Winter 1991

Numerical Modeling of Flame Lift-Off Phenomenon and Calculation of Thermal Loads on a Methane Fuel Injector With Complex Geometry

Taj O. Mohieldin

Old Dominion University

Follow this and additional works at: https://digitalcommons.odu.edu/mae_etds

Part of the Mechanical Engineering Commons

Recommended Citation
https://digitalcommons.odu.edu/mae_etds/253

This Dissertation is brought to you for free and open access by the Mechanical & Aerospace Engineering at ODU Digital Commons. It has been accepted for inclusion in Mechanical & Aerospace Engineering Theses & Dissertations by an authorized administrator of ODU Digital Commons. For more information, please contact digitalcommons@odu.edu.
NUMERICAL MODELING OF FLAME LIFT-OFF PHENOMENON AND CALCULATION OF THERMAL LOADS ON A METHANE FUEL INJECTOR WITH COMPLEX GEOMETRY

BY
TAJ O. MOHIELDIN
M.E. in Mechanical Engineering, August 1987
Old Dominion University
Norfolk, Virginia

A Dissertation Submitted to the Faculty of Old Dominion University in Partial Fulfillment of the Requirements for the Degree of

Doctor of Philosophy
Mechanical Engineering

OLD DOMINION UNIVERSITY

December, 1991

Dr. Sushil K. Chaturvedi (Director)  Dr. Surendra N. Tiwari

Dr. Albert S. Roberts JR.  Dr. Jag J. Singh
ABSTRACT

NUMERICAL MODELING OF FLAME LIFT-OFF PHENOMENON AND CALCULATION OF THERMAL LOADS ON A METHANE FUEL INJECTOR WITH COMPLEX GEOMETRY

Taj O. Mohieldin
Department of Mechanical Engineering and Mechanics
Old Dominion University
Director: Dr. Sushil K. Chaturvedi

A numerical study has been conducted to analyze a fuel injector with three in-line cylinder geometry that has been adopted as a model for investigating the combustion phenomenon in the 8-Foot High Temperature Tunnel (HTT) combustor at the NASA Langley Research Center. The primary objective here is to analyze the flame lift-off phenomenon in the three cylinder fuel injector geometry in two-dimensions. The fluid mechanics model used in the analysis includes the time-averaged Navier-Stokes equations that are employed in conjunction with a two-equation k-ε model for predicting the effects of turbulence. Calculations were performed with three chemistry models, namely fast chemistry, one-step and two-step reaction kinetics. The coupled elliptic, non-linear, partial differential equations are solved by an existing quadratic upwind scheme. Predictions are made for the flame lift-off, injector surface temperature and thermal load resulting from the combustion phenomenon downstream of the fuel injector.
Effects of fuel jet velocity, chemistry model, inlet turbulent intensity and oxygen enrichment on the flame lift-off phenomenon, and the thermal load on the fuel injector are analyzed by considering simultaneously combined convection (outside the cylinders) and conduction (inside the cylinders). Results indicate that as the fuel jet velocity is increased, the flame is transformed from a wrap around configuration to a clearly lifted flame configuration. Of the three chemistry models considered in the present study, only the two-step chemistry model predicts a clearly lifted flame. The results indicate that as the fuel injection velocity is increased the thermal load and peak surface temperature decreases sharply (as the flame gets detached from the injector surface). The effect of oxygen enrichment on the combustion process is very pronounced and causes the establishment of a wrap around flame even at higher injection velocities.
Acknowledgments

The author wishes to express his sincere appreciation to Dr. Sushil K. Chaturvedi, his advisor, for his guidance, support, encouragements, and productive assistance throughout the course of this research. He would like to express his thanks for the many useful comments and suggestions provided by the members of the guidance committee, Drs. S. N. Tiwari, and A. S. Roberts Jr. Special thanks are also due Dr. J. J. Singh for stimulating discussions on various aspects of this work. The author also wishes to acknowledge the financial assistance from NASA Langley Research Center, under contract NAS-1-18584-35, during the course of this study. And last, but not least, the author is grateful to his family and especially to his wife, Sumia E. Mohieldin, for her constant devotion, support, and patience with what must have seemed to her—as it did sometimes to him—to be a never ending research.
# TABLE OF CONTENTS

ACKNOWLEDGEMENTS

| TABLE OF CONTENTS | .......................................................... ii |
| LIST OF TABLES | .......................................................... iv |
| LIST OF FIGURES | .......................................................... v |
| LIST OF SYMBOLS | .......................................................... xi |

Chapter

1 Introduction ........................................ 1

2 LITERATURE SURVEY ................................... 7

3 GOVERNING EQUATIONS ................................... 16

3.1 Physical Model ........................................ 16

3.2 Basic Conservation Equations ....................... 18

3.3 Turbulence Modelling ................................ 18

3.4 Energy Equation ....................................... 23

3.5 Mass Conservation ..................................... 26

3.6 Combustion Models ................................... 27

3.7 Calculation of Physical Properties ............... 33

3.8 General Form of the Governing Differential
Equations .................................................. 34

3.9 Numerical Procedure .................................. 40

3.9.1 Grid System and Discretization
Equation .................................................. 40
3.9.2 Overall Solution Procedure .......... 43
3.9.3 Boundary Conditions .................. 44

4 COMPUTER CODE VALIDATION .......... 46
4.1 Turbulent Flow Past Heated Cylinder .... 46
4.2 Turbulent Flow Between Two Cylinders .... 54
4.3 Reacting Flow in a Suddenly-Expanded
   Combustion Chamber ....................... 54

5 RESULTS AND DISCUSSION ............. 76
5.1 Grid Independency ....................... 76
5.2 Results for Non-Reacting Flows ......... 83
5.3 Combustion Calculations ................ 97
5.3.1 Consideration of Different Chemistry
   Models ................................... 97
5.3.2 The Effect of Fuel Jet Velocity .... 102
5.3.3 Thermal Load Analysis ............... 120
5.3.4 Effect of LOX Injection .............. 126
5.3.5 Effect of Inlet Turbulence Intensity 135
5.3.6 Influence of Far-Field Bondary
   Conditions .............................. 140

6 CONCLUSIONS .......................... 144
REFERENCES ............................... 148
APPENDICES ............................... 160
A STOICHIOMETRIC RELATIONS ............ 161
B QUADRATIC INTERPOLATION ............ 164

iii
LIST OF TABLES

3.1 Turbulence model constants ..................... 22
3.2 Conservation equations corresponding to
equation (3.8-1) .................................. 35
3.3 Chemical kinetics data for fast and one step
reactions ........................................... 36
3.4 Chemical Kinetics data for two step reaction ... 37
3.5 Enthalpy of formation for different species .... 38
3.6 Polynomial coefficients for physical properties. 39
4.1 Geometrical and flow parameters for turbulent
flow past heated cylinder .......................... 47
4.2 Geometrical and flow parameters for air flow
past a pair of cylinders ............................ 53
4.3 Flow parameters for the reacting flow in a
suddenly-expanded combustion chamber ............ 57
5.1 Flow conditions for the non-reacting flow
calculations ......................................... 84
LIST OF FIGURES

1.1 Schematic of the 8-Ft high temperature tunnel .......... 3
1.2 The ring injector for the 8-Ft HTT ..................... 4
3.1 The three in-line cylindrical injectors ............ 17
3.2 Finite difference star for quadratic upstream-weighted scheme ....................... 42
4.1 Physical model for turbulent flow past heated cylinder ........................................ 48
4.2 A comparison of the calculated and measured pressure distribution on a circular cylinder in air flow at Re = 10^6 ........................................ 49
4.3 Local heat transfer coefficient from a circular cylinder to air .................................... 51
4.4 Physical model for non-reacting air flow past a pair of circular cylinders .................... 52
4.5 Velocity distribution about two cylinders spaced 1.58 cm apart .................................. 55
4.6 Schematic of a suddenly-expanded combustion chamber ............................................. 56
4.7 Flame structure for the fast chemistry model ..... 58
4.8 Flame structure for the one-step kinetics model.. 59
4.9 Flame structure for the two-step kinetics model... 60
4.10 Comparison of experimental data of gas temperature profile at an axial location of 9.5 cm with results from three combustion model ..... 62

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
4.11 Radial gas temperature profiles at axial
locations of 9.5 cm and 17.5 cm ................. 63

4.12 Radial gas temperature profiles at axial
locations of 24.6 cm and 32.7 cm ................. 64

4.13 Comparison of experimental data of the
center-line oxygen mole fraction with results
from three combustion models ...................... 65

4.14 Comparison of experimental data of the
center-line methane mole fraction with results
from three combustion models ...................... 67

4.15 Comparison of experimental data of the
center-line methane fraction with numerical
results ............................................. 68

4.16 Radial profiles of \( \text{CH}_4 \) at axial locations of
9.5 cm and 17.5 cm .................................. 69

4.17 Radial profiles of \( \text{CH}_4 \) at axial locations of
24.6 cm and 32.7 cm ................................ 70

4.18 Radial profiles of \( \text{O}_2 \) for various axial
locations ........................................... 71

4.19 Radial profiles of \( \text{CO}_2 \) at several axial
locations ............................................ 73

4.20 A comparison of the calculated and measured CO
mole fraction ....................................... 74

5.1 Typical grid for finite volume calculations ...... 77

5.2 Comparison of the center-line axial velocity
for non-reacting flow for two different grid
sizes ................................................... 79
5.3 Comparison of the center-line axial velocity for reacting flow for two different grid sizes.... 80

5.4 The calculated center-line temperature for two different grid sizes ......................... 81

5.5 The effect of grid refinement on the calculated surface temperature distribution .............. 82

5.6 The flow field for the non-reacting flow at time t = 0.005 s .................................. 85

5.7 The flow field for the non-reacting flow for time t = 0.01 s .................................. 86

5.8 The flow field for the non-reacting flow at time t = 0.05 s .................................. 87

5.9 The flow field for the non-reacting flow at time t = 0.06 s .................................. 88

5.10 The flow field for the non-reacting flow at time t = 0.08 s .................................. 89

5.11 The flow field for the non-reacting flow at time t = 0.1 s .................................. 90

5.12 The steady flow field for the non-reacting flow .. 91

5.13 Comparison of the pressure coefficient on the surface of the middle cylinder obtained from steady state and time dependent calculations ..... 92

5.14 Comparison of the steady state center-line velocity with the time dependent solution ........ 94

5.15 The steady state non-reacting flow field for fuel injection velocity of 60 m/s ............... 95

5.16 The steady state non-reacting flow field for fuel injection velocity of 100 m/s ............... 96
5.17 Flame structure for fast chemistry model ........ 98
5.18 Flame structure for one-step kinetics model ..... 99
5.19 Flame structure for two-step kinetics model ..... 100
5.20 The variation of the temperature along the surface of the middle cylinder ................. 101
5.21 Vertical variation of the combustion product temperature at an axial location of 6.11 cm ..... 103
5.22 Flame structure for 30 m/s fuel jet velocity .... 105
5.23 Flame structure for 60 m/s fuel jet velocity .... 106
5.24 Flame structure for 100 m/s fuel jet velocity ... 107
5.25 The flow field for 30 m/s fuel jet velocity ..... 108
5.26 The flow field for 60 m/s fuel jet velocity ..... 109
5.27 The flow field for 100 m/s fuel jet velocity .... 110
5.28 Comparison of the temperature on the surface of the middle cylinder for three fuel jet velocities. 111
5.29 Vertical variation of combustion products temperature at an axial location of 61.1 mm .... 112
5.30 Vertical variation of combustion products temperature at an axial location of 61.5 mm .... 113
5.31 Vertical variation of combustion products temperature at an axial location of 62.3 mm .... 114
5.32 Flame structure for fuel jet velocity of 150 m/s for one-step reaction ....................... 116
5.33 Flame structure for fuel jet velocity of 150 m/s for two-step reaction ....................... 117
5.34 The temperature variation on the surface of the middle cylinder for fuel jet velocity of 100 and 150 m/s ............................................. 118

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
5.35 Flame structure for the three ring injector using two-step chemical kinetic model and fuel jet velocity of 100 m/s .......................... 119

5.36 Flame structure for three fuel jet velocities . 121

5.37 Heat flux variation on the surface of the cylinder for fuel jet velocity of 30 m/s ....... 122

5.38 Heat flux variation on the surface of the cylinder for fuel jet velocity of 60 m/s ...... 123

5.39 Heat flux variation on the surface of the cylinder for fuel jet velocity of 100 m/s ...... 124

5.40 The surface temperature distribution for the solid injector for three fuel jet velocities ... 125

5.41 Comparison of the surface temperature prediction for the solid and ring injectors for fuel jet velocity of 30 m/s ............... 127

5.42 Comparison of the surface temperature prediction for the solid and ring injectors for fuel jet velocity of 60 m/s ............... 128

5.43 Comparison of the surface temperature prediction for the solid and ring injectors for fuel jet velocity of 100 m/s ............... 129

5.44 Heat flux variation for the solid fuel injector for fuel velocity of 30 m/s ................ 130

5.45 Heat flux variation for the solid fuel injector for fuel velocity of 60 m/s ................ 131

5.46 Heat flux variation for the solid fuel injector for fuel velocity of 100 m/s ............... 132

5.47 Flame structure for 60 m/s fuel jet velocity with LOX injection ......................... 133
5.48 The prediction of temperature on the surface of middle cylinder with and without enriched air.  

5.49 The flame structure for fuel jet velocity of 100 m/s and 3% air turbulent intensity 

5.50 The flame structure for fuel jet velocity of 100 m/s and 24% air turbulent intensity 

5.51 The prediction of the temperature on the surface of the middle cylinder for three air turbulent intensities 

5.52 The vertical temperature variation at an axial position of 6.11 cm for three air turbulent intensities 

5.53 Influence of far-field boundary conditions on the center-line velocity magnitude 

5.54 Influence of far-field boundary condition on center-line temperature distribution 

5.55 Influence of far-field boundary condition on flame structure (L = 20 cm)
LIST OF SYMBOLS

\( A \) = pre-exponential coefficient
\( a \) = constant in the specific heat
\( B \) = constant in combustion model
\( C_P \) = specific heat at constant pressure
\( C_1, C_2, C_\mu \) = constants in turbulence model
\( C_{R_l} \) = constant in combustion model
\( D \) = outside diameter
\( d \) = inside diameter
\( E \) = activation energy
\( g \) = square of fluctuation of concentration
\( G_k \) = generation of \( k \)
\( h \) = enthalpy
\( \delta h \) = enthalpy of formation
\( J \) = mass flux
\( K \) = molecular conductivity
\( k \) = kinetic energy of turbulence
\( K_t \) = turbulent conductivity
\( L \) = length scale of turbulence
\( M \) = molecular weight
\( m \) = mass fraction
\( m_0 \) = mass fraction at the oxidant inlet
\( P \) = pressure
\( Pr \) = Prandtl number
\( Pr_t \) = turbulent Prandtl number
\( R \) = gas constant
\( R \) = reaction rate
\( \bar{R} \) = universal gas constant

\( \text{Re} \) = Reynolds number

\( r \) = radial distance from axis of symmetry

\( \text{Sc} \) = Schmidt number

\( \text{Sc}_t \) = turbulent Schmidt number

\( S_{\Phi} \) = source or sink term of any variable

\( T \) = Temperature

\( t \) = time

\( u \) = axial velocity

\( v \) = vertical velocity

\( x \) = axial co-ordinate

\( y \) = vertical co-ordinate

Greek symbols

\( \Gamma \) = exchange coefficient

\( \gamma \) = dependent variable = \( \frac{m_{fu}}{\frac{m_{ox}}{2}} \)

\( \mu \) = molecular viscosity

\( \mu_t \) = turbulent viscosity

\( \rho \) = density

\( \epsilon \) = dissipation of energy

\( \Theta \) = mixture fraction

\( \Phi \) = general dependent variable

\( \delta_{ij} \) = Kronecker symbol

\( \psi \) = inert species

\( \alpha, \beta \) = concentration exponents

Subscripts

\( \text{eff} \) = effective

\( F \) = fuel stream

\( f_u \) = fuel
\( i,j \) = tensor notation
\( i,j \) = molecular species
\( k \) = reaction
\( 0 \) = oxidizer stream
\( ox \) = oxidant
\( pr \) = product
\( s \) = turbulent
Chapter 1

INTRODUCTION

There has been in recent years a renewed interest in hypersonic flows. The prime motivation for this activity is the goal to develop a hypersonic vehicle, designated as the National Aero-Space Plane (NASP), that is capable of taking-off from a conventional runway for its flight to outerspace [1,2]. The NASP has been the subject of many recent conceptual studies, and an important conclusion of these studies is that a significant portion of this vehicle will have to be designed using computational tools since ground-based test facilities do not exist for all the flight regimes encountered by the aircraft. These developments have thus created growing need for wind-tunnels for testing the aerodynamic and propulsion characteristics of the NASP under regimes ranging from subsonic to hypersonic.

One existing hypersonic test-facility at the NASA Langley Research Center, the Eight-Foot High Temperature Tunnel (HHT), is currently undergoing modifications to accommodate the testing of supersonic combustion engines for the proposed hypersonic aircraft [3]. This blow-down type wind-tunnel employs methane-air combustion to produce the tunnel test medium.

*The numbers in brackets indicate references.
In the modified configuration of the HTT, liquid oxygen (LOX) is injected in an annulus well ahead of the combustion chamber (Fig.1.1). The LOX injection is controlled to produce 20.95% percent oxygen concentration in the combustion products which is an important requirement for the testing of supersonic combustion engines in the tunnel. The modified HTT configuration will enable testing of hypersonic vehicles in a range of Mach numbers from four to seven.

The objective of this study is to solve a problem important to hypersonic research, and make a useful contribution to the field of combustor modeling using computational fluid dynamics. The present study has been undertaken due to the need to better understand the flow structure and temperature and concentration fields in the vicinity of the combustor in the Eight-Foot High Temperature Tunnel.

In the present configuration for the HTT combustor, a multi-ring fuel injector has been used to achieve a total temperature of 2000°C by burning methane fuel in air (Fig.1.2). Since LOX injection in the proposed configuration is likely to cause higher local temperature in the neighborhood of the fuel injector, accurate calculations of thermal load on the ring injector are essential if the fuel injector for safe operation is to be designed and operated for the LOX enriched mode. Since flow field characteristics downstream of the multi-ring injector are important in understanding the combustion phenomenon downstream of the fuel injector, a detailed calculation of flow, temperature, and concentration fields with and without LOX injection has been undertaken in this. In addition, the effects of different chemistry models on vortex stabilized diffusion flames are also analyzed.
Fig. 1.1 Schematic of the 8-Ft High Temperature Tunnel.
Fig. 1.2. The ring injector for the 8-Ft HTT.
A better understanding of fluid flow, heat transfer and turbulent combustion phenomenon should hopefully lead to fuel injector configurations that would sustain stable but lifted flames with acceptable thermal loads resulting from combustion of methane with enriched air.

The next chapter of this dissertation presents a comprehensive review of the previous work on turbulent flows with and without combustion. There has been considerable amount of work in this area, and as a result emphasis is given here to previous work directly related to the current problem. Chapter 3 introduces the general conservation equations and numerical solution procedure for solving the governing equations. The turbulence and chemical kinetics models in the present study are also discussed in some details.

Chapter 4 deals with the computer code validation. Results from the present computer code are compared with experimental and theoretical data available in the literature. Three different physical models considered for this purpose include calculation of turbulent flow and heat transfer characteristics of non-reactive flow around heated circular cylinder, computation of non-reactive flow between an array of two in-line circular cylinders, and calculation of diffusion flame, resulting from a step change geometry in the combustion chamber.

Chapter 5 discusses the current numerical results for the multi-cylinder fuel injector considered in the present study. Results for the effect of non-reactive fuel jet on air are presented first, followed by determination of the characteristics of a quasi-lifted diffusion flame as a function of fuel jet velocity, turbulence level and kinetic.
models. Finally, the effects of LOX injection on thermal load are presented. Chapter 6 concludes this study with some recommendations for future work.
Chapter 2

LITERATURE SURVEY

Simulation of combustion in general requires solution of a set of partial differential equations that mathematically describe the mass, momentum, energy and species transport processes. These coupled equations cannot be solved by conventional analytical procedures due to their non-linearity. As a result, the governing equations are generally solved numerically by employing finite difference, finite volume or finite element methods. The numerical solution is further complicated by vastly different characteristic times for physical processes such as turbulent diffusion and chemical reaction. The modeling of turbulence phenomenon is a difficult problem even in non-reactive flows due to the closure problem. This problem is further complicated by the need to model the interaction between chemistry and turbulence. The mean species production or consumption rate due to chemical reaction needs to be modeled properly to assess the effects of chemical reaction on flow field and vice-versa. Finally, the chemical reactions are quite complex, usually involving multi-step and multi-species chemical kinetics. For example, comprehensive modeling of methane-air combustion would require several dozen intermediate reactions and chemical species. This would certainly cause the cost of numerical modeling of combustion to be prohibitive. Other factors such as radiation, vortex shedding and complex geometrical features also cause the task of combustion modeling to be very challenging. In view of all
these complexities, there is a need to simplify and model the phenomenon in such a way that the problem becomes tractable mathematically without compromising the physics of the problem.

In this chapter, previous analytical and experimental studies in the area of turbulent combustion, with special emphasis on combustor modelling, are reviewed. Numerical and experimental studies in the area of non-reactive turbulent flow at high Reynolds number are considered first. Subsequently the literature on turbulent reactive flow is reviewed and summarized.

The current combustor geometry involves air flow between concentric cylindrical rings, with many small holes drilled in each ring for fuel discharge. The numerical study of air flow past a circular cylinder has a long history. The first study for steady flow past a circular cylinder was reported by Thom[4] for Reynolds number of 10 and 20. Since then a vast number of research efforts have been directed to this problem[5-8]. The comprehensive review of this problem has been given by Fornberg [8]. However, the difficulties involved in computing high Reynolds number flows has produced very few definite results. The flow field contains not only flow separation but also the phenomenon of vortex shedding. Recent development of faster and larger computers have made the computation of these complex flows possible[9-12]. Prominent among these, for Reynolds number in the range from $10^3$ to $10^6$, are the work of Kawamura and Kuwahara [10] and Ishii et al.[12]. Their results indicate that the flow in the supercritical regime are nearly steady, and the separation points shift leeward. Over the years, experimental studies have been carried out by various researches into the nature of vortex shedding from a cylinder in cross-flow regime.
Extensive reviews of this topic have been given by Cantwell[13]. Cantwell and Coles[14] made attempts in this direction when investigating the turbulent wake of a circular cylinder at a Reynolds number of 140,000. By using a flying hot-wire technique, they were able to obtain a series of phase-averaged streamline patterns for the far wake for each stage of vortex shedding. However, Cantwell's results provide very little information for the flow in the near field region where vortices are being formed.

One of the earliest investigation of fluid flow between two cylinders is that of Spivack[15]. His experimental results show that for Reynolds number less than $1.5 \times 10^4$, a non-linear relationship between frequency and velocity indicates a transition in the state of the flow. Above a critical spacing between the cylinders equal to the diameter, the cylinders behaved independently. Zdravkovich[16] critically reviewed investigations in this category and noted that one of the most neglected features of the interference flow was the measurements of vortex shedding from two cylinders in staggered arrangement. Data available to Zdravkovich[16], were those by Hori[17], Ishigai et al.[18,19], Bearman et al.[20], and Okajima[21]. Recently, Kiya et al. [22] investigated experimentally the frequency of vortex shedding from two circular cylinders of the same diameter, in staggered arrangements, at a Reynolds number of $1.58 \times 10^4$. For the side by side arrangement, the most prominent feature shown in their study is that when the non-dimensional spacing exists in the range of 1.4 to 2.0. The gap flow between the cylinders is biased to one side and bistable in nature. When the spacing is less than 1.4, the gap flow between the cylinders becomes very weak and as a result the pair of the cylinders behave as if there is no gap flow. For all transverse spacings greater than two times the diameter, there exists a single frequency in both
wakes which, when reduced to the Strouhal number, approximately the same as for the single cylinder.

Heat transfer between the fluid and a cylinder in cross flow has been the subject of both applied and fundamental studies for many years. The earliest studies of heat transfer were performed in air [23-25]. Recent advances in computational modeling are making it feasible to obtain solution to the heat transfer problem numerically for the whole circumference of a cylinder. So far, satisfactory results have been achieved only for low values of Reynolds number [26]. On the front part of the cylinder, up to the separation point of a laminar boundary layer, the heat transfer can be determined by either approximate or exact analytical techniques[27]. At higher values of Reynolds number, heat transfer gradually increases downstream of the laminar boundary layer separation point and is mainly determined experimentally[28]. Among the earliest contributions to the development of the theory of turbulent heat transfer were those of Giedt[29], Kestin[30], and Lowery[31]. They analyzed the subcritical flow of air in a wide range of Reynold number. Dyban and Epick[32] have measured local heat transfer at different levels of free-stream turbulence, and Hanson and Richardson[33] have investigated the near wake region using a single wire probe. Recently Žukauskas and Ziugzda[34] studied the effect of turbulence level on heat transfer from a cylinder in cross flow. Their results indicate that a higher turbulence level causes heat transfer augmentation on the front part of the cylinder.

Both the heat transfer and the fluid dynamics are highly dependent on blockage factor in the channel in which the cylinders are fitted. The current 8-Ft. HTT fuel injector has concentric rings which cause blockage of air flow through the
spacing between the rings. There are only few experimental and analytical studies of the blockage factor effects reported in the literature [34,35]. The study by Žukauskas [34] covers Reynolds number from $5 \times 10^4$ to $4 \times 10^6$, and it was carried out with water flow. Several studies suggest a close connection between heat transfer and the processes of vortex formation and vortex shedding. Experiments in this area employed auxiliary cylinders and splitter plates to eliminate regular vortex shedding [36,37]. The manner of vortex shedding had a significant effect on the heat transfer from the cylinder, especially in the leeward region of the cylinder.

Despite the rapid advances made in computer technology, a direct solution of the conservation equations for turbulent flows is currently not feasible. Most engineering calculations involve solution of time-averaged conservation equations. This introduces higher order fluctuation terms, and as a result a closure of turbulent flow equations is required.

A survey of the mean-turbulence-field closure models by Mellor and Herring [38] gives an excellent discussion of what has been achieved in the mathematical modelling of turbulence. Different classes of turbulence models have been developed, among these are: Prandtl's mixing-length model [39], the one-differential-equation models of Prandtl [40], Bradshaw, Ferriss and Atwell [41] and Nee and Kovasznay [42], the two-differential-equation models of Kolmogorov [43], Marlow and Nakayama [44], Spalding [45], and Jones and Launder [46], and the more complex models of Chou [47], Kolovandin and Vatutin [48], and Hanjalic and Launder [49].

Several investigators have reviewed current turbulence models and have made recommendations concerning their use [50-53]. Spalding [54] has presented a discussion of solved and unsolved problems in turbulence modeling. He focuses on the $k-\varepsilon$ model and discusses its advantages and shortcomings. A recent
study by Nikjooy and So [55] recommends use of k-ε turbulence model for combustor modeling.

Turbulent diffusion flames occur widely in combustors and as a consequence, knowledge of their physical characteristics is important in design and operation of combustors. Topics related to jet diffusion flames have been widely investigated. The stability and the structure of the turbulent diffusion flame in still air have received some attention in the past[56-58]. The stability of flames of co-flowing streams of hydrogen and air has been studied by Vranos et al. [59]. Takeno and Kotani[60] have conducted similar experiments, but with the aim of understanding the effect of the temperature of the air stream on the stability of the flames. Baev and Yasakov[61] and Annushkin and Severdlov[62] have published papers that concentrate on the blow-out stability characteristics of diffusion flames. Extensive experimental data are presented by Kalaghatgi[63] who gives the blow-out speed for various fuels for a range of nozzle diameters. Almost all previous investigations have considered a single jet diffusion flame, and a majority of these studies are experimental in nature.

In many combustion problems the kinetic mechanisms determine the characteristic space and time scales over which the governing equations must be solved. Kinetic information is generally provided either by a detailed mechanism which attempts to describe the chemistry in a reacting environment on a microscopic or molecular level and which consists of a number of elementary kinetic steps which occur in an overlapping manner. However, for combustion of hydrocarbon fuels usually a large number of species are involved, and thus correspondingly a large number of differential equations, are required for a detailed kinetic representation. In addition, the specific rate constants of the elementary reactions and the
elementary reaction themselves, as currently reported in the literature, are not necessarily well documented for all temperature conditions and thus can be a source of large error.

Despite the emergence of a number of detailed schemes for hydrocarbon combustion [64-67], the use of schemes with smaller number of reactions, capable of accurately describing major flame features, is of considerable importance for many practical problems in the field of combustion. The realistic simulation of kinetics with large number of intermediate reactions and species would require prohibitively large computational time despite rapid advancement in the state of the art of computation. One of the important applications of global reaction schemes is to turbulent combustion, where the fluctuating nature of turbulent flow and the associated turbulence-chemistry interaction introduces severe additional modelling difficulties, as discussed by Libby and Williams [68], and Jones and Whitelaw [69]. In this case, the major problem is caused by the strong non-linearity of typical reaction rate expressions and the need to evaluate the mean time average values in turbulent flows.

A number of investigators, including Dryer and Glassman [70], Westbrook and Dryer [71], Hautman et al. [72], Coffee et al. [73], Eldemann and Fortune [74], Duteque et al. [75], Westbrook and Dryer [76], Paczko et al. [77], Peters and Kee [78], and Jones and Lindstedt [79], have proposed global or quasi-global reaction schemes optimized for a particular combustion model.

Various approaches have been used to account for the effect of mixture inhomogeneity on the rate of combustion in mathematical modeling of turbulent combustion. In the approach taken by Mason and Spalding [80], the local chemical reaction rate is related solely to the local turbulent state, by considering the local fluctuation of fuel mass fraction and a
characteristic time for the breakup of turbulent eddies. Other workers have introduced the joint probability distribution function (pdf) of associated independent variables which may be used in alternative forms to predict features of different type of turbulent flames\[81-83\]. Prediction based on models of pdf, when applied in their most sophisticated forms, call for significantly more complicated mathematical treatment than predictions based on the eddy-break-up model\[84\]. Although, both methods seem to give good predictions in some turbulent combustion problems\[84\], neither of the methods seem to have achieved a break-through by being generally applicable to both premixed and diffusion flames.

Historically, two principal modeling approaches has been used for combustion processes. At one extreme end, chemical kinetics is assumed to be rate controlling and turbulent mixing is considered unimportant \[85,86\]. At the other end of the spectrum, turbulent mixing is treated in detailed, but infinite rate chemistry is assumed\[87\]. Only a few attempts have combined the treatment of finite rate chemistry and detailed turbulent mixing \[88-90\].

The literature survey clearly indicates that most of the previous numerical studies on turbulent subsonic combustion have considered only simple geometry due to the complexity of the problem. The present injector geometry, with fuel jets issuing out of cylindrical injector, has not been analyzed even for the non-reacting case. The prediction of thermal load and flame lift-off distance requires that combustion calculation be carried out by analyzing the conjugate problem which involves simultaneous consideration of heat convection (outside the cylinders) and heat conduction (inside the
cylinders). In addition, the flame lift-off phenomenon will require consideration of both kinetic and diffusion mechanisms. The review of literature reveals that such a problem has not been analyzed. As a result, this problem has been investigated in this study to make contributions to the existing literature. Specifically, we have analyzed the effects of the factors that govern the combustion phenomenon and attendant flame structure and thermal load on methane fuel injector with complex geometry. The details of fuel injector geometry, physical model, governing equations and numerical methodology are described in the next chapter.
Chapter 3

GOVERNING EQUATIONS

The purpose of this chapter is to outline the conservation equations, the chemistry models and the numerical integration methodology used in this study. The equations to be used are for the conservation of mass, momentum, energy and species. These equations govern the chemically reacting flow in two-dimensions. The geometrical features of the models considered here result in large turbulent recirculating regions, and as a result the conservation equations in elliptic form have been used to predict the flow features.

3.1 Physical Model

As stated earlier, the spray bar for the 8-FT HTT has 15 rings, as shown in Fig.1.1. Some of these rings are active while others have been made inactive by plugging in the holes in them. In order to understand the physical phenomenon, and to economize on computational time, a two-dimensional model, employing three in-line cylindrical injectors, was adopted for analysis (Fig.3.1). In order to isolate these three rings from other rings, the symmetry boundary conditions are applied on the axes of symmetry of the first and the third cylinder. However, we note that flow symmetry or asymmetry is not assumed apriori for the middle cylinder, and this condition is predicted as part of the solution procedure.
Fig. 3.1 The three in-line cylindrical injectors.
3.2 Basic Conservation Equations

The equations representing the conservation of mass and momentum in cartesian coordinates assume the following form when written in tensor notation:

\[
\text{Mass Conservation: } \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0 \quad (3.2)
\]

\[
\text{Momentum Conservation: } \quad \frac{\partial}{\partial t} (\rho u_j) + \frac{\partial}{\partial x_i} (\rho u_i u_j) =
\]

\[
\frac{\partial}{\partial x_i} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] - \frac{\partial p}{\partial x_j} \quad (3.3)
\]

The above equations are the unsteady Navier-Stokes equations. The velocity components are the instantaneous ones, and \( \mu \) is the molecular viscosity of the fluid mixture. The need for turbulence modeling was pointed out at the beginning of this chapter. The use of time-averaged equations and the turbulence model adopted in the present study are justified and explained in the next section.

3.3 Turbulence Modelling

The unsteady Navier-Stokes equations are generally considered to be valid for turbulent flows in the continuum regime. However, the complexity and random nature of turbulent motion has made exact analytical solutions of the Navier-Stokes
equations difficult to achieve. Despite major advances in computer technology, computer simulations based the Navier-Stokes equations are beyond the capability of present day computers for most practical problems. This is due to extremely large numbers of grid points that will be required to resolve all time and length scales of turbulent motions. Although several turbulence models of increasing complexities have been proposed, none of them appear to have all the desirable features for modeling of turbulent combustion flows. Sophisticated models of turbulence, incorporating better physical modeling, generally require substantially higher computational efforts.

In turbulent flows, the velocity at a point is considered as a sum of the mean (time-averaged) and the fluctuating components:

$$u_i = \bar{u}_i + u'_i$$  \hspace{1cm} (3.4)

Substitution of Eq.(3.4) into Eqs.(3.2) and (3.3) yields the time-average momentum equations,

$$\frac{\partial}{\partial t} (\rho u_j) + \frac{\partial}{\partial x_i} (\rho u_i u_j) =$$

$$\frac{\partial}{\partial x_i} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] - \frac{\partial \rho}{\partial x_j} + \frac{\partial}{\partial x_i} (-\rho u'_i u'_j)$$  \hspace{1cm} (3.5)

Equation (3.5) has the same form as the fundamental momentum equation (3.3) with velocities now representing time-averaged (or mean-flow) values and the effect of turbulence incorporated through the "Reynolds stresses", $-\rho u'_i u'_j$. 

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
In having to decide on a turbulence model for the present study, we are faced with a familiar dilemma. Should we use a simple model such as the turbulent kinetic energy \((k)\)-dissipation\((\epsilon)\) model, or should we pursue more sophisticated, and complex but not fully tested models such as the Reynolds stress models? It is felt here that the added complexities of a Reynolds stress transport model are unwarranted in view of the fact that these models are still under development. Also their use would increase computational effort considerably. In view of these facts, and the fact that the \((k-\epsilon)\) model has been successfully used in recent years by several researchers for turbulent combustion flows, we have decided to adopt it as the turbulence model in the present study. Choice of this model represents a reasonable balance between requirements of moderate computational efforts and the ability of the model to predict physical phenomena.

The standard \(k-\epsilon\) model relates the individual Reynolds stresses to the mean-flow gradients with the eddy viscosity,

\[-\rho \overline{u'_i u'_j} = -\frac{2}{3} \rho k \frac{\partial u_j}{\partial x_i} + \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)\]  \hspace{1cm} (3.6)

where \(\mu_t\) is the turbulent viscosity and \(k\) is the kinetic energy of turbulence

\[k = \frac{1}{2} \overline{u'_i u'_i}\]  \hspace{1cm} (3.7)
The turbulent viscosity $\mu_t$ is related in the following manner to the two parameters characterizing the local state of turbulence in the $k-\epsilon$ model namely the turbulent kinetic energy $k$ and the dissipation rate $\epsilon$:

$$
\mu_t = \rho \sigma_{\mu} \frac{k^2}{\epsilon} \quad (3.8)
$$

The variations of the turbulence parameters $k$ and $\epsilon$ over the flow field are determined from the following semi-empirical transport equations [91]

$$
\frac{\partial}{\partial t} ( \rho k ) + \frac{\partial}{\partial x_i} ( \rho u_i k ) = 
\frac{\partial}{\partial x_i} \left[ \left( \frac{\mu_1}{\sigma_k} + \mu \right) \frac{\partial k}{\partial x_i} \right] + G_k - \rho \epsilon \quad (3.9)
$$

$$
\frac{\partial}{\partial t} ( \rho \epsilon ) + \frac{\partial}{\partial x_i} ( \rho u_i \epsilon ) = 
\frac{\partial}{\partial x_i} \left[ \left( \frac{\mu_1}{\sigma_\epsilon} + \mu \right) \frac{\partial \epsilon}{\partial x_i} \right] + C_1 \frac{\epsilon}{k} G_k - C_2 \rho \frac{\epsilon^2}{k} \quad (3.10)
$$

where $C_1$, $C_2$, $\sigma_k$, and $\sigma_\epsilon$ are empirical constants and their values used for the present calculations are compiled in Table 3.1 and are identical to those of [54].
Table 3.1 Turbulence model constants

<table>
<thead>
<tr>
<th>constant</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1$</td>
<td>1.44</td>
</tr>
<tr>
<td>$C_2$</td>
<td>1.92</td>
</tr>
<tr>
<td>$C_\mu$</td>
<td>0.09</td>
</tr>
<tr>
<td>$\sigma_k$</td>
<td>1.00</td>
</tr>
<tr>
<td>$\sigma_\epsilon$</td>
<td>1.30</td>
</tr>
</tbody>
</table>
and the quantity $G_k$, the generation of $k$, is given by

$$G_k = \mu_t \left[ 2 \left\{ \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 \right\} + \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 \right] \quad (3.11)$$

### 3.4 Energy Equation

The energy equation in the form of a transport equation for enthalpy $h$ is written as:

$$\frac{\partial}{\partial t} \left( \rho h \right) + \frac{\partial}{\partial x_i} \left( \rho u_i h \right) =$$

$$\frac{\partial}{\partial x_i} \left[ \left( K + K_t \right) \frac{\partial T}{\partial x_i} \right] - \frac{\partial}{\partial x_i} \left( h_j J_{ji} \right) + S_h \quad (3.12)$$

where the pressure work and viscous dissipation terms are neglected. The symbol $K$ is the molecular conductivity, $K_t$ is the turbulent conductivity due to turbulent transport

$$K_t = \frac{h_i c_p}{Pr_t} \quad (3.13)$$

and $h_j$ is the enthalpy of species $j$. The symbol $J_{ji}$ is the flux of species $j$ in the $i$th direction, and $S_h$ is the enthalpy source due to chemical reaction,
where \( h_j^\circ \) is the enthalpy of formation of species \( j \) and \( R_j \) is the volumetric rate of creation of species \( j \) due to chemical reaction.

The mixture enthalpy \( h \), is defined as

\[
h = \sum_j m_j h_j \tag{3.15}
\]

where

\[
h_j = \int_{T_0}^T C_{p,j} \, dT \tag{3.16}
\]

and \( m_j \) is the mass fraction of species \( j \). The specific heat of species \( j \) at constant pressure is expressed by the symbol \( C_{p,j} \).

The heat flux term in Eq. (3.12) can be recast as

\[
K \frac{\partial T}{\partial x_i} = \frac{K}{C_p} \left( \frac{\partial h}{\partial x_i} - \sum_j h_j \frac{\partial m_j}{\partial x_i} \right) \tag{3.17}
\]
where \( C_p \) is the mixture heat capacity, defined as

\[
C_p = \sum_j m_j C_{p,i}
\]  

(3.18)

Substitution of Eq.(3.17) into Eq.(3.12) yields the energy equation in the following form:

\[
\frac{\partial}{\partial t} (\rho h) + \frac{\partial}{\partial x_i} (\rho u_i h) =
\]

\[
\frac{\partial}{\partial x_i} \left( \frac{K}{C_p} + \frac{\mu_i}{\rho r_i} \right) \left( \frac{\partial h}{\partial x_i} - \sum_j h_j \frac{\partial m_j}{\partial x_i} \right)
\]

\[- \frac{\partial}{\partial x_i} \sum_j h_j J_{ji} + S_h
\]

(3.19)

For turbulent flows, the diffusion flux \( J_i \) of species \( j \) is represented by

\[
J_i = - \left( \frac{\mu}{Sc} + \frac{\mu_i}{Sc_i} \right) \frac{\partial m_j}{\partial x_i}
\]

(3.20)

where \( Sc \) and \( Sc_i \) are the molecular Schmidt number and the turbulent Schmidt number respectively. Substitution of Eq.(3.20) into Eq.(3.19) yield the energy equation in the following form:
By assuming that the molecular diffusivities for all species and for heat transfer as equal, Eq. (3.21) can be reduced to the following form:

\[
\frac{\partial}{\partial t} (\rho h) + \frac{\partial}{\partial x_i} (\rho u_i h) = \frac{\partial}{\partial x_i} \left[ \left( \frac{K}{C_p} + \frac{\mu_i}{P_r_i} \right) \frac{\partial h}{\partial x_i} \right] - \frac{\partial}{\partial x_i} \left[ \left( \frac{K}{C_p} + \frac{\mu_i}{P_r_i} \right) \sum_j h_j \frac{\partial m_j}{\partial x_i} \right] + \frac{\partial}{\partial x_i} \left[ \left( \frac{\mu}{S_C} + \frac{\mu_i}{S_{C_i}} \right) \sum_j h_j \frac{\partial m_j}{\partial x_i} \right] + S_h
\]  

(3.21)

By assuming that the molecular diffusivities for all species and for heat transfer as equal, Eq. (3.21) can be reduced to the following form:

\[
\frac{\partial}{\partial t} (\rho h) + \frac{\partial}{\partial x_i} (\rho u_i h) = \frac{\partial}{\partial x_i} \left[ \left( \frac{K}{C_p} + \frac{\mu_i}{P_r_i} \right) \frac{\partial h}{\partial x_i} \right] + S_h
\]  

(3.22)

3.5 Mass Transport Equations

The conservation equations for the transport of species takes the following form:

\[
\frac{\partial}{\partial t} (\rho m_i) + \frac{\partial}{\partial x_i} (\rho u_i m_i) = \frac{\partial}{\partial x_i} \left( \frac{\mu}{S_C} + \frac{\mu_i}{S_{C_i}} \frac{\partial m_i}{\partial x_i} \right) + R_i
\]  

(3.23)

where \( m_i \) is the mass fraction of chemical species \( i \), and \( R_i \) is the mass rate of creation or depletion by chemical reaction.
3.6 Combustion Models

The source of chemical species \( i \) due to reaction, \( R_i \), in Eq. (3.23) is computed as the sum of the reaction sources over the \( k \) reactions that the species may participate in, i.e.,

\[
R_i = \sum_k R_{ik}
\]  

(3.24)

For a chemically-inert species \( R_i \), by definition, is zero.

The calculation of reaction rates \( R_i \) is the principal source of difficulty particularly when considering turbulent flows. First of all, combustion is a process in which many species and reactions are involved. A detailed description of the combustion process requires the knowledge of all the intermediate species and the intermediate reaction steps. However, only for single hydrocarbon fuels reaction schemes are available in the literature, and even for these simple fuels, the number of species and reactions to be considered in the combustion process is too large for presently available computer resources. Also, there are physical situations where the great amount of data generated by a detailed chemical reaction mechanism is not warranted and a global mechanism will suffice. This global reaction is often a convenient way of approximating the effects of the many elementary reactions which actually occur. The instantaneous consumption rate of fuel, \( R_{fu} \), for the single step (global)
reaction is usually represented by the Arrhenius equation [70]

\[ R_{fu} = A \rho^2 \left[ m_{fu} \right]^{\alpha} \left[ m_{ox} \right]^{\beta} \exp \left( -\frac{E}{RT} \right) \quad (3.25) \]

Where \( m_{fu} \) and \( m_{ox} \) are the instantaneous mass fractions of the fuel and the oxidizer respectively, \( E \) is the activation energy, \( A \) is the pre-exponential rate, \( \alpha \) and \( \beta \) are the concentration exponents. For laminar flows the above equation will suffice in many physical situations. However, for turbulent flows, the effect of turbulence on the combustion process and consequently on reaction rates must be accounted for. In turbulent flows, properties such as concentrations and temperature fluctuate in space and time. In order to obtain a time-mean reaction rate, the time-averaging on highly non-linear Arrhenius equation will be required. Four different approaches have been used to model the effect of turbulence on the rate of combustion.

1. In this simplest approach, \( \bar{R} \), the time-mean rate of formation, is calculated from the time-mean variables. This is done by simply substituting mean values of concentration and temperature in Eq. (3.25). As shown by Spalding [93], this method does not yield good results, since the effects of the fluctuation components in form of higher order correlations, are not considered.

2. In the moment closure approach [55], the mean formation rate \( \bar{R} \) is obtained by applying the Reynolds decomposition with appropriate simplifications. This results in a large number of higher order correlations such as \( \bar{m} \bar{i} m_{ij} \), \( \bar{\rho} \bar{i} m_{ij} \), \( \bar{T} \bar{i} m_{ij} \), etc. which requires large number of equations for
these variables. This approach causes difficulty in modeling since usually a large number of extra varaibles need to be included for proper physical modeling.

3. This third category of models are based on a statistical description of fluctuations of the mixture fraction and this approach in the literature is known as the probability density function (pdf) approach[81]. Predictions based on this approach, when applied in their most sophisticated forms, call for significantly more complicated mathematical treatment and tremendous computational cost, since extra transport equations governing the pdf and other variables related to mixture fraction would be required [81].

4. In the fourth approach, based on heuristic ground, the rate of reaction is assumed to be controlled by the rate of break up of fuel eddies from large size to the molecular level where the chemical reaction occurs (eddy-break-up model). This method is simple, and it gives good predictions in many turbulent combustion problems[85].

In the present study, the reaction rate $R_i$ is controlled either by an Arrhenius kinetic rate expression, or by the mixing of the turbulent eddies containing fluctuating species concentrations (eddy-break-up model) depending whether the reaction is locally diffusion or kinetically controlled. Three levels of complexity for simulating the chemical kinetics are considered:
**Single-Step Kinetics**

In this model, one step chemical kinetic reaction mechanism for methane combustion is represented by [70]

$$\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} \quad (3.26)$$

An important consequence of the simple chemical reaction assumption is that the mass rates of creation by chemical reaction of fuel and oxidant $R_{fu}$ and $R_{ox}$ are related through

$$R_{fu} = \frac{1}{2} R_{ox} \quad (3.27)$$

We note here that the single step model will not be able to predict the concentration of carbon monoxide which may be an important parameter in certain applications.

Combining Eqs. (3.27) and (3.23), a source-free equation having a single dependent variable $\theta$ (mixture fraction) is obtained [55] (see Appendix A)

$$\frac{\partial}{\partial t} (\rho \theta) + \frac{\partial}{\partial x_i} (\rho u_i \theta) = \frac{\partial}{\partial x_i} \left[ \left( \frac{\mu}{\text{Sc}} + \frac{\mu_l}{\text{Sc}_l} \right) \frac{\partial \theta}{\partial x_i} \right] \quad (3.28)$$

The mixture fraction $\theta$ is defined as

$$\theta = \frac{(\gamma - \gamma_o)}{(\gamma_F - \gamma_o)} \quad (3.29)$$
where $\gamma$ is given by

$$\gamma = m_{fu} - \frac{m_{pr}}{2} = m_{fu} + \frac{m_{pr}}{3}$$  \hspace{1cm} (3.30)$$

where $m_{pr}$ is the mass fraction of the product, and subscripts $P$ and $O$ stand for fuel and oxidant stream, respectively.

Thus, for one-step kinetic reaction there are five species, namely, CO$_2$, O$_2$, N$_2$, H$_2$O and CH$_4$ participating in the combustion phenomenon. Another equation for the fuel fraction $m_{fu}$ is written as

$$\frac{\partial}{\partial t} \left( \rho m_{fu} \right) + \frac{\partial}{\partial x_i} \left( \rho u_i m_{fu} \right) = \frac{\partial}{\partial x_i} \left[ \left( \frac{\mu}{S_{C_2}} + \frac{\mu_l}{S_{C_1}} \right) \frac{\partial m_{fu}}{\partial x_i} \right] + R_{fu}$$  \hspace{1cm} (3.31)

Four additional algebraic equation can be obtained from stoichiometric relations (see Appendix A).

The reaction rate $R_{fu}$ is controlled either by an Arrhenius expression Eq.(3.25), or by the mixing of the turbulent eddies containing fluctuating species concentration, depending on whether the reaction is locally kinetically or diffusion controlled. The eddy break-up model of Spalding [94] can be written as

$$R_{fu} = C_{RI} \rho g^{1/2} \frac{\varepsilon}{k}$$  \hspace{1cm} (3.32)

where $C_{RI}$ is an empirical constant, and $g$ represents the local mean-square concentration fluctuation and is represented by
\[ g^{1/2} = \min \left( m_{f_u}, \frac{m_{f_u}}{2}, \frac{B}{3} m_{pr} \right) \]  \hspace{1cm} (3.33)

where B is an empirical constant.

For turbulent flows, the reaction rate is given by [94]

\[ R_{f_u} = \min \left[ C_{R1} \rho g^{1/2} \frac{\varepsilon}{K}, A \rho^2 \left[ m_{f_u} \right]^\alpha \left[ m_{ex} \right]^\beta \exp \left( -\frac{E}{RT} \right) \right] \]  \hspace{1cm} (3.34)

Two-Step Reaction Model

The one-step reaction model, may be replaced by a more sophisticated kinetics model which allows for prediction of local mass fraction of carbon monoxide. The two-step model for methane, is represented by [76]

\[ \text{CH}_4 + \frac{3}{2} \text{O}_2 \rightarrow \text{CO} + 2\text{H}_2\text{O} \]  \hspace{1cm} (3.35)

\[ \text{CO} + \frac{1}{2} \text{O}_2 \rightarrow \text{CO}_2 \]  \hspace{1cm} (3.36)

There are six species (CH4, O2, CO2, CO, H2O and N2) involved in this model which have to be determined. Three properties, namely mixture fraction \( \theta \), mass fraction of fuel \( m_{\text{CH}_4} \), and mass fraction of carbon monoxide \( m_{\text{CO}} \), are obtained from three differential equations similar to Eqs.(3.25) and (3.26). Three additional algebraic equations are obtained from the stoichiometric relations (see Appendix A).
The reaction rate of the fuel $R_f$, is obtained from Eq. (3.34). The reaction rate for carbon monoxide, $R_\text{e}$, is obtained from equation similar to Eq. (3.6-11).

**Diffusion-Controlled Combustion (Fast Chemistry)**

When the reaction rate is infinite, the physical variables in combustion process approach equilibrium values very quickly. Since chemical kinetics need not be considered under this assumption, the complete chemical state can be determined from the local thermodynamic state, and solution of only one source-free conservation equation for the mixture fraction $\Theta$. Once the $\Theta$-equation, has been solved, the mass fractions of the other species are obtained from algebraic equations (see Appendix A).

### 3.7 Calculation of Physical Properties

The density is computed based on the ideal gas law as

$$
\rho = \frac{P}{\bar{R} T \sum_i \frac{m_i}{M_i}} 
$$

(3.37)

where $\bar{R}$ is the universal gas constant, $M_i$ is the molecular weight of species $i$ and $P$ is the operating pressure.

The specific heat is defined as a function of temperature using polynomial fit as follows:
\[ C_p = a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4 \]  (3.38)

The thermal conductivity and the laminar viscosity of the mixture are also defined by equations similar to Eq.(3.38). The constants for the polynomials for the specific heat, thermal conductivity and laminar viscosity are given in Table 3.6.

### 3.8 General Form of the Governing Differential Equations

The governing partial differential equations for the conservation of mass, momentum, energy and chemical species, are rearranged into a general form which can be written as:

\[
\frac{\partial}{\partial t} (\rho \Phi) + \frac{\partial}{\partial x_i} (\rho u_i \Phi) = \frac{\partial}{\partial x_i} (\Gamma_{\Phi} \frac{\partial \Phi}{\partial x_i}) + S_{\Phi} \]  (3.39)

The corresponding values for \( \Phi, \Gamma_{\Phi} \) and \( S_{\Phi} \) are indicated in Table 3.2. The constants in the turbulence model are given in Table 3.1, and the chemical kinetics data for fast, one-step and two-step kinetics models are given in Tables 3.3, 3.4 and 3.5.
Table 3.2 Conservation equations corresponding to equation (3.7-1)

<table>
<thead>
<tr>
<th>Conservation of</th>
<th>$\Phi$</th>
<th>$\Gamma$</th>
<th>$S_\Phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>X-Momentum</td>
<td>$u$</td>
<td>$\mu + \mu_t$</td>
<td>$\frac{\partial}{\partial x}(\mu_{eff} \frac{\partial u}{\partial x}) + \frac{\partial}{\partial y}(\mu_{eff} \frac{\partial v}{\partial x})$ $- \frac{\partial P}{\partial x} - \frac{3}{2} \rho K$</td>
</tr>
<tr>
<td>Y-Momentum</td>
<td>$v$</td>
<td>$\mu + \mu_t$</td>
<td>$\frac{\partial}{\partial x}(\mu_{eff} \frac{\partial u}{\partial y}) + \frac{\partial}{\partial y}(\mu_{eff} \frac{\partial v}{\partial y})$ $- \frac{\partial P}{\partial y} - \frac{3}{2} \rho K$</td>
</tr>
<tr>
<td>K-Transport</td>
<td>$K$</td>
<td>$\mu + \frac{\mu_t}{\sigma_k}$</td>
<td>$G_k - \rho \epsilon$</td>
</tr>
<tr>
<td>$\epsilon$-Transport</td>
<td>$\epsilon$</td>
<td>$\mu + \frac{\mu_t}{\sigma_\epsilon}$</td>
<td>$G_k \frac{\epsilon}{K} - C_2 \rho K$</td>
</tr>
<tr>
<td>Enthalpy</td>
<td>$h$</td>
<td>$\frac{K}{C_p} + \frac{\mu_t}{Pr_t} \sum_j \frac{\partial}{\partial x} R_j$</td>
<td></td>
</tr>
<tr>
<td>Mixture Fraction</td>
<td>$\Theta$</td>
<td>$\left( \frac{\mu}{Sc} + \frac{\mu_t}{Sc_t} \right)$</td>
<td>0</td>
</tr>
<tr>
<td>Mass Fraction</td>
<td>$m_{fu}$</td>
<td>$\left( \frac{\mu}{Sc} + \frac{\mu_t}{Sc_t} \right)$</td>
<td>$R_{fu}$</td>
</tr>
<tr>
<td>Mass Fraction</td>
<td>$m_{co}$</td>
<td>$\left( \frac{\mu}{Sc} + \frac{\mu_t}{Sc_t} \right)$</td>
<td>$R_{co} - \frac{28}{16} R_{fu}$</td>
</tr>
</tbody>
</table>
Table 3.3 Chemical kinetics data for fast and one step reactions [70]

<table>
<thead>
<tr>
<th>Constant</th>
<th>Fast Chemistry</th>
<th>One-step model</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$, $\frac{\text{Kg}}{\text{m}^3 \cdot \text{sec.}}$</td>
<td>$1. \times 10^{15}$</td>
<td>$1.6 \times 10^{17}$</td>
</tr>
<tr>
<td>$E$, $\frac{J}{\text{Kg} \cdot \text{mol}}$</td>
<td>100</td>
<td>$2.02312 \times 10^{8}$</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>1</td>
<td>0.7</td>
</tr>
<tr>
<td>$\beta$</td>
<td>1</td>
<td>0.8</td>
</tr>
<tr>
<td>$C_{R1}$</td>
<td>4.0</td>
<td>4.0</td>
</tr>
<tr>
<td>$B$</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>Constant</td>
<td>$R_{ju}$, $\frac{Kg}{m^3 \cdot sec.}$</td>
<td>$R_{co}$, $\frac{Kg}{m^3 \cdot sec.}$</td>
</tr>
<tr>
<td>----------</td>
<td>---------------------------------</td>
<td>---------------------------------</td>
</tr>
<tr>
<td>$A$, $\frac{Kg}{m^3 \cdot sec.}$</td>
<td>$5.28 \times 10^15$</td>
<td>$1.68 \times 10^{10}$</td>
</tr>
<tr>
<td>$E$, $\frac{J}{Kg \cdot mol}$</td>
<td>$2.2403 \times 10^8$</td>
<td>$1.03716 \times 10^8$</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>$0.5$</td>
<td>$1.0$</td>
</tr>
<tr>
<td>$\beta$</td>
<td>$1.0$</td>
<td>$1.0$</td>
</tr>
<tr>
<td>$C_{R1}$</td>
<td>$4.0$</td>
<td>$4.0$</td>
</tr>
<tr>
<td>$B$</td>
<td>$0.5$</td>
<td>$0.5$</td>
</tr>
</tbody>
</table>
Table 3.5 Enthalpy of formation for different species (T_o=298 k)

<table>
<thead>
<tr>
<th>Species</th>
<th>( \Delta_h^o ) J Kg-mol</th>
<th>( \Delta_s^o ) J Kg-mol</th>
</tr>
</thead>
<tbody>
<tr>
<td>CIH_4</td>
<td>-0.7489 E+8</td>
<td></td>
</tr>
<tr>
<td>CO</td>
<td>-1.1044 E+8</td>
<td></td>
</tr>
<tr>
<td>CO_2</td>
<td>-3.9369 E+8</td>
<td></td>
</tr>
<tr>
<td>H_2O</td>
<td>-2.4195 E+8</td>
<td></td>
</tr>
<tr>
<td>O_2</td>
<td>0.0</td>
<td></td>
</tr>
<tr>
<td>N_2</td>
<td>0.0</td>
<td></td>
</tr>
</tbody>
</table>
Table 3.6 Polynomial coefficients for physical properties

<table>
<thead>
<tr>
<th>Constant</th>
<th>$C_p$</th>
<th>$K$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_0$</td>
<td>1.14497 E+3</td>
<td>0.01125</td>
</tr>
<tr>
<td>$a_1$</td>
<td>-0.4642</td>
<td>2.9218E-5</td>
</tr>
<tr>
<td>$a_2$</td>
<td>7.2862 E-4</td>
<td>7.7298E-9</td>
</tr>
<tr>
<td>$a_3$</td>
<td>-3.12839 E-7</td>
<td>-3.9906E-12</td>
</tr>
<tr>
<td>$a_4$</td>
<td>4.4635 E-11</td>
<td>4.7413E-16</td>
</tr>
</tbody>
</table>
3.9 Numerical Procedure

The general partial differential equations represented by Eq. (3.39) and Table 3.2, are integrated over a small control volume to obtain an algebraic difference equations which can be solved numerically.

Several methods have been proposed for solving the Navier-Stokes equations in arbitrary configurations in conjunction with orthogonal and nonorthogonal grid systems. These methods differ in the choice of grid layout (staggered versus non-staggered) and the dependent variable in the momentum equations (cartesian versus curvilinear velocity components). Most of the methods, however, use the SIMPLE algorithm [95] or its variants for determining pressure distribution that satisfies mass conservation equation.

3.9.1 Grid System and Discretization Equation

Before integrating the standard equations over the flow domain, a satisfactory grid is required. In the present work, a cartesian grid is used in the computer code. For hybrid differencing purposes the computer code ‘‘FLUENT’’[97] uses a staggered grid in which velocities are evaluated at the boundaries of scalar variable (P, k, , ... etc.) cells. Hence separate grids define the locations of the u-
and \( v \)-velocities. A portion of these grid is shown in Fig. 3.2. The equations are reduced to their finite-difference analogues by integrating partial differential equations over the computational cells into which the domain is divided. The resulting algebraic equations can be written in the following common form [95]

\[
\Phi_{i,j} \sum_k (A_k - S_{i,j}) = \sum_k (A_k \Phi_k) - S_c \tag{3.40}
\]

where the summation is over the neighbouring finite difference cells \( i \). The \( A \)'s are coefficients which contain contributions from the convective and diffusive fluxes and \( S_c \) and \( S_{i,j} \) are the components of the linearized sources,

\[
S_\Phi = S_c + S_{i,j} \Phi_{i,j} \tag{3.41}
\]

A quadratic upwind scheme (QUICK) is used for interpolating between grid points and to calculate derivatives of the flow variables [96]. This scheme aims in principle at combining the relatively high accuracy of centra difference with the stability property of the upwind scheme. Such a combination is achieved by evaluating any face \( \Phi \)-value on the basis of a conventional quadratic interpolation between \( \Phi \)-values at three nodes, two located on either side of the face considered and the third being removed one mesh width away in the upstream direction. The scheme thus requires the 9-point star shown in Fig. 3.2 and must, as the upwind scheme, take the sign of all face velocities into account. Using quadratic interpolation for
Fig. 3.2 Finite difference star for quadratic upstream-weighted scheme.
the dependent variable $\Phi$, it can be shown that the finite difference form of any convective-diffusive equation is reduced to [55,96],

$$
\begin{align*}
A_{i,j} \Phi_{i,j} &= A_{i+1,j} \Phi_{i+1,j} + A_{i-1,j} \Phi_{i-1,j} + A_{i,j+1} \Phi_{i,j+1} + \\
&\quad A_{i,j-1} \Phi_{i,j-1} + A_{i+2,j} \Phi_{i+2,j} + A_{i-2,j} \Phi_{i-2,j} + \\
&\quad A_{i,j+2} \Phi_{i,j+2} + A_{i,j-2} \Phi_{i,j-2} + S_c
\end{align*}
$$

(3.42)

where

$$
\begin{align*}
A_{i,j} &= A_{i+1,j} + A_{i-1,j} + A_{i,j+1} + A_{i,j-1} + \\
&\quad A_{i+2,j} + A_{i-2,j} + A_{i,j+2} + A_{i,j-2} + S_p
\end{align*}
$$

(3.43)

The derivation of $\Phi_{i-1,j}$ is given in detail in Appendix B and the form of $\Phi$ at the other faces is similar to the one presented here.

### 3.9.2 Overall Solution Procedure

The set of simultaneous algebraic equations is solved by a semi-implicit iterative scheme [95] which starts from arbitrary initial conditions (except at the boundaries) and converges to the correct solution, which satisfies the governing equations after performing a number of iterations. The reader is referred to [97] for more details of the iterative procedure.
The degree of convergence is measured through the calculation of the residual for each conservation equation by summing the imbalance in the equation for all cells in the domain. The residual R is defined as

\[
R = \sum_{ij} \left[ A_{i+1,j} \Phi_{i+1,j} + A_{i-1,j} \Phi_{i-1,j} + A_{i,j+1} \Phi_{i,j+1} + A_{i,j-1} \Phi_{i,j-1} + A_{i+2,j} \Phi_{i+2,j} + A_{i-2,j} \Phi_{i-2,j} + A_{i,j+2} \Phi_{i,j+2} + A_{i,j-2} \Phi_{i,j-2} + \Phi_{i,j} S_u - A_{i,j} \Phi_{i,j} \right]
\quad (3.44)
\]

The solution is said to be converged when R is in the range of \(10^{-5}\) to \(10^{-6}\).

### 3.9-3 Boundary Conditions

Due to elliptic nature of the conservation equations, boundary conditions must be specified at all boundaries of the domain considered. Uniform boundary conditions are prescribed for the velocity, temperature and concentration at the inlet boundary. The inlet values of the kinetic energy of turbulence, \(k\), and the dissipation rate \(\epsilon\), are estimated from the specified turbulence intensity at the entrance section as follows[97]

\[
k = 1.5 \left( \bar{u} I \right)^2 \quad (3.45)
\]

\[
\epsilon = C_\mu 0.75 \frac{k^{0.5}}{L} \quad (3.46)
\]
where \( I \) is the inlet turbulence intensity and \( L \) is a characteristic length of turbulence in the given flow geometry. The wall-function approach is used for satisfying the \( u \)-velocity and temperature conditions at the solid boundaries[51].
Chapter 4

COMPUTER CODE VALIDATION

The computer code, "FLUENT", used in the present study [97], has been validated for several non-reacting flow situations [98]. However, very little information is available regarding its predictive capabilities for situations involving turbulent chemically reacting flows in systems with complex geometrical features similar to the physical model considered in the present study. In order to gain confidence in the predictive capabilities of the code a comprehensive efforts was directed towards validation of the code. To achieve this goal, results obtained from the present computer code for several physical models are compared in this chapter with corresponding experimental results available in the literature.

4.1 Turbulent Flow Past Heated Cylinder

Figure 4.1 shows the physical model of turbulent flow past a heated cylinder. The geometrical and flow parameters for this case are also shown in Table 4.1. Through this model, we have tested the capability of the computer code for predicting the local convective heat transfer and pressure coefficients on the cylinder surface. We note here that the cylindrical surface was generated by a large number of cartesian steps with very fine step sizes. The pressure coefficient results obtained numerically are compared with experimental results [34] in Fig.4.2. The results were obtained for two inlet turbulence intensities namely 1.2 and 7 percent. The comparison with
Table 4.1 Geometrical and flow parameters for turbulent flow past heated cylinder

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( d ), cm</td>
<td>1.0</td>
</tr>
<tr>
<td>( H ), cm</td>
<td>9.0</td>
</tr>
<tr>
<td>( L ), cm</td>
<td>25.0</td>
</tr>
<tr>
<td>( T_f ), K</td>
<td>293</td>
</tr>
<tr>
<td>( \mu_f ), ( \frac{Kg}{m.s} )</td>
<td>1.81 E-5</td>
</tr>
<tr>
<td>( K_f ), ( \frac{W}{m.K} )</td>
<td>0.0259</td>
</tr>
<tr>
<td>( C_p ), ( \frac{J}{Kg.K} )</td>
<td>1005</td>
</tr>
<tr>
<td>( P ), ( \frac{N}{m^2} )</td>
<td>1.4 E+7</td>
</tr>
</tbody>
</table>
Fig. 4.1 Physical model for turbulent flow past heated cylinder.
Fig. 4.2 A comparison of the calculated and measured pressure distribution on a circular cylinder in air flow at Re = 10.
experimental results for pressure coefficient are excellent. The pressure trough and pressure recovery to a plateau are very well predicted. In fact, the generation of cylindrical surface with very fine cartesian steps has not affected the physical phenomenon, as illustrated by local comparison of pressure coefficient in Fig.4.2.

Figure 4.3 shows the variation of Nusselt number along the cylindrical surface at a Reynolds number of $7.7\times10^5$. The results indicate that the Nusselt number is predicted within $\pm 12\%$ of the experimental results in the angular range of $60$ to $180^\circ$. The results in $0$ to $60^\circ$ range differs by about $35\%$. This deviation can be traced to use of a cruder grid upstream of the cylinder. This grid cannot capture the thin laminar boundary layer developing over the leading part of the cylinder. Since the combustion process occurs behind ring injector, it is encouraging to know that convective heat transfer mechanism is being accurately modeled in the neighborhood of the rear stagnation point. The discrepancy in the leading part of the cylinder can be reduced or eliminated by choosing a much finer grid, upstream of the cylinder. However, due to parabolic nature of the flow in the leading part of the cylinder, the flow field downstream of the cylinder is not affected significantly by the crude grid upstream. We also note that the code successfully predicts two troughs and one peak in the heat transfer coefficients. The first trough is due to increasing thickness of the boundary layer. The heat transfer coefficient then increases due to transition of the laminar boundary layer to a turbulent boundary layer. The further decrease occurs due to thickening of the turbulent boundary layer followed by increase due to flow recirculation.
Fig. 4.3 Local heat transfer coefficient from a circular cylinder to air.
Fig. 4.4 Physical model for non-reacting air flow past a pair of circular cylinders.
<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(d), cm</td>
<td>3.48</td>
</tr>
<tr>
<td>(D), cm</td>
<td>3.81</td>
</tr>
<tr>
<td>(G), cm</td>
<td>1.58</td>
</tr>
<tr>
<td>(\mu_f), Kg m^{-1}s^{-1}</td>
<td>1.814 E-5</td>
</tr>
<tr>
<td>(u_a), m s^{-1}</td>
<td>12.19</td>
</tr>
<tr>
<td>(P), N m^{-2}</td>
<td>1.01e+5</td>
</tr>
</tbody>
</table>

Table 4.2 Geometrical and flow parameters for turbulent flow past a pair of circular cylinders.
4.2 Turbulent Flow Between Two Cylinders

Figure 4.4 shows the physical model for non-reacting air flow past a pair of cylinders for which the measured velocity data has been reported in the literature[15]. The geometrical and flow parameters for this case are also shown in Table 4.2. The computed axial velocity profile in the wake of the cylinders at an axial position \( x = 6d \), is compared with the experimental results in Fig. 4.5. It is noted that the results for this complex geometry, obtained with a 132x96 grid, are in good agreement with the hot wire data reported in [15].

4.3 Reacting Flow in a Suddenly-Expanded Combustion Chamber

Since the physical model, to be considered in the present work, requires modeling of chemistry effects, further validation of the computer code needs to be done for a chemically reacting case. Experimental results for this case have been reported by Lewis and Smoot[99]. The geometrical features of the suddenly-expanded combustion chamber are given in Fig. 4.6 while the flow parameters for the case are given in Table 4.3. The fuel, town gas, is injected from an axially located tube, while air is introduced from a concentric annulus at the inlet. The results were calculated for three chemistry models, namely equilibrium, one-step reaction kinetics and two-step reaction kinetics models. This was done to identify the chemistry model which predicts results closest to experimentally observed results.
Fig. 4.5 Velocity distribution about two cylinders spaced 1.58 cm apart.
Fig. 4.6 Schematic of a suddenly-expanded combustion chamber.
Table 4.3 Flow parameters for the suddenly expanded combustion chamber

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_a$, m/s</td>
<td>34.3</td>
</tr>
<tr>
<td>$T_a$, K</td>
<td>589</td>
</tr>
<tr>
<td>$u_F$, m/s</td>
<td>21.3</td>
</tr>
<tr>
<td>$T_F$, K</td>
<td>300</td>
</tr>
<tr>
<td>$P$, $\frac{N}{m^2}$</td>
<td>0.94 $\times 10^5$</td>
</tr>
<tr>
<td>Air flow rate, $\frac{m^3}{s}$</td>
<td>36.3</td>
</tr>
<tr>
<td>Gas flow rate, $\frac{m^3}{s}$</td>
<td>2.84</td>
</tr>
</tbody>
</table>
Fig. 4.7 Flame structure for the fast chemistry model.
Fig. 4.8 Flame structure for the one-step kinetics model.
Fig. 4.9 Flame structure for the two-step kinetics model.
The chemical kinetics data for single and two step reaction models are given in Tables 3.3, 3.4 and 3.5. We note here that no attempt was made during the investigation to fine tune various constants to achieve better accord with Figures 4.7-4.9 show the flame structure for fast or equilibrium chemistry, one-step and two-step reaction models. We note that the flame shapes are quite different for equilibrium chemistry case, where the flame is nearly attached with the high temperature combustion zone approaching the fuel injection port area. The one-step and the two-step reaction models show significantly lifted flames in Figs. 4.8 and 4.9. In fact, the flame lift-off in the two-step kinetics model is quite pronounced due to the slower second reaction step involving formation of carbon monoxide.

Figure 4.10 shows the radial variation of gas temperature at an axial location $x=9.5\text{cm}$. The results obtained numerically from the three chemical models are compared with the experimental data of Lewis and Smoot[99]. It is noted that the two-step model produces results that are in best agreement with the experimental results. The fast chemistry model produces unrealistically high gas temperature near axial locations due to fast consumption of fuel implicit in the chemistry model. The single-step model also approximately replicates the variation of experimentally observed temperature profile but the degree of agreement is worse compared to the one predicted with the two-step model. At locations significantly removed from the combustor axis, the equilibrium model grossly underestimates the observed temperature profile. The comparison of the three chemistry models at several axial locations shows similar trends in Figs. 4.11 and 4.12.

Figure 4.13 shows the variation of oxygen concentration
Fig. 4.10 Comparison of experimental data of gas temperature profile at an axial location of 9.5 cm with results from three combustion models.
Fig. 4.11 Radial gas temperature profiles at axial locations of 9.5 cm and 17.5 cm.
Fig. 4.12 Radial gas temperature profiles at axial locations of 24.6 cm and 32.7 cm.
Fig. 4.13 Comparison of experimental data of the center-line oxygen mole fraction with results from three combustion models.
along the axis as obtained from the three chemistry models considered in the present study. The results from a numerical calculation employing probability density function (pdf) approach, taken from Smith and Smoot [100], are also included. The results from these four models are compared with experimental results reported in [99]. It should be noted that experimental and numerical studies in [99] and [100] have been conducted by the same group of researchers. The two-step reaction model once again produces results, including the peak O₂ concentration magnitude and its location, that are in excellent agreement with experimental results. The pdf model greatly underestimates the O₂ concentration initially, and then overestimates it at the far field axial locations. The fast chemistry model, as expected, shows a near zero O₂ concentration, a value far removed from observed O₂ concentration values.

Figure 4.14 shows the variation of centerline concentration of methane. The two-step kinetics model once again produces results that are closest to the experimental results. The pdf and fast chemistry models predict results that are significantly higher than the observed values in the near field axial location. Only in the far field, these models produce results that asymptotically approach observed methane concentration. Figure 4.15 shows the comparison of present numerical results (two-step model) with those of Nikjooy and So [55]. The results in [55] are obtained by employing physical and computational models similar to the ones used in the present study. The result of Nikjooy and So deviate from the experimentally observed trends more than the present study. The reason for this apparent discrepancy is not evident to the author at the present time.

Figures 4.16 and 4.17 show the radial variation of methane concentration at several axial locations. Numerical results,
Fig. 4.14 Comparison of experimental data of the center-line methane mole fraction with results from three combustion models.
Fig. 4.15 Comparison of experimental data of the center-line methane fraction with numerical results.
Fig. 4.16 Radial profiles of CH$_4$ at axial locations of 9.5 cm and 17.5 cm.
Fig. 4.17 Radial profiles of CH$_4$ at axial locations of 24.6 cm and 32.7 cm.
Fig. 4.18 Radial profiles of $O_2$ for various axial locations.
obtained from fast, one-step and two-step chemistry models, are compared with data[99]. The results from one-step and two-step models compare very favorably with experimental results for the first two axial locations. It is also evident that the fast chemistry model grossly overestimates the observed values at all four axial locations. At the next two axial locations (x=24.6 and 32.7cm), all three models overpredict the experimental results, but the departure of results from the two-step model from data is smaller compared to other two models.

Figure 4.18 shows the radial oxygen concentration profile at four axial locations indicated in the figure. The numerical results are obtained from two models, namely pdf model [100] and two-step reaction model of present study. These results are compared with experimental results from[99]. It is noted that the two-step model produces best results in the near axis locations where the combustion zone exists. The departure from experimental trends becomes quite significant at locations farther away from the centerline. Only at x=32.7cm, the oxygen concentration is predicted well by the two-step reaction model for the entire radial coordinate range. In contrast, the pdf model has widest departure from experimental results in the near axial locations where combustion zone is located. Overall, the two-step model of present study predicts results that are in better accord with experimental results as compared to results predicted from the pdf model.

Figure 4.19 shows the radial profile of CO$_2$ concentration at four axial locations namely x = 32.7, 47.6, 63.2 and 78.1 cm. The two-step chemistry model produces good results in the near-field axial locations while the results produced by the pdf model deviate significantly from CO$_2$ data in the near-field locations. In the far field locations, both models overestimate the CO$_2$ concentration.
Fig. 4.19 Radial profiles of CO$_2$ at several axial locations.
Fig. 4.20 A comparison of the calculated and measured CO mole fraction.
Figure 4.20 shows the radial profile of CO concentration at two axial locations, namely $x=47.6$ and $63.2\text{cm}$. The carbon monoxide profile is drawn through results predicted from the two-step chemistry model of present study, and the results predicted by Nikjooy and So [55]. Although at $x=63.2\text{ cm}$ axial location, the present model predicts results that are in good agreement with data, the numerical results at $x=47.6\text{cm}$ show significant departure from the data. It is interesting to note that the present model predicts CO concentration well near axial locations. In comparison, the results of Nikjooy and So deviate more from data as compared to results from the present study.

The above discussion indicates that the FLUENT code has the capability of predicting physical phenomenon that involves complex geometrical feature as well as chemical reactions due to combustion of fuel. The results for non-reacting flow past a heated cylinder yielded results for pressure coefficient and Nusselt number that are in reasonable agreement with the data. Since cylindrical geometry was generated by very small cartesian steps, these results further indicate that the physics of the problem is not compromised by this expediency introduced in the computational procedure.

Comparison of the results for the reacting case with data published in the literature indicates that the fast chemistry model is inadequate for predicting the observed temperature and concentration profiles in the combustion zone. The two-step reaction model produced results that are in closest agreement with the data. The one-step model also approximately replicated the variation of experimentally observed temperature and concentration profiles, but the degree of agreement is inferior to the two-step model.
Chapter 5

RESULTS AND DISCUSSION

The numerical schemes and physical models described in Chap. 3 and validated in Chap. 4, are applied to obtain results for the three ring injector represented by the physical model shown in Fig. 3.1. Results were first obtained for the non-reactive flow of air around the three ring injector, followed by prediction of the effect of non-reacting fuel jet on the vortex pattern behind the cylinder. For the reactive flow, effects of various parameters governing the surface temperature distribution, flame lift-off and thermal load were assessed. Finally calculations were made to determine the effects of LOX injection on thermal load on the ring injector.

5.1 Grid Independency

Computations in the present study were done using a nonuniform grid in order to concentrate grids in the combustion zone where large gradients of physical properties occurred. Also, to resolve the steep gradients near the walls, the grid points were densely packed in their vicinity. A typical discretized domain is shown in Fig. 5.1. Most of the results presented here have been obtained using 218x144 grid points along the x-y axes. A coarser grid with 101x75 grid points was also employed to establish grid independency of results. For all results for reacting cases, the grid independency calculations were obtained with a single-step chemistry model. The two-equation turbulence model and QUICK numerical scheme were employed for all results obtained in the present study.
Fig. 5.1 Typical grid for finite volume calculations.
Figures 5.2 and 5.3 compare the code predictions of the center-line axial velocity for non-reacting and reacting flows respectively for two different grid sizes. Figure 5.2 shows that the center-line velocity is not sensitive to the grid sizes employed. For example, doubling the grid size has only slight impact on the results. The only difference between the two results seems to be in the far-field region where a coarser grid has been used. It is also interesting to note that the magnitude of the velocity minimum, and its location in the vortical flow downstream of the cylinder are predicted reasonably well by both grids. Corresponding calculations for the reacting flow (Fig.5.3) also shows virtually no difference for grid sizes of 218x144 and 101x75.

The calculated center-line temperature for reacting case is shown in Fig.5.4 for grid sizes of 101x75 and 218x144. The results for 101x75 grid are quite similar to the center-line temperature distribution generated with 218x144 grid except for small deviations in the mid-axial locations. The effect of grid refinement on the calculated surface temperature distribution for the middle cylinder is shown in Fig.5.5. Because the grid is fairly refined for most of the cylinder surface, except the front portion, differences between the results corresponding to the two grid sizes are minor except for the upstream portion where the 101x75 grid represents a very crude discretization of the physical domain. It is concluded based on extensive experimentation with numerical grids, that the 218x144 grid provides grid independent results for both chemically reacting and non-reacting cases involving the three cylinder injector geometry. Instead of using the coarser grid (101x75), the finer grid (218x144) was employed for all computations in this study so that better accuracy throughout all regions of interest can be achieved.
Fig. 5.2 Comparison of the center-line axial velocity
for non-reacting flow for two different grid sizes.
Fig. 5.3 Comparison of the center-line axial velocity for reacting flow for two different grid sizes.
Fig. 5.4 The calculated center-line temperature for two different grid sizes.
Fig. 5.5 The effect of grid refinement on the calculated surface temperature distribution.
All calculations for the present work have been done on a VAX 8550 computer at NASA Langley. Typical computer times (CPU) required to produce a solution with 218x144 grid points for reacting flow are in the range of 1200 to 1300 min.

5.2 Results for Non-Reacting Flows

The characterization of flow conditions downstream of the ring injector is important in understanding and predicting the flame lift-off phenomenon. Also, the flow conditions downstream of the ring injector govern the thermal loads on the ring structure. In this section some numerical results for the non-reacting flows will be presented. The flow parameters for this case are given in Table 5.1.

The time dependent flow field of air around the cylinder for six time steps is shown in Figs. 5.6-5.11. The flow field behind the cylinders is dominated by the vortical flow patterns generated by the circular shape of the rings. As the time increases the length of the vortices downstream of the cylinder increases and subsequently decreases until it reaches the steady state solution. Fig. 5.12 shows the results obtained from steady state calculation. Comparison of the steady state results (Fig. 5.12) with the time dependent solution for large time limit (Fig. 5.11) confirms that the time dependent solution in the large time limit approaches the steady state solution.

Figure 5.13 compares the pressure coefficient on the surface of the middle cylinder obtained from steady state calculations with the corresponding time dependent results for the large time limit. Comparison of the predictions for these two cases indicates that a steady state solution for the problem exists, and that it can be reached asymptotically in the large time limit by solving the transient problem.
Table 5.1 Flow parameters for the non-reacting case

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_a$, m/s</td>
<td>2.0</td>
</tr>
<tr>
<td>$T_a$, K</td>
<td>277</td>
</tr>
<tr>
<td>$I_a$</td>
<td>12%</td>
</tr>
<tr>
<td>$T_F$, K</td>
<td>277</td>
</tr>
<tr>
<td>$I_F$</td>
<td>6%</td>
</tr>
<tr>
<td>$p$, $\frac{N}{m^2}$</td>
<td>1.37 E+7</td>
</tr>
</tbody>
</table>
Fig. 5.6. The flow field for the non-reacting flow for time $t = 0.005$ S.
Fig. 5.7 The flow field for the non-reacting flow for time $t = 0.01 \text{ S}$. 
Fig. 5.8 The flow field for the non-reacting flow for time $t = 0.05\, S$. 

Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
Fig. 5.9 The flow field for the non-reacting flow for time $t = 0.06$ S.
Fig. 5.10 The flow field for the non-reacting flow for time $t = 0.08 \text{ S}$. 
Fig. 5.11 The flow field for the non-reacting flow for time $t = 0.1$ S.
Fig. 5.12 The steady flow field for the non-reacting flow
Fig. 5.13 Comparison of the pressure coefficient on the surface of the middle cylinder obtained from steady state and time dependent calculations.
Figure 5.14 compares the steady state center-line velocity with the time dependent solution for the large time limit for two time steps. For the smaller time-step the time dependent solution shows almost exact agreement with the steady solution. However, for the large time-step, the time dependent solution underpredicts the steady state solution significantly. This indicates that for larger time step the time dependent solution needs to be carried out to even larger time to achieve the steady state limit.

Figure 5.15 shows the steady state non-reacting flow field for a fuel injection velocity of 60m/s. We note that the strong entrainment by the jet, injected from the leeward axial location on the cylinder, causes the vortex pattern behind the cylinder to decay considerably. In fact, only a very small recirculation, with flow reattachment on the cylinder, remains in presence of the jet. The jet entrainment also causes two large recirculation regions to appear downstream of the middle and other cylinders. The direction of rotation of these large eddying regions is opposite to the recirculation regions located on the cylinder surface. Figure 5.16 shows the corresponding case for the non-reacting fuel jet velocity of 100m/s. Compared to 60m/s case, the flow is nearly attached on the cylinder surface, with only slight recirculation on the cylinder surface. However, the recirculating eddy for downstream of the cylinder gets stronger and larger.
Fig. 5.14 Comparison of the steady state center-line velocity with the time dependent solution.
Fig. 5.15 The steady state non-reacting flow field for fuel injection velocity of 60 m/s.
Fig. 5.16 The steady state non-reacting flow field for fuel injection velocity of 100 m/s.
5.3 Combustion Calculations

In this section results for the reactive flow are presented. Results for the effect of chemical kinetic models on flame lift-off are presented first, followed by the investigation of the fuel jet velocity effect on temperature distribution and thermal load on the fuel injector surface. The effect of LOX injection on thermal load is discussed subsequently. Finally, results obtained for different inlet turbulence intensities are presented.

5.3.1 Consideration of Different Chemistry Models

Figures 5.17-5.19 show enlarged views of the flame structure for fast chemistry, one-step and two-step reaction models respectively. The chemical kinetics data are similar to those given in Tables 3.2 and 3.3. The fuel jet velocity for these cases has a constant value of 100m/s. The flame shapes are different for equilibrium and kinetics models. For example, in the equilibrium chemistry case, the flame is attached with the high temperature combustion zone approaching the fuel injection port area. The one-step reaction model also shows slight attachment to the surface of the cylinder, and the flame thickness near the surface is reduced. The two-step reaction model predicts a lifted flame, and smaller flame thickness near the fuel injection port. In fact, the flame lift-off predicted by the two-step kinetic model is quite-pronounced due to the slower second step reaction model involving formation of carbon monoxide.

Figure 5.20 shows the variation of the temperature along the surface of the middle cylinder for above three cases. Near the fuel injection point, the fast chemistry model produces
Fig. 5.17 Flame structure for fast chemistry model.
Fig. 5.18 Flame structure for one-step kinetics model.
Fig. 5.19 Flame structure for two-step kinetics model.
Fig. 5.20 The variation of the temperature along the surface of the middle cylinder.
unrealistically high surface temperature due to the fast consumption of fuel implicit in the chemistry model. The difference in the prediction of the maximum surface temperature using one-step and two step reaction model is about 100°C near the fuel injection port. However, far from the fuel injection point prediction of the three models is quite similar.

Figure 5.21 shows the vertical variation of combustion product temperature at an axial location \( x = 6.11 \text{cm} \) slightly downstream of the injector point. As expected, the difference between predicted results from the equilibrium and the two-step reaction models near the fuel injection port is quite significant.

5.3.2 The effect of Fuel Jet Velocity

In this section the effect of fuel jet velocity on the flame structure and thermal load is presented. The results are for the case where convection (outside the cylinder surface) and conduction (inside the cylinder) are considered simultaneously for the chemically reacting case. The ring injector is modeled as a composite cylinder. The inner cylinder is assumed to have stagnant methane. In reality, the methane moves slowly through the cylinder towards the injection point. However, consideration of slow convective phenomenon inside the cylinder will be prohibitive from a computational point of view. As a result, we have modeled the heat transfer process inside the cylinder by pure conduction. This procedure is acceptable since it is likely to produce conservative (higher) estimates of surface temperature. To obtain the converged solution, the adiabatic wall solution case was first employed as the starting field for iteration for the conjugate case. On the cylinder wall the heat flux continuity condition involving equality of convective and conductive heat fluxes is imposed.
Axial Position 6.11 cm

Fig. 5.21 Vertical variation of the combustion product temperature at an axial location of 6.11 cm.
Figures 5.22-5.24 show the flame structure for fuel injection velocities of 30, 60 and 100m/s respectively. At the lowest injection velocity the vortical flow pattern downstream of the cylinder is large and well defined. The reversed flow region is responsible for transporting the hot combustion products towards the cylinder, thus producing the flame anchoring with a large wrap around the leeward portion of the cylinder. As the fuel jet velocity is increased, the vortical flow pattern behind the cylinder becomes somewhat smaller and weaker, and as a result the flame wrap around region diminishes and it nearly disappears for the 100m/s fuel velocity case. It is interesting to note that similar flame regimes here have been observed qualitatively for the three cylinder discrete injection case [101] Figures 5.25-5.27 show that the flow field for the three jet velocities changes significantly for the combustion cases. For the 30m/s case, a large well organized vortex system on the leeward portion of the cylinder is clearly indicated. As the fuel jet velocity is increased, the vortical flow pattern behind the cylinder weakens. Thus the flow field patterns are consistent with the flame structure shown in Figs.5.22-5.24. The comparison of the flow field for reacting cases (Fig.5.26 and 5.27) and non-reacting cases (Figs.5.15 and 5.16) also yields important information. Where as in the non-reacting case, there is very small recirculating regions near the cylindrical surface, a well defined recirculating region exists for the reacting case. This keeps the flame anchored to the injector by providing recirculated combustion products to the oncoming jet to sustain combustion phenomenon.

The temperature on the surface of the middle cylinder are compared for the three jet velocity cases in Fig.5.28. We note that the lowest velocity case produces the highest temperature on the surface of the cylinder near the fuel injection port.
Fig. 5.22 Flame structure for 30 m/s fuel jet velocity.
Fig. 5.24 Flame structure for 100 m/s fuel jet velocity.
Fig. 5.27 The flow field for 100 m/s fuel jet velocity.
Fig. 5.28 Comparison of the temperature on the surface of the middle cylinder for three fuel jet velocities
Fig. 5.29 Vertical variation of combustion products temperature at an axial location of 61.1 mm.
Fig. 5.30 Vertical variation of combustion products temperature at an axial location of 61.5 mm.
Fig. 5.31 Vertical variation of combustion products temperature at an axial location of 62.3 mm.
Figures 5.29-5.31 show the vertical variation of combustion products temperature for three injection velocities at three axial locations namely x=61.1, 61.5 and 62.3 mms respectively. Once again, as expected the lowest injection velocity results in the maximum combustion products temperature near the fuel injection port.

Figures 5.32 and 5.33 show the flame structure for fuel injection velocity of 150 m/s for one-step and two-step reaction models respectively. For one-step model, the flame is still attached at a point near the fuel injection port. However, the flame lift-off predicted by the two-step model is quite pronounced. Comparison of Figs. 5.33 and 5.19 shows the effect of fuel injection velocity on flame lift-off distance. Both figures confirm that the methane flame lift-off can be modeled by using the two-step chemical kinetics model. The higher fuel injection velocity shows a clear flame lift-off. It is also evident that the flame lift-off distance increases with increasing injection velocity. This raises the possibility of predicting computational blow-off of the flame if one uses a compressible flow model due to higher subsonic Mach numbers at higher injection velocities. The clear evidence of flame lift-off is also illustrated in Fig. 5.34 where the surface temperature is shown for fuel jet velocity of 100 and 150 m/s, using two-step reaction model. We note that there is a collapse in the values of surface temperature as the injection velocity is increased from 100 to 150 m/s. As a result we can term the flame at 150 m/s as clear lifted flame, while the flame at 100 m/s can be regarded as only slightly lifted or quasi-lifted.

Figure 5.35 shows the flame structure for the three ring injector using two-step chemical kinetic model for the fuel jet velocity of 100 m/s. Comparison of Fig. 5.35 and 5.24 indicated that there are some differences in the flame structure prediction of the two model. For the one-step, models the
Fig. 5.32 Flame structure for fuel jet velocity of 150 m/s for one-step reaction.
Fig. 5.33 Flame structure for fuel jet velocity of 150 m/s for two-step reaction.
Fig. 5.34 The temperature variation on the surface of the middle cylinder for fuel jet velocity of 100 and 150 m/s.
Fig. 5.35 Flame structure for the three ring injector using two-step chemical kinetic model and fuel jet velocity of 100 m/s.
flame is attached to the cylinder surface near the injection point and the flame is symmetric for the three ring. For the two-step reaction model, the flame is quasi-lifted flame and somewhat asymmetric.

5.3.3 Thermal Load Analysis

The thermal load is analyzed for two types of fuel injector, namely the ring type injector discussed in the previous section and the solid injector. For the solid injector case, the fuel injector is assumed to be a solid cylinder with thermal conductivity equal to that of the ring injector wall material. This model requires much less computational effort, and was considered here to examine if this model predicts results that are in comparable with results obtained for the ring injector model. For both cases, the turbulence was modeled by the two-equation (k-ε) model, and chemistry was modeled by the single-step kinetics model. The continuity of temperature and heat flux conditions were applied at the fluid-solid interfaces in both cases.

Figure 5.36 compares the flame structure for the middle cylinder for fuel injection velocity of 30, 60 and 100m/s respectively. The results indicate that for the 30m/s jet velocity case, the maximum temperature inside the injector is of the order of 900 K, a much higher value compared to the other fuel jet velocity cases. Figures 5.37-5.39 show the heat flux variation on the surface of the middle cylinder, for the three fuel jet velocities. As expected, a significant reduction in the incoming heat flux results as the fuel jet velocity is increased. The heat flux for the 100m/s velocity case is almost negligible compared to that obtained for the 30m/s fuel injection velocity.
Fig. 5.37 Heat flux variation on the surface of the cylinder for fuel jet velocity of 30 m/s.

Scale: 1 cm = 326 kw/m²
Fig. 5.38 Heat flux variation on the surface of the cylinder for fuel jet velocity of 60 m/s.

Scale: 1 cm = 326 kW/m²
Fig. 5.39 Heat flux variation on the surface of the cylinder for fuel jet velocity of 100 m/s.
Fig. 5.40 The surface temperature distribution for the solid injector for three fuel jet velocities.
Figure 5.40 shows the surface temperature distribution for the solid injector for three fuel jet velocity. The peak temperatures are lower for solid injector when compared with corresponding results for hollow cylindrical (ring) injector case (Fig.5.28). As a result, the use of the solid cylinder model, despite its computational advantages, is not realistic since it does not yield conservative results for surface temperature. Figures 5.41-5.43 compare further the surface temperature predictions for the solid and ring fuel injectors for different fuel jet velocities. At low velocity, the ring injector predicts a 200°C higher temperature near the fuel injection port than that for the solid injector. This is due to the fact that methane gas with its low thermal conductivity acts as an insulation to the heat flux going into the injector. As the fuel jet velocity increases to higher values, the difference in the temperature prediction of the solid and ring injector becomes negligible. We note here that we have used the ring injector in most of the present calculations to obtain more conservative results, and to model the physical situation more realistically.

Figures 5.44-5.46 show the heat flux distribution obtained for the solid fuel injector. Comparison of the predictions for the ring and solid injector cases indicated somewhat higher level of heat flux for the solid fuel injector which is consistent with trends in surface temperature presented earlier.

5.3.4 Effect of LOX injection

The results presented in the previous sections were for combustion of methane with air. In this section the effect of combustion of methane with enriched air on thermal load is discussed. The enriched air is modeled with a uniform \( \text{O}_2 \) concentration of 47% by mass at the inlet section of the combustor.
Fig. 5.41 Comparison of the surface temperature prediction for the solid and ring injectors for fuel jet velocity of 30 m/s.
Fig. 5.42 Comparison of the surface temperature prediction for the solid and ring injectors for fuel jet velocity of 60 m/s.
Fig. 5.43 Comparison of the surface temperature prediction for the solid and ring injectors for fuel jet velocity of 100 m/s.
Scale: 1 cm = 326 kW/m²

Fig. 5.44 Heat flux variation for the solid fuel injector for fuel velocity of 30 m/s.
Fig. 5.45 Heat flux variation for the solid fuel injector for fuel velocity of 60 m/s.

Scale: 1 cm = 326 kW/m²
Fig. 5.46 Heat flux variation for the solid fuel injector for fuel velocity of 100 m/s.

Scale: 1 cm = 326 kW/m²
Fig. 5.47 Flame structure for 60 m/s fuel jet velocity with LOX injection.
Fig. 5.48 The prediction of temperature on the surface of middle cylinder with and without enriched air.
Fig. 5.49 The flame structure for fuel jet velocity of 10 m/s and 3% air turbulent intensity.
Fig. 5.50. The flame structure for fuel jet velocity of 100 m/s and 24% air turbulent intensity.
Fig. 5.51 The prediction of the temperature on the surface of the middle cylinder for three air turbulent intensities.
Fig. 5.52 The vertical temperature variation at an axial position of 6.11 cm for three air turbulent intensities.
5.3.6 Influence of Far-Field Boundary Conditions

Boundary conditions must be specified at the outlet section of the flow. The sensitivity of location of this boundary on the results was also tested. Since the gradient $\frac{\partial \rho}{\partial x}$ was set to zero at the exit, the axial length of the domain was varied to see if far-field boundary condition and its location affected the combustion phenomenon in the near field. Figure 5.53 shows the center-line velocity variation with axial distance for two combustor lengths, namely 36.5 and 20 cms. Corresponding distribution of center-line temperature are presented in Fig.5.54. Examination of Figs. 5.53 and 5.54 shows that significant differences are not observed in the magnitude of the two sets of results. Comparison of Figs. 5.55 and 5.24 further indicates that the flame structure for the shorter axial length is essentially similar to that of axial length of 36.5m. Although, the results in the present study were obtained with the larger combustor length, it is recommended that all future calculations, specifically in three-dimensions should be carried out with shorter length to reduce computational time.
Fig. 5.53 Influence of far-field boundary conditions on the center-line velocity magnitude.
Fig. 5.54 Influence of far-field boundary condition on center-line temperature distribution.

Temperature, K

Axial Distance, cm

--- L = 36.5 cm

00000 20
Fig. 5.55 Influence of far-field boundary condition on flame structure.
Chapter 6

CONCLUSIONS

This study presents a numerical analysis of a three in-line cylindrical fuel injector that has been adopted as a model for investigating combustion phenomenon in the 8-Ft High Temperature Tunnel at the NASA Langley Research Center. The primary objective here is to investigate the flame lift-off phenomenon and to predict thermal loads on the three cylinder fuel injector geometry in two-dimensions.

The "FLUENT" computer code used in the present study is first tested for its predictive capabilities for both reacting and non-reacting cases. The code was subjected to several physical situations that involved complex geometrical features as well as chemical reactions due to combustion of fuel. The case of non-reacting flow past a heated cylinder yielded results for pressure coefficient and Nusselt number that are in reasonable agreement with the experimental data. Since cylindrical geometry was generated by very small cartesian steps, these results further indicate that the physics of the problem is not compromised by this expediency introduced in the computational procedure.

The reacting case involved the suddenly expanded combustor geometry, and the results were obtained for three chemistry models, namely fast chemistry, one-step reaction and two-step reaction models. The results predicted from the computer code were compared with data published in the literature. The present results indicate that fast chemistry model is inadequate for predicting the observed temperature and
concentration profiles in the combustion zone. The two-step reaction model produced results that are in best agreement with the data. The results from the present two-step model calculation for the suddenly expanded combustor geometry were also compared with two other numerical results that exist in the literature. The results obtained from the present computer code are in general closer to the data when compared to computational results of Nikjooy and So[55] and Smith and Smoot[92].

The validated computer code 'FLUENT' has been applied to obtain the results for the three cylinder fuel injector configuration. The effects of fuel injection velocity, chemistry model, turbulence intensity and oxygen enrichment on flame structure and thermal load were analyzed in some details. The numerical results indicate that fuel injection velocity has significant effect on the combustion phenomenon in the vicinity of the fuel injector. As the fuel injection velocity is increased, the flame transforms from a wrap around the cylinder configuration to a clearly lifted flame configuration. The associated thermal load and peak surface temperature also decrease sharply as the flame gets detached from the injector surface.

The present study indicates that the choice of chemistry model is also critical in the prediction of flame lift-off phenomenon. For example, only the two-step chemistry model predicts a clearly lifted flame while the fast chemistry and one-step reaction chemistry models predict attached flames for all fuel injection velocities considered in the present study. The flame lift-off is also clearly indicated by a precipitous drop in thermal loads or peak surface temperature.
The effect of turbulence intensity variation appears to be limited to thinning of the flame base. As a result the thermal loads and peak surface temperature reduce slightly as the turbulence intensity is increased. The overall flame structure remains nearly the same for all three intensity levels considered in the present study. The effect of oxygen enrichment on the combustion process is very pronounced and is reflected in a 200°C rise in the peak surface temperature. The oxygen enrichment causes the establishment of a wrap around flame even at higher injection velocity of 60 m/s.

This study demonstrates the effectiveness of CFD modelling of the extremely complex turbulent reactive flows encountered in the combustor. It may be concluded from the present study that the two-step reaction kinetics model is essential for prediction of lifted flame on the injector considered in the present study. Based on the present study, the following recommendations are suggested.

(1) It is shown here that while considerable computational advantage can be derived by using one-step kinetics model to predict the flame structure and the thermal load, its capability for predicting of flame lift-off is questionable, and for this reason the two-step kinetics model should be used, especially for any future three dimensional studies.

(2) The flow in the present investigation is assumed to be two-dimensional, but in actuality the flow is three dimensional. The two-dimensional model was considered to understand the basic physics of the problem due to the present constraints of limited computational time.

(3) The prediction of other turbulence models such as the algebraic stress model should be tested and compared with prediction of the present k-ε model.
(4) More parametric studies should be carried out to investigate the flame lift-off leading to computational flame blow-off.

(5) Extension of the chemistry model for four steps will be useful in determining if more intermediate reaction steps are important in predicting more accurately the observed temperature and concentration profile.
REFERENCES


148


APPENDICES
APPENDIX A

STOICHIOMETRIC RELATIONS

The linear relation between the inert species $\psi$ and the mixture fraction $\theta$ can be expressed as:

$$\frac{\psi - \psi_0}{\psi_F - \psi_0} = \frac{\theta - \theta_0}{\theta_F - \theta_0} \quad (A.1)$$

where $\psi$ stands for $m_C$, $m_O$, $m_H$, and $m_N$, $o$ and $F$ indices represent $o$ and $F$ inlet, respectively.

One-Step Reaction:

For one-step kinetic model there are five species participating in the mixture composition viz: (CH$_4$, O$_2$, N$_2$, CO$_2$ and H$_2$O). If two differential equations (mass fraction, $\theta$ and fuel CH$_4$) are solved, four additional algebraic equations can be obtained from equation (A.1).

If the mass fraction of CH$_4$ in the fuel stream is 1 and the mass fraction of oxidant in the air stream is $m_0$, the linear relations for atomic elements are:

$$m_C = \frac{3}{4} \theta \quad (A.2)$$

$$m_H = \frac{\theta}{4} \quad (A.3)$$
\[ m_0 = m_0 (1 - \theta) \quad (A.4) \]

The stoichiometric relations can be written as:

\[ m_C = \frac{3}{4} m_{fu} + \frac{12}{44} m_{CO_2} \quad (A.5) \]

\[ m_{II} = \frac{1}{4} m_{fu} + \frac{1}{9} m_{H_2O} \quad (A.6) \]

\[ m_0 = m_{O_2} + \frac{16}{18} m_{H_2O} + \frac{32}{44} m_{CO_2} \quad (A.7) \]

Combining Eq. (A.2) and (A.5) \( m_{CO_2} \) can be calculated.

From Eqs. (A.3) and (A.6) \( m_{H_2O} \) and from (A.3) and (A.7) \( m_{O_2} \) can be determined.

\[ m_{H_2O} = \frac{9}{4} (\theta - m_{fu}) \quad (A.8) \]

\[ m_{CO_2} = \frac{11}{4} (\theta - m_{fu}) \quad (A.9) \]

\[ m_{O_2} = m_0 (m_{fu} - \theta) + 4 (m_{fu} - \theta) \quad (A.9) \]
Two-Step Reaction

There are six species (CH₄, O₂, CO, CO₂, H₂O and N₂) involved in the two-step reaction which have to be determined at each control cell. Three properties, namely the mixture fraction θ, mass fraction of fuel $m_{CH}$, and mass fraction of carbon monoxide $m_{CO}$, are obtained from the differential equations. Three additional equations are obtained from the stoichiometric relations:

\[ m_{O_2} = \frac{7}{4} m_{CO} + m_{\theta} (1 - \theta) + 4 (m_{fu} - \theta) \quad (A.10) \]

\[ m_{CO_2} = \frac{11}{4} (\theta - m_{fu}) - \frac{11}{4} m_{CO} \quad (A.11) \]

\[ m_{H_2O} = \frac{9}{4} (\theta - m_{fu}) \quad (A.12) \]
For the calculation of \( \Phi_{i-1,j} \), a second degree polynomial is used:

\[
\Phi = c_0 + c_1 (x - x_{i,j}) + c_2 (x - x_{i,j})(x - x_{i-1,j}) \tag{A.1}
\]

where the constants \( c_0 \), \( c_1 \) and \( c_2 \) are determined from the neighbouring points. Consider the situation for positive axial velocity in which case calculation of \( \Phi_{i-1,j} \) is biased toward the upwind node at \( \Phi_{i-2,j} \), then:

\[
c_0 = \Phi_{i,j} \tag{A.2}
\]

\[
c_1 = \frac{\Phi_{i-1,j} - \Phi_{i,j}}{x_{i-1,j} - x_{i,j}} \tag{A.3}
\]

\[
c_2 = \frac{\Phi_{i-2,j} - \Phi_{i,j}}{x_{i-2,j} - x_{i,j}} - \frac{\Phi_{i-1,j} - \Phi_{i,j}}{x_{i-1,j} - x_{i,j}} \left( \frac{1}{x_{i-2,j} - x_{i-1,j}} \right) \tag{A.4}
\]

and for the case when the axial velocity is negative, the coefficients in Eq. (A.1) are calculated using values of \( \Phi \) at the grid node \( i-1,j, i+1,j \) and \( i+1,j \), so that

\[
c_0 = \Phi_{i,j} \tag{A.5}
\]

\[
c_1 = \frac{\Phi_{i-1,j} - \Phi_{i,j}}{x_{i-1,j} - x_{i,j}} \tag{A.6}
\]

\[
c_2 = \frac{\Phi_{i+1,j} - \Phi_{i,j}}{x_{i+1,j} - x_{i,j}} - \frac{\Phi_{i-1,j} - \Phi_{i,j}}{x_{i-1,j} - x_{i,j}} \left( \frac{1}{x_{i+1,j} - x_{i-1,j}} \right) \tag{A.7}
\]