; the value appears to be higher for the oil experiments. In all of these experiments the CO remained relatively low.
Figure 6.5 NO & CO Emissions vs $S_T$ in Phase II Experiments
6.1.5 Air Distribution

The flows presented in Figures 5.8, 5.11, and 5.12 illustrate important principles related to the mass flow distribution in the burner. First, comparison of Figures 5.8 and 5.11 demonstrates the previously described principles relating the flow field to $Re_p$ and $Re_{H,T}$. However, when the amount of secondary air is increased and the geometry remains the same, these effects lose their robustness. From the normalized stream function contours it seems that that primary and secondary air jets initially behave jointly. It is expected that the secondary air jet would compliment the primary air jet in its effect on the flow. In Figures 5.8, 5.12, and 5.11 the two jets have the same swirl number and a net mass flow of 23%, 19.2%, and 12% respectively. Surprisingly, the flow pattern in Figure 5.12 is not an intermediate case between the other two; the increased secondary air mass flow greatly increases the penetration of the primary air jet through the IRZ$_o$ rather than decreasing it as would occur if the secondary air jet acted jointly with the primary. The increase in the centerline penetration does however correlate with the ratio of the primary and secondary air Reynolds number. For Figures 5.8, 5.12, and 5.11 the centerline penetration is 0%, 9.3%, and 4.1% while $Re_{H,P}/Re_{H,S}$ is 14.6, 1.61, and 6.45 respectively. These insights highlight the importance of the radial air distribution established by the burner. Decreasing the effective radial separation of the tertiary air jet from the inner jets increases flame length. The low secondary air mass flow is one method of increasing the effective separation between the jets. When there is a physical change in the radial spacing of the tertiary air jet the same effect is observed. This is can be seen by comparing Figures 5.1 and 5.6.
6.1.6 Fuel Droplet Size

The flame is shown to be quite sensitive to atomization since a change in droplet size changed the flame shape. Figures 5.13A, B, and C show that the air flow operating parameters have the major influence on determining the flow field, and the droplets, especially small ones, follow the streamlines to a large extent. However, the droplet interaction with the flow field can be significant when the flow field is sensitive. This occurs in Figures 5.14 and 5.15 when the flame shape changes from B to C by increasing the droplet size. This effect can be explained based upon the principles discussed previously. The initial droplet velocity is the same in both cases; so the net momentum being introduced by the droplets is the same. However, when the droplets are larger there are fewer of them, and they transfer momentum to the flow further downstream. The droplets are only indirectly affected by the adverse pressure gradient. The result is that axial momentum is transferred to regions that were formerly unaffected by the droplets. The increase in axial momentum from the oil droplets decreases the effective swirl number locally. As was shown before, a decrease in swirl can increase the mass flow penetration along the centerline. This is exactly the effect of increasing fuel droplet size. The increase in flow penetration on the centerline is accompanied by an increase in flame length and an increase in CO emissions.

6.1.7 Atomizer Spray Angle

The spray angle of the atomizer was shown to effect the centerline penetration through the IRZ_o. A small spray angle gives the oil spray greater axial momentum which then gets transferred to the primary air jet. A larger axial momentum reduces the effective swirl number and results in increased centerline penetration as was demonstrated. Larger spray angles give the oil droplets a higher radial velocity on the average. When the spray
angle is large the droplets mix into the tertiary air stream more quickly; this reduces the fuel's separation. Together, the effects of increasing spray angle on radial velocity and axial momentum contribute to an increase in NO emissions. The increase in radial velocity allows more fuel to mix with the tertiary air jet early in the flow and produce NOx. The decrease in axial velocity associated with the increase in spray angle decreases the residence time of the fuel in the fuel-rich zone; this also increases NOx emissions.

6.2 Design Parameter Analysis

Most of the design parameters that were studied relate to the burner quarl. The divergent quarl is important to burner systems because it can increase the strength and size of an IRZ without increasing the pressure drop through the burner. Design limitations constrain quarl exit area and quarl length; so, it is important to understand which aspects of the quarl design can not be compromised so as to maintain a low NOx flame.

Increasing the quarl length, shifts the IRZ₀ further downstream and increases its strength. While the tertiary air jet remains within the quarl it can only entrain on one side; so, it entrains less than if it were free to entrain on both sides. After leaving the quarl the tertiary air jet spreads out. In the modeling jets exiting a long quarl had a smaller spreading angle than jets exiting a short quarl. This is related to the differences in the jets rotational energy at the quarl exit. When a jet entrains the surrounding fluid, it does work on the fluid and loses some of its energy. Therefore, the jets emerging from a long quarl will have less rotational energy; and this keeps them from spreading as quickly. The spreading of the jet promotes vortex breakdown. The computational results confirm that the jets which spread more slowly experience vortex breakdown further downstream. In addition to this, the jet which spreads out more slowly will entrain less and retain more of its energy. This is the

168
reason that the jets with long quarls were capable of exhibiting a stronger vortex breakdown.

With regard to RSFC burner performance, long quarls contribute two important effects. They can lengthen flame shape B and increase the residence time of the fuel in the fuel rich zone by moving the IRZO further downstream. Long quarls also enhance downstream mixing and promote better fuel burnout by increasing the strength of the vortex breakdown. This means quarl length has a positive correlation to both NO and CO emissions.

Changes in the quarl divergence angle had no predictable effect on the flow field. A larger divergence angle may seem like a convenient way of shortening the quarl, but total quarl length, i.e. including the divergence, is important to the burner's performance. If the quarl is allowed to protrude into the furnace, a larger divergence angle can reduce the space requirements for retrofit.

Decreasing the tertiary air radial spacing decreased the strength of the IRZo and increased flame length. The effect is consistent with the decrease in effective air distribution described in Section 6.1.5. Although the quarl length changed in the cases presented, a subsequent case with constant quarl length demonstrated the same change in the IRZo and flame length.

Increasing the quarl exit area strengthens the IRZo, but only to a small degree for the RSFC burner. With regard to burner design, a smaller quarl size is acceptable since it evidences no effect on flame length or IRZo position. However, a smaller quarl is likely to decrease flame stability; so, the size must be considered carefully.

6.3 RSFC Burner Scaling Criteria

The kinematic similarity criteria proved to be the best guideline for scaling flame shape B while maintaining the same swirl numbers for the burner. The jet Reynolds
numbers are also maintained through kinematic scaling. This leads to the conclusion that
the critical primary air Reynolds number is the same for all burners of kinematic similarity.
In Section 6.1.1 the primary air Reynolds number was noted for its strong influence on
penetration through the IRZ₀. For chemical similarity the jet Reynolds numbers scale
according to the following relationship:

\[ Re = s^{2/3} Re_0 \]  \hspace{1cm} (6.1)

When thermal similarity criteria are applied, the Reynolds numbers for the burner’s jets scale according to Equation 6.2:

\[ Re = \sqrt{s} Re_0 \]  \hspace{1cm} (6.2)

The models in Figures 5.23, 24, and 25 were scaled down by a factor of s=0.7. If the
critical primary and secondary air jet Reynolds numbers happen to be the same for all scales of the burner, jet penetration would increase when the burner is scaled down
according to the rules of chemical and thermal similarity. Furthermore, scaling down
according to chemical similarity criteria would increase the jet penetration more than with
thermal similarity. Since, this was precisely the relationship observed in the models, the
supposition is supported. Figure 6.6 illustrates the percent of the burner mass flow
penetrating the IRZ₀ on the centerline in relationship to the primary air Reynolds number
when the burner model is scaled down from 21 MW to 15 MW using the three scaling
criteria being considered. The relationship between penetration and jet Reynolds number is
the same as was observed in the parametric studies shown in Figure 5.4. Similarity in
geometry, relative flow rates, and swirl numbers is believed to be responsible for making
the relationship to Reₚ collinear among the three scaling criteria.

The parametric studies indicated that the primary and secondary air jet Reynolds
numbers were only related to the penetration indirectly. They showed that the penetration
Figure 6.6 Penetration vs Primary Air Re for Scale-Down from 21 MW
could be similarly altered under conditions of constant Reynolds number and changing swirl number. The functional relationship is described in Equation 6.3:

$$\dot{m} = f(Re_p, Re_s, S_p, S_s)$$ (6.3)

In the parametric studies it was concluded that the observed dependence on these nondimensional parameters was indicative of the importance of the angular momentum, $M_\theta$, of the primary and secondary air jets. An increase in penetration was obtained by decreasing $M_{\theta_p}$ either by decreasing $Re_p$ and keeping $S_p$ constant or by decreasing $S_p$ and keeping $Re_p$ constant.

Because the scaling studies demonstrated changes in flame shape consistent with the findings of the parametric studies, an additional condition was developed for each of the scaling methods by which flame shape could theoretically be maintained at different scales. Jet angular momentum is believed to be of primary importance. Kinematic similarity with constant swirl numbers scaled the angular momentum in a manner that maintained the flame shape. The scaling relationship for angular momentum is given in Equation 6.4:

$$M_\theta = sM_{\theta_0}$$ (6.3)

If this is the only criteria for maintaining the flame shape and the penetration of the primary and secondary air jets, the primary and secondary jet swirl numbers must be adjusted in the following ways depending on the scaling method used:

$$S = S_0 / \sqrt{s} \quad \text{Thermal}$$
$$S = S_0 / s^{2/3} \quad \text{Chemical}$$
$$S = S_0 \quad \text{Kinematic}$$ (6.4)

The validity of the relationship for kinematic scaling has already been demonstrated. Additional modeling work was done to test this relationship for other similarity criteria.
The validity of the proposed criteria is best demonstrated through a comparison of centerline mass flow penetration with both the firing rate and the angular momentum of the primary and/or secondary air jet. Figure 6.7a shows the predicted relationship between centerline penetration, firing rate normalized by the 21 MW reference case, \( Q/Q_0 \), and angular momentum normalized by the 21 MW reference case, \( M_{\theta}/M_{\theta,0} \). When Equation 6.4 is used in RSFC burner scale up to determine the swirl numbers, the relationship between angular momentum and scale is the same as the relationship between the firing rate and scale. Therefore, the iso-penetration lines are defined by Equation 6.5:

\[
\frac{M_{\theta}}{M_{\theta,0}} = \frac{Q}{Q_0}
\]

(6.5)

The proposed scaling criteria was evaluated for burners of thermal similarity. Figure 6.7b gives the computational results for 5 burners related by the thermal similarity criteria. The condition in Equation 6.4 was proved to be accurate when the reference burner was scaled down but not entirely valid when the burner was scaled up. Maintaining constant swirl numbers with scale-up changed the flow field to flame shape A. This at least shows that the actual scale-up relationship for burners of thermal similarity lies somewhere between maintaining constant swirl numbers and applying the relationship in Equation 6.4.

In the parametric studies the tertiary air jet was shown to be primarily responsible for the formation and positioning of the IRZ_\( \omega \). When the burner is scaled up, it is desirable that the position of the IRZ_\( \omega \) change according to the change in length scale. Since, the spreading of a turbulent jet typically scales with its diameter, geometric similarity should be sufficient. If the tertiary air swirl number remains constant, the tangential velocity scales in the same manner as the axial velocity. Darmofal [30] notes that
Figure 6.7a Theoretical Iso-Penetration Lines for RSFC Burners

Figure 6.7b %Penetration for RSFC Burner Models with Thermal Similarity
increasing the swirl number of a vortex increases its susceptibility to vortex breakdown. Therefore, maintaining a constant swirl number for the turbulent tertiary air jet should keep the IRZ₀ at nearly the same non-dimensional axial position. Comparison of Figures 5.23a and 5.24a validates this point. The figures describe flows with the same firing rate and the same swirl numbers, but they have different geometric scales. The IRZ₀ is shown to have the same non-dimensional axial position in both cases.

6.4 Significance of Modeling Density Stratification
In this section density stratification in jets with swirl is examined. The capabilities and limitations of a standard incompressible CFD code to model these flows are discussed, and the practical implications of density stratification are reviewed.

6.4.1 Stratified Isothermal Jet
The isothermal stratified turbulent jet studies by Beér and Chigier pointed out the importance of annular flow rotation in reducing turbulent shear stresses in the vicinity of a turbulent jet. With or without density stratification in the annular flow, experimental results showed that annular flow rotation significantly turbulent shear stresses in the jet. When density stratification is also present, the turbulence damping was more pronounced.

Similar conclusions can be drawn from the modeling studies even though the results differ in some obvious ways. The \( \rho u' \nabla v' \) shear stresses are the common parameter used to compare the models and the experiments. Rotation in the annular air stream reduced the jet width by dampening the shear stresses in the jet boundary. This differs from the complete reduction reported in the experimental results, but the trend is the same. Furthermore, the peak shear stresses in the jet models were slightly attenuated by the introduction of rotation. The difference in the magnitude of this effect is one of the most significant differences between the experiments and the modeling studies, but again the trend is the same for both. An important contrast between the experiments and modeling
studies was that in the model the effects of rotation were more pronounced for the air jet but in the experiments the effects of rotation they were more pronounced for the Helium jet. The strong decreases in shear stress with rotation that were measured imply that the Helium jet in the experiments had large values of Ri*, i.e. greater than 0.04, in the interior of the jet. In contrast the Helium jet in the model had low values of Ri* in its interior. This difference highlights the point that radial density gradients and swirl in the annular flow do not necessarily lead to turbulence damping unless the high magnitude regions coincide. The second Helium jet model with increased tangential velocity in the vicinity of the jet confirms this point. Furthermore, the original model of the Helium jet experiments demonstrates smaller changes due to rotation in the annular flow because it is physically narrower than the corresponding air jet, and therefore it experiences weaker swirl effects in the same swirling annular flow field.

It is concluded that solid body flow rotation in the vicinity of the jet reduces turbulent shear stress in that region, and this effect is complimented by superimposing a positive radial density gradient on the same region. The standard incompressible CFD code models turbulence damping related to rotation alone and neglects the complimentary effects of density stratification. The modified CFD code accounts for both effects. Turbulence damping at the jet boundary results in reduced jet entrainment. The secondary effects of this are a slower decay in the jet velocity, and when the jet has a lower density than the surrounding air, the rate of decay in the centerline concentration is also reduced.

The discrepancies between the experimental data and the model are not fully understood. Analysis of the experimental profiles of radial density and air jet axial velocity demonstrated they are physically unreasonable. The generation of significant shear stresses in the rotating annular flow away from the jet is believed to represent a significant flow disturbance in that region; a recirculation zone is suspected. A recirculation zone, however,
would be inconsistent with the flat axial velocity profile measured experimentally for that region. The differences in the amplitude of $\rho \overline{u'v'}$ can be attributed in part to the shortcomings of the turbulence model, however, the strong damping of $\rho \overline{u'v'}$ also suggests that the tangential velocities were larger than the measured values in the vicinity of the jet. The non-zero values of $\rho \overline{v'w'}$ in the absence of rotation can not be reproduced by the RSM turbulence model. Modeling and comparison with additional sets of swirling stratified flow turbulence data is needed to determine the full shortcomings of the modified code.

6.4.2 RSFC Burner Density Stratification

Application of the modified CFD code to the RSFC burner model demonstrated that density stratification effects have a significant influence on the IRZ$_o$. The IRZ$_o$ characterizes the vortex breakdown of the tertiary air jet. The regions of significant Ri* are on the interior side of the annular tertiary air jet. The code modification reduces shear stresses in this region, and therefore reduces entrainment by the tertiary air jet in this part of the flow field. Reducing entrainment allows the jet to retain more energy because it does less work on the surrounding fluid.

The reduced entrainment and increased swirl energy brought about by the code modification has an understandable effect on the tertiary air jet’s behavior. Increasing the jet’s swirl energy allows it to exhibit a stronger vortex breakdown; this was also demonstrated by lengthening the quarl. However, in contrast to quarl lengthening, density stratification slightly increases the spreading angle of the jet at the quarl exit. This occurs because the jet has more swirl energy at the quarl exit due to reduced entrainment. Lengthening the quarl increases the jet’s entrainment relative to the quarl exit. Previously, it was believed that density stratification would reduce the spreading angle of the jet.
because of reduced entrainment on the jet's surface. In the model the spreading of the jet
appeared to be governed more strongly by the forces associated with swirl than with the
effects of entrainment. If this is physically accurate density stratification serves to increase
the spreading angle of the tertiary air jet rather than lessen it. This is not known
conclusively however because the modified code is still inaccurate in predicting the
spreading angle of the tertiary air jet.

The burner model overestimates the spreading angle of the RSFC flame. The
shortcomings of the k-ε turbulence model are a significant part of the problem. The burner
flow field calculations with the RSM turbulence model could not meet the same
convergence criteria as were required of the k-ε models, but the RSM turbulence model
changed the flow field in a manner that more accurately resembled the experiments.
However, further study needs to be done to obtain satisfactorily converged solutions and
assess the significance of the changes.

Reduced entrainment by the tertiary air jet helps delay vortex breakdown until
further downstream. This was shown to be true for quarl extension as evidenced in Figure
5.20. Similarly, the IRZ₀ position shifted as a result of introducing density stratification
effects to the code. However, this effect was very small; the IRZ₀ shifted downstream by
no more than 0.1 burner diameters.

For the burner the primary significance of density stratification is related to NOx
formation. Limiting entrainment on the inner boundary of the tertiary air jet is essential to
preventing early burnout of the fuel. Without stratification the fuel would mix into the air
more rapidly and bound nitrogen species would convert to NO. The present study of oil
diffusion flame aerodynamics for the RSFC burner did not delve into the modeling
specifics of NOx formation chemistry; instead, the aerodynamic requirements of the
burner to operate in a low NO\textsubscript{x} state were considered.
CHAPTER 7

Summary, Conclusions, and Recommendations

7.1 Summary

Having observed the ability of the RSFC burner to reduce NOx emissions for heavy oil diffusion flames, a thorough computational study was conducted to better understand the flow field characteristics of the low NOx tulip-shaped flame. The flow field of this optimal flame was modeled, and the sensitivity of the flow field to relevant operating and design parameters was assessed. The criteria for scale-up of the tulip-shaped flame were also examined. Density stratification plays a crucial role in lowering the NOx emissions of this flame. The influence of density stratification on jet behavior was examined for isothermal, swirling, stratified jets and for the tulip-shaped flame.

The CFD code that was used in the modeling studies is described in Chapter 4. The physical parameters that were incorporated into the model are also recorded. In Chapter 3 the constituent equations and modeling assumptions of the CFD code are presented. Additionally, the contributions of density fluctuations to the constituent equations is presented, and a re-formulation of the governing equations with algebraic evaluation of the density fluctuation source terms is described.

In Chapter 4 the models for several components of the burner-furnace system are described and compared to the experimental set-up and conditions. The operating conditions for 4 reference cases are presented as well. In Chapter 5 data describing the flow field in the furnace as a result of parametric changes in the operating conditions and
design parameters is presented. In Chapter 6 the data is analyzed and its implications for NO and CO reduction are discussed.

An assessment was made of the capability of the CFD code to describe the effects of density stratification. In Chapter 4 the experimental set-up and computational models for isothermal jet experiments are described. The reported experimental results are compared with the modeling results in Chapter 5. In Chapter 6 the results are analyzed and the modified computational code is assessed.

Stratification in the RSFC burner was studied by examining the modified Richardson number contours in the model and applying the modified code to the burner model. Chapter 5 presents these results, and they are analyzed in Chapter 6.

7.2 Conclusions

Insights into the performance of the low NOx RSFC burner and its proclivity for being modeled were obtained as a result of these investigations. Conclusions can be drawn which provide important guidelines for optimizing burner performance and scale-up. Additionally, the insights obtained in the density stratification modeling studies provide important guidance for understanding the establishment of the low NOx RSFC flow field and can guide future low NOx burner development. This section answers the principle hypotheses which guided this research. They are as follows:

1) The jet dynamics for the tulip-shaped RSFC burner flame associated with optimal low NOx experimental performance can be described in a useful manner using the k-ε turbulence model and a single-step reaction mechanism.

2) Mass flow penetration through the recirculation zone established by the tertiary air jet is the primary cause for increased RSFC flame length and CO emissions and can also be associated with increased opacity. The angular momenta of the primary and secondary air jets are the most influential operating parameters for mass flow penetration, and they are inversely proportional to mass flow penetration. The effect of the
angular momentum increases as the ratio of primary to secondary air Reynolds number, $\text{Re}_{\text{HL,p}}/\text{Re}_{\text{HL,s}}$, increases.

3) Algebraic modeling of density fluctuations does not change the computed RSFC burner flow field in an appreciable manner; so, reduced entrainment effects are concluded to be of only secondary importance in influencing the spreading and vortex breakdown of the RSFC tertiary air jet.

4) Density stratification does play a significant role in determining the spreading of a jet when entrainment is of primary importance in governing the jet’s behavior and modified Richardson numbers greater than 0.04 exist within a significant cross-section of the jet.

5) With regard to RSFC burner design, tertiary air swirl must lie above the critical swirl number of 0.65 in order to establish the flow field necessary for low NOx performance. Additionally, the computational results indicate that a quarl length greater than 0.35 burner diameters can delay vortex breakdown to an extent that is believed to have a positive influence on NOx reduction in the stratified flame.

6) The flow pattern of the RSFC burner can be maintained during scale-up if the swirl for the primary and secondary air jets is kept between the extremes of either maintaining a constant swirl number or increasing the jets’ angular momenta proportionally with the scaling factor.

7) Atomizers that produce small oil droplets within a narrow spray angle are best for assisting the low NOx performance of the RSFC burner.

7.3 Recommendations for Future Work

Reacting flows incorporate several physical phenomena which are only approximated by numerical models. Efforts to improve modeling capabilities are ongoing. With regard to the RSFC burner the capabilities of the RSM turbulence model need to be assessed more fully. Ultimately, the modeling approach which gives the best prediction of the tertiary air jet spreading angle while requiring the least computational time is desired.

Although significant characteristics of the RSFC burner flow field could be represented with the code used in this study, it is desirable to know how accurately the code represents the actual flow field. Species and temperature mapping of an RSFC oil diffusion flame has been performed by Shihadeh [19], but velocity profile measurements
were lacking. A detailed flame mapping of the RSFC burner which includes average velocity measurements is desirable for better assessment of the model’s accuracy and as a reference for code improvement.

Predicting exit NOx levels for the burner is the ultimate goal of burner flow field modeling. Separate from the issue of flow field accuracy is the incorporation of NOx formation chemistry into the code. Ehrhardt [31] used a zone modeling technique on the burner flow field to apply NOx reburn chemistry to a model of an oil diffusion flame. Application of this method to the flow field of the RSFC burner could provide a useful quantitative assessment of the NOx emissions. A more cumbersome approach would be to incorporate the chemical reactions governing thermal, prompt, fuel NO formation and NO reburn into the flow field calculations.
References


