INFORMATION TO USERS

This manuscript has been reproduced from the microfilm master. UMI films the text directly from the original or copy submitted. Thus, some thesis and dissertation copies are in typewriter face, while others may be from any type of computer printer.

The quality of this reproduction is dependent upon the quality of the copy submitted. Broken or indistinct print, colored or poor quality illustrations and photographs, print bleedthrough, substandard margins, and improper alignment can adversely affect reproduction.

In the unlikely event that the author did not send UMI a complete manuscript and there are missing pages, these will be noted. Also, if unauthorized copyright material had to be removed, a note will indicate the deletion.

Oversize materials (e.g., maps, drawings, charts) are reproduced by sectioning the original, beginning at the upper left-hand corner and continuing from left to right in equal sections with small overlaps. Each original is also photographed in one exposure and is included in reduced form at the back of the book.

Photographs included in the original manuscript have been reproduced xerographically in this copy. Higher quality 6" x 9" black and white photographic prints are available for any photographs or illustrations appearing in this copy for an additional charge. Contact UMI directly to order.
LARGE EDDY PROBABILITY DENSITY FUNCTION (LEPDF) SIMULATIONS FOR TURBULENT REACTIVE CHANNEL FLOWS AND HYBRID ROCKET COMBUSTION INVESTIGATIONS

by

Jianwen Yi

Copyright © Jianwen Yi 1995

A Dissertation Submitted to the Faculty of the DEPARTMENT OF AEROSPACE AND MECHANICAL ENGINEERING In Partial Fulfillment of the Requirements For the Degree of DOCTOR OF PHILOSOPHY WITH A MAJOR IN MECHANICAL ENGINEERING In the Graduate College THE UNIVERSITY OF ARIZONA

1995
As members of the Final Examination Committee, we certify that we have read the dissertation prepared by Jianwen Yi entitled Large Eddy Probability Density Function (LEPDF) Simulations For Turbulent Reactive Channel Flows And Hybrid Rocket Combustion Investigations and recommend that it be accepted as fulfilling the dissertation requirement for the Degree of Doctor of Philosophy.

Kumar Ramohalli
Alfonso Ortega
Warren Dowler

Final approval and acceptance of this dissertation is contingent upon the candidate's submission of the final copy of the dissertation to the Graduate College.

I hereby certify that I have read this dissertation prepared under my direction and recommend that it be accepted as fulfilling the dissertation requirement.

Dissertation Director
Kumar Ramohalli
STATEMENT BY AUTHOR

This dissertation has been submitted in partial fulfillment of requirements for an advanced degree at The University of Arizona and is deposited in the University Library to be made available to borrowers under rules of the library.

Brief quotations from this dissertation are allowable without special permission, provided that accurate acknowledgement of source is made. Requests for permission for extended quotation from or reproduction of this manuscript in whole or in part may be granted by the copyright holder.

SIGNED: ________________

[Signature]
ACKNOWLEDGMENTS

The author considers himself fortunate in having the opportunity to work with Professor Kumar Ramohalli. His bright ideas, extraordinary patience, timely encouragement, and generous financial support ensure the success of this research.

He is grateful to Dr. A. Ortega, Dr. S. Z. She, Dr. H. Fasel, Dr. M. M. Rai (NASA AMES Research Center), Dr. C. L. Chan, Dr. T. Balsa, and Dr. C. F. Chen. Even a brief discussion with them can save considerable search time in the libraries. He wishes to express his respectful gratitude to Professor Warren Dowler, particularly for his detailed advice during his visits to the University of Arizona.

The author thinks the lectures by Dr. Stephen Mahaney and Dr. Mary Bailey are very important part of his education. These lectures helped him to get important background in computer science.

The special thanks are directed to Mr. Bill Escher (NASA HQ), Mr. Ben Goldberg, and Mr. Jery Cook (NASA MSFC) for their years of consecutive funding for the experimental part of this research.

The author feels that help from the following colleagues is invaluable: Mr. Milton Schick, Mr. Mario Rascon, Mr. Matt Hilbert, Mr. Brian Wygle, Ms. Teresa Dereniak, Mr. Gary Honea, Mr. Ron Bates, Mr. In-Kyung Sung, and Mr. Mike Jones. It is author's pleasure to thank Dr. Yongsheng Yang, for his generous suggestions.

The support of his wife, Feng Ren, and his son Hubert, has abated the task immensely. There is no better place than to dedicate the dissertation to them.
# TABLE OF CONTENTS

LIST OF FIGURES ........................................................................... 10

ABSTRACT ................................................................................. 14

CHAPTER 1: INTRODUCTION ......................................................... 16

1.1 Characteristics of Turbulent Flows ........................................... 17
1.2 Characteristic Length and Time Scales in Turbulent Flows ..... 20
  1.2.1 Integral Length Scale .................................................... 20
  1.2.2 Taylor Microscale ........................................................ 21
  1.2.3 Kolmogorov Microscale ............................................... 23
  1.2.4 Length and Time Scales For Turbulent Reactive Flows ... 24
1.3 Turbulence Energy Spectrum ................................................. 26
1.4 Turbulent Reactive Flows ...................................................... 32
1.5 The Present Advancements in State-of-The-Art ..................... 36

CHAPTER 2: NUMERICAL SIMULATION APPROACHES FOR TURBU-

LENT REACTING FLOWS .......................................................... 40

2.1 DNS Approach ...................................................................... 41
2.2 Moment Approach .................................................................. 44
2.3 PDF Approach ....................................................................... 47
2.4 LES Approach ....................................................................... 49
2.5 LEPDF Method ...................................................................... 54
CHAPTER 3: FORMULATION OF LE PDF METHOD ................................................. 57
3.1 Velocity Flow Field ................................................................. 58
  3.1.1 Filtered Equations .......................................................... 58
  3.1.2 Filter Discussion ............................................................. 60
  3.1.3 Subgrid Scale Modeling .................................................. 61
3.2 Passive Scalar Transport ...................................................... 63
  3.2.1 Filtered PDF Equation ..................................................... 63
  3.2.2 Modeling for PDF Transport Equation .............................. 64
  3.2.3 Chemistry Consideration .............................................. 65

CHAPTER 4: NUMERICAL SIMULATION TECHNIQUES ................................. 67
4.1 Numerical Scheme ............................................................... 67
  4.1.1 Numerical Schemes for the Velocity Flow Field ............... 68
  4.1.2 Monte Carlo Method for Scalar PDF Equation ................. 88
4.2 Initial and Boundary Conditions .......................................... 98
  4.2.1 Boundary Conditions ..................................................... 98
  4.2.2 Initial Conditions ........................................................ 102
4.3 Supercomputing Techniques ................................................ 104

CHAPTER 5: LES SPATIAL SIMULATIONS FOR FULLY DEVELOPED
  TURBULENT CHANNEL FLOWS .................................................... 108
5.1 Code Verifications ............................................................ 109
5.2 Generation of Initial and Inflow Conditions ........................... 111
5.3 Mean-Velocity Profile and Turbulence Statistics ...................... 114
   5.3.1 Mean-Velocity Profile ............................................... 114
   5.3.2 Turbulence Intensity ................................................ 115
8.2.1 Gas Phase Theory .................. 172
8.2.2 Condensed Phase Theory ............. 176

CHAPTER 9: POLYMER OXIDATIVE DEGRADATION MODEL ...... 181
9.1 Kinetics of Polymer Oxidative Degradation ............... 183
9.2 Surface Regression Correlation .................... 188
9.3 Results and Discussions .......................... 191
   9.3.1 Polymer Inert Degradation ................. 192
   9.3.2 Polymer Oxidative Degradation ............. 194

CHAPTER 10: SOLID ROCKET COMBUSTION SIMULATOR AND ENVIRONMENTAL IMPACT OF HYBRIDS ............... 198
10.1 Solid Rocket Combustion Simulator .................. 198
10.2 Hybrids As An Environmental Solution for Solids ....... 203

CHAPTER 11: HYBRID ROCKET INTERNAL BALLISTICS INVESTIGATIONS .................. 210
11.1 Regression Rate Variation Along Fuel Grain ............... 210
11.2 Experimental Investigation of Scale-up Principles ....... 210
11.3 Catalytic Combustion of Metallized Fuel ................. 212
   11.3.1 HTPB Degradation Kinetics ............... 212
   11.3.2 Oxidative Degradation of Metallized Fuel ...... 214
   11.3.3 Experimental Test Matrix .................. 216
   11.3.4 Results And Discussion ................... 218

CHAPTER 12: PRESENT ADVANCEMENTS ...................... 221
12.1 Present Advancements ........................... 221
APPENDIX A: HYBRID ROCKET OXIDIZER FEED SYSTEM ANALYSIS 224
  A.1 Flow Analysis for Nozzle .......................... 225
  A.2 Flow Analysis for Combustion Chamber ............... 226
  A.3 Flow Analysis for Oxidizer Feed Duct ................ 230
  A.4 Results and Discussion ................................ 232

APPENDIX B: DESIGN OF HYBRID ROCKETS AND EXPERIMENTAL
  SET-UP ...................................................... 240

APPENDIX C: HYBRID ROCKET FUEL MANUFACTURE TECHNOLOGY 243

REFERENCES .................................................. 247
# LIST OF FIGURES

1.1 Typical Eddies in a Turbulent Boundary Layer .......................... 20
1.2 Turbulence Energy "Cascading" Process ................................. 30
1.3 Normalized Energy and Dissipation Spectra for $Re = 200,000$, Ref. 2 33
1.4 Overall Plan for Numerical Simulations of Engineering Combustion
   Systems ........................................ 38

2.1 Projected Use of Simulations in Turbulence Physics (left) and Aerothermodynamics (right), Ref. 14 ................................. 43
2.2 Turbulent Boundary Layer on a Wall (above), Large-scale structure
   in a turbulent mixing layer(below), Ref. 35 ................................ 51
2.3 Homogeneous Turbulence Behind a Grid, Ref. 35 ........................ 52

4.1 Schematic of Reacting, Spatially Developing Channel Flow ............ 68
4.2 Staggered Grid Showing Physical Locations at Which the Dependent
   Variables Are Defined ........................................ 80

5.1 Mean-Velocity Profile From LES Spatial Simulation and Experimental
   Data .................................................. 115
5.2 Turbulence Intensity in Streamwise Direction ........................... 116
5.3 Turbulence Intensity in Normal Direction ................................ 117
5.4 Turbulence Intensity in Spanwise Direction ............................. 118
5.5 Normalized Reynolds Stress in the Near Wall Region .................. 119
11.4 HTPB TGA Results in O2 Containing Atmosphere .......... 214
11.5 HTPB/Pyrogallic Acid Fuel TGA Results .......... 217
11.6 HTPB/Calcium Compound Fuel TGA Results .......... 218
11.7 The Metallic Ions Effects On HTPB Pyrolysis .......... 219
11.8 The CuO Effects On HTPB Pyrolysis .......... 220
A.1 The Schematic of Hybrid Rocket Systems .......... 225
A.2 Differential Element of The Combustion Chamber .......... 226
A.3 Friction Factor(4f) vs. Re. (Fig 5.2 of Ref. [162]) .......... 233
A.4 $M_3$ vs. $\frac{A_I}{A_t}$ .......... 235
A.5 $M_2$ vs. $\frac{A_I}{A_t}$ .......... 236
A.6 $M_1$ vs. $M_2$ .......... 237
A.7 $\frac{G}{P_c}$ vs. $\frac{A_I}{A_t}$ .......... 238
A.8 $\frac{P_d A_d}{A_d}$ vs. $M_2$ .......... 239
B.1 Schematic Structure of Experimental Hybrid Rocket .......... 241
B.2 A Firing Experimental Hybrid Rocket .......... 242
C.1 Baker-Perkins APV Rocket Fuel Mixer .......... 244
C.2 Flow Chart of Rocket Fuel Manufacture Process .......... 245
ABSTRACT

A new numerical simulation methodology, Large Eddy Probability Density Function (LEPDF), and corresponding numerical code have been developed for turbulent reactive flow systems. In LEPDF, large scale of turbulent motion is resolved accurately. Small scale of motion is taken care of by a modified Smagorinsky subgrid scale model. Chemical reaction terms are resolved exactly without modeling. A numerical scheme to generate inflow boundary conditions has been proposed for spatial simulations of turbulent flows. Monte-Carlo scheme is used to resolve filtered PDF (Probability Density Function) evolution equation.

The present turbulent simulation code has been successfully applied in the simulations of transpired and non-transpired fully developed turbulent channel flows. It more accurately predicts turbulent channel flows than the existing temporal simulation code with only 27% of the grid size of the temporal simulation code. It has been shown that "Ejection" and "Sweep" are two dominant events in the wall region of turbulent channel flows. They are responsible for about 120% of the total turbulent production. Their interactions have negative contributions to the turbulent production, thereby keeping the total 100%. Counter-rotating vortex is a major mechanism responsible for turbulent production in boundary layer.

It has also shown that injection from channel side walls increases the boundary layer thickness and turbulence intensities, but decreases the wall friction and heat transfer. Suction has opposite effects.
A state-of-the-art hybrid rocket research laboratory has been established. Lab-scale hybrid rockets with fuel port diameters ranging from 0.5 to 4.0 inches have been designed and constructed. Rocket testing facilities for routine measurements and advanced combustion diagnosis techniques, such as infrared image technique and gas chromatography, are well developed. A computerized data acquisition/control system has been designed and built.

A new Cu^{++} based catalyst is identified which can improve the burning rate of general HTPB based hybrid rocket fuel by 15%. Scale-up principles are developed through a series of experimental testing on different sizes of hybrid rockets. A polymer (rocket fuel) degradation model with consideration of catalytic effects of small concentration of oxidizer near fuel surface is developed. The numerical predictions are in very good agreements with experimental data.
CHAPTER 1

INTRODUCTION

Turbulent flow is a very common flow phenomena, most of flows in nature and in engineering applications are turbulent. Everyday life gives us an intuitive knowledge of turbulence in fluids: the smoke of a cigaret or smoke over a fire exhibits a disordered behaviour characteristic of the motion of the air which transport it. Generally speaking, the boundary layer in the earth’s atmosphere is turbulent, so are the jet streams in the upper troposphere and cumulus clouds. The water currents below the surface of the ocean are turbulent; the gulf stream is a turbulent wall-jet kind of flow. Another very important example is the boundary layer growing on aircraft wings.

Most combustion processes involve turbulence and often even depend on it. Turbulent boundary layer is a typical example of turbulent combustion flow. It plays an important role in a variety of practical engineering problems ranging from simple fires to ablation of reentry vehicles. The hybrid rocket, as a promising alternative chemical rocket propulsion system, is a somewhat specialized example of the boundary combustion.

Aerospace scientists investigate the origin and the development of the turbulence in order to delay or to completely avoid turbulent boundary flow on the wing, thus to decrease the drag. Chemical engineers use turbulence to mix and homogenize
fluid mixtures and to accelerate chemical reaction rates in liquids or gases. Study of turbulence is clearly an interdisciplinary activity, which has a very wide range of applications.

1.1 Characteristics of Turbulent Flows

Although it is probably not wise to make a rigid definition of a turbulent flow, the flows we call turbulent do have certain properties in common. For example, waves on the surface of water should not be classified as turbulence. There are too many mechanisms that generate waves, and the active interaction of the air complicates this flow. It does not possess the mechanisms and characteristics of the typical type of turbulent flows.

Turbulent flows have irregular fluctuations of velocity in all three directions. The intensity of the fluctuations is variable, but is customarily 15% or less of the mean velocity. A time history of the velocity at a point looks like a random signal. Nevertheless, there is structure to the fluctuations. Strictly speaking, the turbulent fluctuations are not random (mathematicians have a definition of the term “random variable”, which turbulent irregularities do not meet).

The irregularities in the velocity field have certain spatial structures known as eddies. This is a vague term that may be applied to any spatial flow pattern that persists for a short time. An eddy may be like a vortex, an imbedded jet, a mushroom shape, or any other recognizable form. Large eddies are quite evident in the picture of the boundary in Fig. 1.1. Eddies are not isolated; small eddies are inside larger eddies, and even smaller eddies exist inside the small eddies. Such small-scale motions are also visible in Figure 1.1. One of the main characteristics of turbulence is a continuous distribution of eddy sizes. A flow where the irregularities are limited
to a few separated frequency bands cannot be identified as a turbulent flow.

The turbulence in a flow is self-sustaining. The processes, which are not well defined or understood, generate more turbulence and maintain the irregular motion. Once a flow becomes unstable and turbulence develops, it does not simply die out and repeat the process as a limit-cycle oscillation. Turbulence, once initiated, continues and perpetuates itself without diminishing. Thus, in sustaining turbulence, the transition mechanisms or the original instability, do not have much influence to the subsequent flow field.

A gradient in the mean velocity profile is another characteristic. This mean shear is a necessary condition for the turbulence to be self-sustaining. Otherwise the turbulence, as in the case of the grid turbulence, will die out eventually. In shear layer, boundary layer, jets, and wakes, the region where turbulence exist coincides with the region of mean shear.

In confined flows, turbulence may grow to cover the entire flow, but in all other cases the turbulent region has a limited extent. This is not to say that some fluid is always turbulent and other is always nonturbulent. Another characteristic of turbulent flows is that they entrain nonturbulent fluid, so that the extent of the turbulent region grows. Consider the jet as an example. The fluid that composes the jet continues to increase by entrainment as the jet extends further from the origin.

Turbulent flows are diffusive. Just as random molecular motions in a gas are responsible for viscous diffusion, thermal diffusion, and mass diffusion, a turbulent eddy can transport fluid from a region of low momentum and deposit it in a region of high momentum. Although the actual process is more complicated than that, it is clear that turbulence tends to mix fluid and thereby has a diffusive effect. The term
Eddy diffusion is frequently used to distinguish this effect from molecular diffusion. Eddy diffusion can be 10 or 100 times stronger than the molecular diffusion.

All turbulent flows involve processes that change the length scale of the eddies. Once again, the mechanism of these processes is not well understood, but it is certain that they are a major characteristic of turbulent flows. These processes act in both directions. A modest-size irregularity or eddy grows and become a large eddy. The largest eddies in a flow are about as large as the thickness of the turbulent region. The size of the largest eddies in a boundary layer is about \( \delta \), the boundary layer thickness, and that of the largest eddies in a jet is about equal to the local jet diameter. On the other hand, there are processes that reduce the eddy size. Turbulent eddies are continually formed with smaller and smaller length scales. Viscosity puts a lower limit on the eddy size. When the size of an eddy becomes very small, viscous forces, because of the steep velocity gradient, become very important. The viscous force tend to destroy the smallest eddies. This lower limit of the eddy scale is called kolmogorov scale.

The last major characteristic of turbulent flows is that they are dissipative. Any flow with viscosity has viscous dissipation, but turbulent flows have much more of it because the small-scale eddies have steep velocity gradients. The energy dissipated in the small eddies dominates that dissipated in the largest eddies and in the mean flow. Since the small eddies dissipate energy and tend to destroy themselves, the scale-changing which produces smaller eddies is a necessary element of self-sustaining turbulence.
1.2 Characteristic Length and Time Scales in Turbulent Flows

1.2.1 Integral Length Scale

Most flows have at least one characteristic velocity, \( u \), and characteristic length scale, \( L \), of the device in which the flow takes place. As mentioned earlier, there is a continuous distribution of length scales associated with the turbulent fluctuations of velocity components and of state variables. First, there is a length, \( l \), characterizing the large eddies, those with low frequencies and short wave lengths. Experimentally, \( l \), can be defined as a length scale beyond which various fluid-mechanical quantities become essentially uncorrelated, typically, \( l \), is less than, \( L \), but of same order of magnitude. This length scale, \( l \), is called integral length scale. The integral length
scale together with velocity fluctuation, $u$, is used to define a turbulence Reynolds number,

$$R_l = \frac{ul}{\nu}$$  \hspace{1cm} (1.1)$$

which has more direct bearing on the structures of turbulence in flows than does $R_e$ ($R_e = U*L/\nu$). The cascade view (discussed later) of turbulence dynamics is restricted to large values of $R_l$. Generally $R_l < R_e$. The role of integral length scale can also be viewed through the scale relation,

$$\frac{\partial U_i}{\partial x_j} \sim \frac{u}{l}$$  \hspace{1cm} (1.2)$$

where $U_i$ is the mean flow velocity, $u$ the velocity fluctuation, and $l$ the integral length scale.

### 1.2.2 Taylor Microscale

There is at least two ways to define the Taylor microscale. One definition is associated with the shape of the velocity autocorrelation function. Here we adopted the definition associated with the energy dissipation. The dissipation of energy is proportional to $\overline{S_{ij}S_{ij}}$; this consists of several terms like $(\overline{\partial u_i \partial x_j})^2$, most of which can not be measured conveniently. However, the small-scale structure of turbulence tends to be isotropic. In isotropic turbulence, the dissipation rate is equal to

$$\epsilon = 2\nu \overline{S_{ij}S_{ij}}$$

$$= 15\nu \left( \frac{\partial u}{\partial x_1} \right)^2$$  \hspace{1cm} (1.3)$$
The coefficient 15 in Eq. (1.3), is considerably larger than one because so many components are involved. Let us define a new length scale $\lambda$ by:

\[
\left( \frac{\partial u_1}{\partial x_1} \right)^2 \equiv \frac{u_1^2}{\lambda^2} = \frac{u^2}{\lambda^2}
\]

(1.4)

The length scale is called the Taylor microscale in honor of G. I. Taylor, who first defined Eq. (1.4). The substitution $\overline{u_1^2} = u^2$ can be made because in isotropic turbulence $\overline{u_i^2} = \overline{u_j^2} = \overline{u_3^2}$, so that $u^2$, which was defined as $\frac{1}{3}\overline{u_iu_i}$, is equal to $\overline{u_1^2}$. Since the small-scale structure of turbulence at large Reynolds number $R_l$ is always approximately isotropic, we use

\[
\epsilon = 15\nu \frac{u^2}{\lambda^2}
\]

(1.5)

A relationship between $\lambda$ and $l$ can be obtained from the simplified energy budget equation. The turbulent energy budget, reads

\[
U_j \frac{\partial}{\partial x_j} \left( \frac{1}{2} \overline{u_iu_i} \right) = -\frac{\partial}{\partial x_j} \left( \frac{1}{\rho} \overline{u_j P} + \frac{1}{2} \overline{u_iu_iu_j} - 2\nu \overline{s_{ij}s_{ij}} \right) - \frac{1}{\rho} \overline{u_iu_jS_{ij} - \nu s_{ij}s_{ij}}
\]

(1.6)

where, as always, the capitalized letters are for mean flow field properties, lower case letters for the turbulent fluctuation quantities. It can be seen that the rate of change of $\frac{1}{2} \overline{u_iu_j}$ is that due to pressure-gradient work, transport by turbulent velocity fluctuations, transport by viscous stresses, and two kinds of deformation work.
In a steady, homogeneous, pure shear flow (in which all averaged quantities except \( U_j \) are independent of position and in which \( S_{ij} \) is a constant), the Eq. (1.6) reduces to

\[
-\bar{u}_i \bar{u}_j S_{ij} = 2 \nu \bar{s}_{ij} \bar{s}_{ij}
\]  

This equation states that in this flow the rate of production of turbulent energy by Reynolds stress equals the rate of viscous dissipation. It should be noted that in most shear flows production and dissipation do not balance, though they are nearly always of the same order of magnitude. If \( S_{ij} \) is of order of \( u/l \) and if \(-\bar{u}_i \bar{u}_j \) is of order of \( u^2 \), together with Eq. (1.5), we obtain,

\[
Au^2 \frac{u}{l} = 15 \frac{\nu u^2}{\lambda^2}
\]  

The ratio

\[
\frac{\lambda}{l} = \left( \frac{15}{A} \right)^{\frac{1}{2}} \left( \frac{u l}{\nu} \right)^{-\frac{1}{2}} = \left( \frac{15}{A} \right)^{\frac{1}{2}} R_t^{-\frac{1}{2}}
\]  

In Eq. (1.7 & 1.8) \( A \) is an undetermined constant, which is presumably of order one. Because in all turbulent flows, \( R_t \ll 1 \), the Taylor microscale \( \lambda \) is always much smaller that the integral scale \( l \). Again we see that dissipation of energy is due to the small eddies of turbulence.

1.2.3 Kolmogorov Microscale

The Taylor microscale \( \lambda \) is not the smallest length scale occurring in turbulence. The smallest scale is the Kolmogorov microscale \( \eta \), which is defined as
The Kolmogorov micro scales of time and velocity are defined as

\[ T = \left( \frac{\nu^3}{\epsilon} \right)^\frac{1}{4} \]  

\[ u = \left( \frac{\nu}{\epsilon} \right)^\frac{1}{4} \]  

So, the Kolomogrov Reynolds number

\[ R_\eta = \frac{\eta u}{\nu} = \left( \frac{\nu^3}{\epsilon} \right)^\frac{1}{4} \left( \frac{\nu}{\epsilon} \right)^\frac{1}{4} \equiv 1 \]  

The ratio of Kolmogorov length scale and the integral scale can be obtained directly by the definition of the Kolmogorov length scale,

\[ \frac{l}{\eta} = \frac{l}{\nu^3/\epsilon^\frac{3}{4}} = \left( \frac{u}{\nu} \right)^\frac{3}{4} = R_t^\frac{3}{4} \]  

1.2.4 Length and Time Scales For Turbulent Reactive Flows

There are more characteristic length and time scales associated with reactive flows in addition to the characteristic scales associated with the "cold" flows. One length
scale is the characteristic thickness of a premixed laminar flame, denoted here by \( \delta \). It may be expected that the nature of turbulent reactive flows may differ considerably, depending on whether \( \delta < \eta, \eta < \delta < \lambda, \lambda < \delta < l, \) or \( l < \delta \) (\( \lambda \) and \( l \) are Taylor microscale and integral length scale). wrinkled laminar flames may occur when \( \delta < \eta \) and broadly distributed reactions when \( l < \delta \). The nature of turbulent flames implied by these various inequalities has not been completely explored. In theories it is often assumed that \( \delta < \eta \).

Characteristic times for chemical conversion can be defined directly from chemical reaction rate expressions. To be specific, consider the bimolecular reaction with the rate constant given by Arrhenius formulation. With characteristic temperature \( T_c \) representative of temperatures at which the reaction occurs, as well as representative reactant concentration, \( Y_{10} \) and \( Y_{20} \), the characteristic chemical conversion time \( \tau_c \) can be expressed as

\[
\tau_c = \left( Y_{10} Y_{20} \rho_0 B e^{-\frac{T_{\infty}}{T_c}} \right)^{-1}
\]

(1.14)

Chemical lengths may be constructed from this as \( U \tau_c \) or \( u \tau_c \). Comparison of an appropriate chemical length (or time) with a fluid-dynamical length (or time) provides a nondimensional parameter that has a bearing on the relative rate of the chemical reaction. Nondimensional parameters of this conventional type are termed Damköhler numbers, or more precisely, Damköhler's first similarity group.

An example is

\[
D = \frac{l}{u \tau_c}
\]

(1.15)

For large Damköhler numbers, chemistry is fast and reaction sheets (very thin reaction zone) may develop. For small Damköhler numbers, chemistry is slow, and
“well-stirred” flows may occur.

1.3 Turbulence Energy Spectrum

The energy exchanges between the mean flow and the turbulence is governed by the dynamics of the large eddies. Large eddies contribute most of the turbulence production, because the turbulence production increases with the eddy size. The energy extracted by the turbulence from the mean flow thus enters the turbulence mainly at scales comparable to the integral scale $l$.

The viscous dissipation of turbulent energy, on the other hand, occurs mainly at scales comparable to the Kolmogorov microscale $\eta$. This implies that the internal dynamics of turbulence must transfer energy from large eddy scales to small eddy scales. All of the available experimental evidence suggests that this spectral energy transfer proceeds at a rate dictated by the energy of the large eddies (which is of order $u^2$) and their time scale (which is of order $l/u$).

A turbulent flow field can (conceptually, at any rate) be imagined as divided into all eddies smaller than a given size and all eddies larger than that size. The smaller eddies are exposed to the strain-rate field of the larger eddies. Because of the stretching, the vorticity of the small eddies increases, with a consequent increase in their energy at the expense of the energy of the larger eddies. In this way, there is a flux of energy from larger to smaller eddies.

It is well known that an autocorrelation and the corresponding spectrum are a Fourier-transform pair. If the correlation is a function of spatial separation, the spectrum is a function of wave number. A certain eddy size, say $l$, is thus associated with a certain wave number, say $k$. An “eddy” of wave number $k$ may be thought of as some disturbance containing energy in the vicinity of $k$. It seems reasonable to
think of an eddy as a disturbance contributing a narrow spike to the spectrum at k. However, a narrow spike in the spectrum creates slowly damped oscillations (of wavelength $2\pi/k$) in the correlation. Such a correlation is characteristic of wavelike disturbances, but not of eddies. We expect eddies to lose their identity because of interaction with others within one or two periods or wavelengths. Therefore the contribution of an eddy to the spectrum should be a fairly broad spike, wide enough to avoid oscillatory behavior in the correlation.

It is convenient to define an eddy of wave number k as a disturbance containing energy in a range of wave number, say 0.62k and 1.62k. This choice centers the energy around k on a logarithmic scale, between $\log(1.62k/k) = \log(k/0.62k) = 0.5$. It also makes the width of the contribution to the spectrum equal to k.

The transform of a narrow band around k is a wave of wavelength $2\pi/k$, with the envelop whose width is the inverse of the bandwidth. Now, because the bandwidth selected is k, the width of the envelop of the eddy is of order $1/k$.

The energy of all eddies of size $2\pi/k$ is roughly proportional to $E(k)$ times the width of the eddy spectrum, which is k. Hence, a characteristic velocity is given by $(kE(k))^{1/2}$. The size of the eddy is about $2\pi/k$, so that the characteristic strain rate (and the characteristic velocity) of an eddy of wave number k is given by

$$ s(k) = \frac{(kE(k))^{1/2}}{2\pi/k} = \frac{(k^3E(k))^{1/2}}{2\pi} \tag{1.16} $$

The strain rate of large eddies, which contain most of energy, is of order $u/l$, while the small-scale strain-rate fluctuations are of order $u/\lambda$ ($\lambda$ is a Taylor microscale). Therefore, we should expect that the strain rate $s(k)$ increases with wave number.
The energy spectrum is continuous; for the purposes of this discussion, however, we may think of the spectrum as being made up from eddies of discrete size. The strain rate imposed on eddies of wave number $k$ due to the eddies of the next large size (which extends from $0.24k$ to $0.62k$ centered around $0.38k$) is $s(0.38k)$, which is about $\frac{1}{2}s(k)$ if $s(k)$ is proportional to $k^{2/3}$. It can be shown in the same way that the strain rate due to eddies two size larger than $2\pi/k$ is again about half as large. So we conclude that of the total strain rate felt by an eddy of wave number $k$, one-half comes from eddies of the next larger size, and another quarter from the next larger size. Therefore, we expect that most of the energy crossing a given wave number comes from eddies with slightly smaller wave number.

The question now is which eddies benefit most from the energy transfer across wave number $k$. Energy transfer depends on the ability of the strain rate to align the smaller eddies so that the velocity components become different. The strain rate has to overcome the tendency of eddies to equalize the velocity components. This tendency of eddies is called “return to isotropy”; the lack of isotropy (or anisotropy) that can be generated by the strain rate depends on the time scale for return to isotropy relative to the time scale for the straining motion. Because the strain rate has dimensions of $time^{-1}$, the time scale of return to isotropy is roughly $1/s(k)$ for eddies of wave number $k$. This means that those eddies would return to isotropy in a time of order $1/s(k)$, if the strain rate were removed. Because smaller eddies have larger strain rates, small eddies return isotropy rapidly.

If $p$ is the combined strain rate of all eddies with wave number below $k$, the time scale of the applied strain rate is of order $1/p$. It appears reasonable to assume that the degree of anisotropy is proportional to $p/s(k)$. It can be shown that the energy transferred from all larger eddies to an eddy of wave $k$ is then approximately
The energy absorbed by the eddies of next smaller size is only one-fourth of the above energy. Eddies of wave number $k$ thus receive about two-third of the total energy transfer, those of next smaller size receive about one-sixth and all smaller eddies combined also receive about one-sixth.

A crude picture in Fig. 1.2, is beginning to emerge. Most of the energy that is exchanged across a given wave number apparently comes from the next larger eddies and goes to the next smaller eddies. It seems fair to describe the energy transfer as cascade, much like a series of waterfalls, each one filling a pool that overflows into the next one below. This concept proves to be exceptionally useful, because the largest eddies and the smallest eddies clearly have no direct effect on the energy transfer at intermediate wave numbers.

We have found that the anisotropy of eddies depends on the time-scale ratio $p/s(k)$. The strain rate of the large, or "energy-containing" eddies is comparable to the strain rate of the mean flow ($\partial U/\partial y \sim u/l$). Therefore, large eddies have a steady anisotropy due to the strain rate of the mean flow, which maintains a steady orientation. On the other hand, the strain rate of small eddies is large compared to that of the mean flow and of the large eddies, so that no permanent anisotropy can be induced at small scale. This does not mean that small eddies are isotropic, because energy transfer is possible only if eddies are aligned with a strain rate. However, the anisotropy is temporary; eddies of a given size are stretched mainly by somewhat larger eddies, whose strain-rate field is constantly shifting in magnitude and direction. As the eddy size becomes smaller, the permanent anisotropy decreases, so that at small scales the strain-rate field itself may be expected to be isotropic in the mean. In other words, turbulence is increasingly "scrambled" at small scales, and any permanent sense of direction is lost. This concept is called
Figure 1.2: Turbulence Energy "Cascading" Process
local isotropy; it was proposed by A. N. Kolmogorov in 1941 [2]. The adjective "local" refers to small scales (large wave number).

Local isotropy does not exist if the Reynolds number is not large enough. The strain rate of the mean flow is of order $u/l$; the strain rate of the smallest eddies is of order $u/\lambda \sim (\varepsilon/\nu)^{1/4}$. We probably need $u/l \geq 10u/l$ in order to have local isotropic at the smallest scales. Consequently, $l/\lambda \sim Re^{1/4}$ needs to be at least 10, giving a Reynolds number of at least 100. Similarly $\lambda/\eta \sim 10$. This means that the Taylor microscale length is at least 10 times larger than Kolmogorov length scale.

In the part of the spectrum in which local isotropy prevails, time scales are short compared to those of the mean flow. This means that small eddies respond quickly to changing conditions in the mean flow. Therefore, small eddies always are in approximate equilibrium with local conditions in the mean flows, even though the latter may be evolving. For this reason, the range of wave numbers exhibiting local isotropy is called equilibrium range. It begins at a wave number where $s(k)$ first becomes large compared to the mean strain rate, and it includes all higher wave numbers.

In the equilibrium range, time scales are so short that the details and the energy transfer between the mean flow and the turbulence (which occurs mainly at large scales) can not be important. However the amount of energy cascading down the spectrum should be a major parameter. Because all energy is finally dissipated by viscosity, the total amount of energy transfer must be equal to the dissipation rate and the second major parameter should be viscosity itself. Most of the viscous dissipation of energy occurs near the Kolmogorov microscale $\eta$, as we discussed before.

In the large-scale range, the spectrum scales in a different way. If the spectral
Reynolds number \( s(k) / k^2 \nu \) is large, we do not expect viscosity to be relevant. The principal parameters are those that describe the energy transfer from the mean flows to the turbulence and the energy transfer from large to small scales.

There exists a scale range called inertial-subrange between equilibrium range and the large-scale range. In this range, the two limiting ranges for Kolmogorov range and for large-scale range overlap. In other words, we should be able to go to the small-scale end of the large-scale spectrum and to the large-scale end of the Kolmogorov spectrum simultaneously. It can be shown that the energy spectrum in the inertial subrange is

\[
E(k) = \alpha \varepsilon^{\frac{3}{2}} k^{-\frac{5}{3}}
\]  

Experimental data indicate that \( \alpha = 1.5 \) approximately. In the inertial subrange, no energy is added by the mean flow and no energy is taken out by viscous dissipation, so that the energy flux across each wave number is constant. In other words, the central part of the energy cascade is conservative. The normalized energy and dissipation spectrum is shown in Fig 1.3.

1.4 Turbulent Reactive Flows

Turbulent reactive flows are difficult to predict for the simple reason that neither turbulent transport nor chemical kinetics, the two important phenomena which form their base, are themselves adequately understood. Turbulent reactive flows are generally very complex, involving the interactions of chemical, thermodynamic, and fluid mechanical processes. As mentioned before, the turbulence increases mixing, which can significantly speed up the overall chemical reaction, while the heat release and the induced density and pressure changes can significantly affect the turbulent
Figure 1.3: Normalized Energy and Dissipation Spectra for $Rl = 200,000$, Ref. 2
structures. As discussed in the section of the turbulent scales, the relative magnitude of the chemical reaction time scale and the turbulent mixing time scale is of dominant role in the turbulent reactive flows. If the time scales of the chemical reactions are much greater than the time scales of turbulent mixing, the reactant will be well mixed before significant chemical reaction takes place. This category of reactive flows are called premixed flow. On the other hand, if the time scales of the chemical reactions are of the same order as, or much less than, the turbulent mixing time, the reaction rates are controlled by the ability of the turbulence to bring the chemical species together. This is called nonpremixed flame (or traditionally called “diffusion flame”) which are often the cases in the industrial applications. For nonpremixed flame, the overall reaction rates depends more on the turbulent mixing rates and less on the specific reaction rates.

The evident importance of turbulent flows involving mixing and chemical reactions has stimulated a wide variety of theoretical approaches, as revealed in a number of reviews [3, 4, 5]. Both the NASA Ames and NASA Langley research centers are very active in the simulations of the turbulent reacting flows [6, 7].

In order to understand and predict the complex, turbulent reactive flows, statistical methods are generally introduced and one of two main approaches is usually used: the moment equation or the probability density function methods. In the moment equation method (e.g. $k - \epsilon$ method), averages (usually time averages) of the relevant chemical/fluid mechanical equations are averaged. This gives a rise to a closure problem, wherein there are more unknown quantities than equations. This problem is resolved (to some extent) by introducing ad hoc assumptions relating various unknown quantities and thus closing the system of equations [3]. The main stumbling block for this method is in proposing a reasonable closure model. This is
especially true for the reaction rate terms in the equations for the chemical species concentrations. As discussed later, even for very simple one step binary reaction, the averaging of chemical reaction rate will introduce many new unknowns. For each new unknown, a closure relation needs to be proposed to relate the new unknown to the primary unknowns such as temperature, velocity components, and species concentrations.

The second major approach, the probability density function (pdf) approach, relies on the equation for the (joint) pdf for the relevant physical variables [8]. The closure problem for the reaction rate term is totally avoided. However, closure problems for other terms do appear. Moreover, the major large structure, coherent structure is not well resolved. The numerical solution of the resulting equations can become very difficult. This is because the independent variables in this approach are the usual independent variables together with the dependent variables in the original problem. Thus their number could be very large. In order to avoid this problem, Monte Carlo methods have been introduced [9, 10]. Hybrid methods have also been employed. For example, the pdf approach of Janicka and Kollman [11] use moment equations for the turbulent kinetic energy and dissipation rates in addition to the equation for the pdf.

With the development of the modern computer technologies, more memory and higher computational speed are available in the advanced supercomputers. Nowadays, direct numerical simulations (DNS) emerge as a very powerful numerical simulation technology. Direct numerical simulations involve the numerical solution of the time development of the detailed, unsteady structures in a turbulent flow field. With very efficient algorithm, the fully nonlinear governing equations are solved directly without any turbulence model involved. The greatest advantage of this technology
is that the closure problems for the flow quantities and chemical reaction quantities are circumvented totally. The main disadvantage is that only limited spatial and temporal resolution can be achieved with today's computer resource, which limits the range of space and time scales. In order to make the simulation accurate and meaningful, the smallest resolved computation scale should be down to the Kolmogorov scale. Evidently the resolved largest scale is the scale of the computational domain. The grid point limitation in each computational direction (imposed by the computer resource) will be transferred to the limitation of the ratio of the largest resolved scale to the smallest resolved scale. The ratio is related to the turbulent Reynolds number through the Eq. (1.13) discussed in the section of turbulent scales. Nevertheless, the direct numerical simulations have been used widely to improve our understanding of the physics of turbulence.

As discussed early that the small scale turbulence tends to be universal, but the large scale turbulence varies dramatically from one flow to another. The large eddy simulation (LES) is based on the above two facts of the turbulent flows. In the large eddy simulation the large scale structure of turbulent flow is resolved exactly, while the small scale (subgrid scale) is accounted by a subgrid scale model. The greatest advantage of this scheme is that the computational domain can be much bigger than that of direct numerical simulation with today's computer resource. The main disadvantage with this method is same as the one with the moment method. The closure problems related to chemical reaction rate still needs to be solved.

1.5 The Present Advancements in State-of-The-Art

In the present study, a new numerical simulation method, Large Eddy Probability Density Function (LEPDF) scheme, is developed for turbulent reactive flows. With
the LEPDF method, the momentum is integrated by the LES method. The species transport and chemical reaction contribution are resolved by pdf method. Accordingly, the large scale motion, coherent structure, scalar macro transport are resolved EXACTLY, the subscale motion tend to be very universal and is taken care of by the subgrid (SGS) model as in the LES method. The molecular mixing, the turbulent mixing, and chemical reaction are well resolved by the PDF approach. The major closure problem related to the chemical reaction rate is finally AVOIDED in the pdf method. The chemical reaction term is resolved exactly without any model involved.

A 3-D simulation code has been developed (based on the temporal channel flow code by Rai and Moin [12]) for spatially developing, chemically reacting turbulent flow systems. The numerical techniques include highly accurate (6th order) finite difference scheme and spectral method. The main advantage of the finite difference scheme is the flexibility of the flow field geometries. The code has been optimized in terms of vectorization and parallelization.

The overall plan for the numerical simulations of turbulent combustion systems is divided into five stages. In the first stage, typical fully developed turbulent channel flows is simulated with consideration of streamwise development of turbulent flow fields. Turbulent statistical quantities and turbulence structures are predicted and compared with experimental data. In the second stage, mass transpiration from the side walls of turbulent channel flows is considered. The effects of transpiration rate on the turbulent statistical quantities and turbulent structures are studied in details. In the third stage, the mixing between the main stream and secondary stream from side walls will discussed. In the fouth stage, the combustion processes between oxidizer and fuel will be investigated in details. In the final stage, practical
OVERALL PLAN FOR NUMERICAL SIMULATIONS FOR TURBULENT REACTING FLOWS

Figure 1.4: Overall Plan for Numerical Simulations of Engineering Combustion Systems
engineering combustion system will be simulated. Some guidance to improve system performance (efficiency) is expected to be developed.

At the time of this dissertation, the code for turbulent reacting flow systems has been designed, implemented, and tested. The first two stages of the above overall plan have been finished completely. The third stage is under investigation.
CHAPTER 2

NUMERICAL SIMULATION APPROACHES FOR TURBULENT REACTING FLOWS

As discussed in Chapter 1, there is a continuous distribution of length scales associated with turbulent flows. There are certain size of eddies corresponding to each length scale. The large eddies "withdraw" turbulence energy from mean flow, then pass the energy to the next smaller eddies. Then this turbulence energy will be passed to the even smaller eddies until the eddies reach Kolmogorov length scale, where the dissipation of the turbulence energy is equal to the energy feed from the larger eddies. Another way to look at the turbulence dynamics is that the mean flow generates large eddies. The large eddies will break down into smaller eddies and the smaller into even smaller ones until the eddies lose their identity in the flow field, which is identical to Kolmogorov scale. This scale is far above the molecular scale, however. For reaction flows, the molecular mixing takes place in the smallest eddy size scale.

In turbulent reactive flows, the fuel or oxidizer consumption rate depends on both the ability to bring the reactants together and the chemical reaction rate. The chemical reaction occurs only if all the necessary reactants mix well in the molecular scales. If the chemical reaction rate is greater than the turbulent mixing rate, the species conversion rate is mainly dominated by the mixing process. In the limiting
case, when the chemical reaction rate is much much greater than the mixing rate, the reaction zone is a very very thin “sheet”. On the other hand, if the mixing rate is much greater than the chemical reaction rate, the species conversion rate depends mainly on the chemical reaction rate.

With this picture in mind, it is clear that for numerical simulation of turbulent reactive flows to be accurate, the spatial resolution will be fine enough to resolve the smallest eddies and also small enough to resolve the chemical reaction zone structure. The representative length scale for the chemical reaction zone structure is the zone thickness. As discussed earlier, the smallest eddy size decreases with the increase of the Reynolds number. It is easily understood that the reaction zone thickness decreases with the increase of Damköhler number. The higher the Reynolds number and Damköhler numbers are, the more challenging the numerical simulation will be.

### 2.1 DNS Approach

Since turbulent combustion is governed by the same known conservation equations, the question: can turbulent combustion be computed from the first principles? is reduced to a question of computational power. By the term “direct numerical simulation (DNS)”, we mean a numerical calculation that solves for the time development of the detailed, unsteady structures in a turbulent flow field. In the DNS turbulence simulation, all of the dynamically significant length and time scales of motion are included. This implies resolving length scales in the range of those at which viscous dissipation and chemical reaction occur. To illustrate the requirements for the computational power for DNS method, we take a simple nonreactive turbulent flow as an example. We can obtain an estimate of this range of scales for the nonreactive flows by examining the ratio of a length scale characterizing the energy-containing
range \((l)\) to the Kolmogorov length scale \((\eta)\), which characterizes the dissipation range. From eq. (2.1), the ratio of the energy-containing scale to the Kolmogorov scale is approximately

\[
\frac{l}{\eta} = R_l^{\frac{3}{4}} \tag{2.1}
\]

We see that this ratio of length scales is proportional to \(R_l^{\frac{3}{4}}\), where \(R_l = \frac{ul}{\nu}\) is a Reynolds number based on the energy-containing range of scales. Therefore, the number of grid points \(N\) in a particular direction is expected to be proportional to \(R_l^{\frac{3}{4}}\), so that, in a three-dimensional simulation, the total number of grid points will be proportional to \(R_l^{\frac{3}{4}}\). Most technological flows have Reynolds numbers in the tens of thousands or more, which would require more grid points than computers of present or near future could handle. To the best of our knowledge, the most grid points used so far is 17,357,664 in Rai and Moin's spatially developing compressible turbulent boundary layer [12]. Vincent and Meneguzzi [13] used \(240^3\) (13,824,000) grid points in their homogeneous turbulence simulation, the corresponding Reynolds number \(R_l\) is 1000. The current computer resource limits the DNS approach to basic research studies. Fig. 2.1 [32] shows the projected use of simulation physics and aerothermodynamics. It illustrates and predicts the computer power requirements for different flow simulations.

Reynolds [14] made a thorough discussion about the potential and limitations of the direct numerical simulations and large eddy simulations. Direct Numerical Simulations originated with the work of Orszag and Patterson [15], who studied homogeneous decaying turbulence and the validity of certain analytical theories of turbulence. The approach has been employed further in the studies of turbulent structure [16, 81], turbulent modelling [18], turbulence control, evaluation of new concepts, and even as the calibration for experiment device [20]. DNS is widely
Figure 2.1: Projected Use of Simulations in Turbulence Physics (left) and Aerothermodynamics (right), Ref. 14
used in the _a priori_ technique in the LES method [19]. In addition, DNS has been successfully used in the studies of instability and turbulence transition process [21, 22].

DNS is beginning to be used for turbulent reactive flows. For simplicity, most of this work has been done for incompressible flows in which the effect of chemical reaction on the turbulence is not accounted. Riley, Metcalfe, and Orszag [23] used DNS to study reactions in the time-developing mixing layer between two chemical streams. McMurtry et al [24] used DNS to study a two-dimensional compressible mixing layer undergoing a simple-step chemical reaction with heat release. Leonard and Hill [25] studied two-species, second-order, irreversible, isothermal reactions in "box" (periodic boundary conditions in all three spatial directions) turbulence. In Flow Research Inc., Givi, Jou, McMurtry, and Metcalfe [26, 27, 28] put a series of efforts to use DNS to study turbulent jet flame. They investigated the spatial convolution of a reacting mixing layer under the influence of nonequilibrium chemical reactions with their two-dimensional spectral-element code. They also used DNS to study a reaction type $A+B \rightarrow \text{products}$ in a homogeneous turbulent flow in which the influence of molecular mixing was isolated and studied in detail.

### 2.2 Moment Approach

The accurate prediction of turbulent flows at high Reynolds numbers and Damköhler numbers remains a formidable challenge for computational fluid dynamics (CFD). Because of the rapid increase in the range of length scales with increasing Reynolds number, direct numerical simulation is not feasible for prediction of turbulence at high Reynolds number or high Damköhler number turbulent flows of engineering interest. These predictions can only be obtained by solving some suitably averaged
(filtered) form of the Navier-Stokes equations. In fact, averaged turbulent qualities are of great engineering interest. Moment method is one of the methods to predict only the statistical quantities (averages, fluctuations,...). The main point for the moment method is to solve the averaged momentum equation, continuity equation, and the scalars (temperature and species) conservation equations. However, averaging the governing equations gives rise to the correlation of turbulent quantities which must be modeled using various levels of approximations.

The simplest solution to the closure problem involves the direct assumption of gradient transport in the governing equations. Such an assumption is usually made in connection with time-averaged quantities. For the flux of a scalar quantity q, gradient transport assumes that \( u_i''q'' = \nu_t \partial q / \partial x_i \), while for the component of a vector quantity, e.g., \( u_j \), the flux is \( u_i''u_j'' = \nu_t (\partial u_i / \partial x_j + \partial u_j / \partial x_i) \). Here, \( \tilde{\cdot} \) stands for fluctuations and overbar for averaged turbulent quantities. In both expressions \( \nu_t \) is a turbulent exchange coefficient, an expression for which is to be obtained through modelling in some fashion.

Over the years, several empirical hypothesis have been used. Eddy-viscosity and mixing length concepts are among the more popular and extensive used concepts. Bossinesq (in 1877) was the first to attack the problem of finding a model for Reynolds shear stress by introducing the concept of eddy viscosity. In the early 70's, \( k-\epsilon \) was developed and has been widely used since then. In the \( k-\epsilon \) model, the turbulence exchange coefficient \( \nu_t \) is modelled as the combination of \( k \) and \( \epsilon \). One typical example of this model is:

\[
\nu_t = C_{nu} \frac{k^2}{\epsilon}
\]

where \( k \) is the turbulence energy and \( \epsilon \) is the dissipation rate.
In spite of the tremendous effort that has been put into developing turbulence models, progress in this area has been limited. The major shortcoming of turbulence models used in most Reynolds-averaged Navier-Stokes computations is that they are designed to model all scales of turbulent structures. However, the large structures are highly dependent on the particular geometry and flow conditions of interest; it is therefore difficult, if not impossible, to develop a universal turbulence model that accounts for all the scales of motion. Moreover, the basis of gradient transport approximations resides in small length scales associated with the turbulent fluctuations relative to the length scales of the mean flow. Unfortunately, this situation seldom prevails in turbulent flows of practical interest, and consequently there is no good basis for the common closure scheme.

In addition to the difficulties mentioned above, the closure problem for chemical reaction rates is another major stumbling block for the moment method to be used in turbulent reactive flows. The mean chemical production term that appears in the species and energy conservation equations requires special consideration. Even for a very simple chemical reaction, the expression for the mean chemical reaction rate will be very complicated. Thus, consider the simple reaction

\[ M_1 + M_2 \xrightarrow{k} M_3 \]

The species \( M_1 \) can be considered fuel, \( M_2 \) the oxidizer, and \( M_3 \) a single product of reaction. The mean consumption rate of species \( M_1 \) can be written as

\[
-\overline{S_1} = (\rho^2 K_f)(Y_1 Y_2 + Y_1'' Y_2'') + (\rho^2 K_f)'' Y_2'' Y_1' + (\rho^2 K_f)'' Y_1'' Y_2' + (\rho^2 K_f)'' Y_1'' Y_2''
\]

(2.4)
In the above expression some more unknown fluctuation quantities are introduced. These will raise more questions about modelling. In the practical applications, the chemistry will be much more complicated than the single step reaction, the expression for the mean chemical reaction rate will be extremely difficult.

2.3 PDF Approach

Realizing the difficulty associated with chemical reaction rate in the $k - \epsilon$ method, the probability density function (pdf) method was proposed to overcome the shortcomings. Lundgren [29] and Monin [30] laid the foundations of the pdf approach. The pdf approach attracted the interest of those studying turbulent reactive flows when Dopazo [31] showed that reaction terms are closed in the pdf formulation. In the probability density function method, only the statistical quantities are determined. The state of the flow and scalar fields are described by a complete description of the joint probability density function. The pdf methods can be further classified into three categories. They are, respectively, the joint pdf of composition $f_{\phi}(\bar{\psi}; x, t)$; the joint pdf of velocity and composition $f_{ug}(V, \psi; x, t)$, and, the joint pdf of velocity, dissipation and composition $f(V, \xi, \psi; x, t)$. Here $V \equiv \{V_1, V_2, V_3\}$ and $\xi$ are independent (sample-space) variables corresponding to velocity, and to the instantaneous mechanical dissipation $\epsilon(x, t)$.

Their success, then, revolves around two issues. The first is the tractability of the numerical method to solve the modelled pdf evolution equations, especially if realistic chemical kinetics or complex flow-geometry is involved. The second is the accuracy of the modelling, especially that of molecular mixing.

While the composition joint pdf $f_{\phi}$ provides a complete one-point statistical description of the composition field, it contains no information about the velocity
field. Consequently, in addition to the modeled equation for $f_\phi$, a turbulence model (normally, k-ε method) is needed to determine the mean-velocity and turbulence fields. Among many researchers, Chen et al [51] applied this method to study the turbulent nonpremixed methane jet flames.

The velocity-composition joint pdf approach has the advantage that all forms of convective transport are treated exactly, since the corresponding term in the transport equation for $f_\phi$ is in closed form. Consequently the assumption of gradient-diffusion transport is avoided. Pope & Correa [52] and Masri & Pope [53] have successfully used this approach in their studies of turbulent nonpremixed flames. However, it is still necessary to introduce some kind of modelling to account for the turbulent length and time scales, such as turbulent mixing scales.

In contrast to the above two pdf approaches, the method based on the joint pdf of velocity, dissipation and composition $f(V, \xi, \phi; x, t)$ provides a complete closure: the single modelled equation for $f$ is closed. Hence the incompleteness of the velocity-composition joint pdf approach is remedied, and the need for the modelling equation for $< \epsilon >$ is obviated. But generally some theoretical statistic model should be introduced to describe the pdf evolution processes.

In summary, in the joint composition pdf method, the flow field solver generally involves the gradient-diffusion assumption. It is very important to point out that the gradient-diffusion model used here intends to model all the length scales, while the one used in LEPDF method is only intended to model the small scale fluctuations. It is obvious that the gradient-diffusion assumption here is significantly in error since the flame length scales are much smaller than the turbulence integral scale. In the joint velocity-composition pdf method, the joint pdf contains no information about turbulent length scales or time scales. Consequently, additional assumptions
or model equations are required. For several free shear flows, the assumption has been made [54, 55, 52, 56] that the turbulent time scale \( T = k / \langle \varepsilon \rangle \) is uniform across the flow. In the joint velocity, composition, and dissipation pdf method, the dissipation rate is treated as a random variable, and the joint pdf contains length-scale and time-scale information. However, there is lot of work needed to do for a reasonable and widely accepted statistical model for \( \varepsilon \) to apply in a variety of flows, especially for the inhomogeneous, anisotropic flows.

After all, in all the pdf methods, only the statistical information is sought. The large scale motion (or coherent structure) is not properly resolved in the pdf approach, even though the macroscale mixing is mainly controlled by the large scale motion.

### 2.4 LES Approach

Large-eddy simulation (LES) is a relatively new approach to the calculation of turbulent flows. The basic idea stems from two experimental observations. First, the large-eddy structure of turbulent flows varies greatly from flow to flow (e.g. jets vs. boundary layers [35] Fig. 2.2) and is consequently difficult, if not impossible, to model in a general way. Secondly, the small-scale turbulence structures are nearly isotropic, very universal in character [35] (Fig. 2.3), and hence more amenable to general modelling. This universal property of small scale motion can easily be seen from the turbulence spectrum [34, 43] (Fig. 1.3). In LES, one actually calculates the large-scale motions in a time-dependent, three-dimensional computation, using the large-scale field dynamical equations that incorporate simple models for small-scale turbulence. Only the part of the turbulence field with scales that are small relative to overall dimensions of the flow field is modelled. This is in contrast to
phenomenological turbulence modelling (like $k$-$\epsilon$), in which all the deviations from the mean velocity profile are modelled.

In large-eddy simulations we decompose the flow variables into a large scale (or resolved) component, denoted by an overbar, and a subgrid scale component. The large scale component is defined by the filtering operation:

$$
\overline{f}(x_1, x_2, x_3) = \int_D \Pi_{i=1}^3 G_i(x_i, x_i') f(x_1', x_2', x_3') dx_1' dx_2' dx_3'
$$

where the integral is extended over the entire domain $D$ and $G_i$ is the filter function in the $i$th direction. The filtered Navier-Stokes, continuity, and scalars (temperature, species concentration) conservation equations, which described the evolution of the large, energy-carrying eddies, can be obtained by applying the filtering operation to the Navier-Stokes, continuity, and scalar conservation equations (will be discussed later). The effect of the subgrid scales appears in the residual quantities, such as the residual stress, $\tau_{ij} = \overline{u_i u_j} - \overline{\bar{u}_i \bar{u}_j}$. Smagorinsky [37] model is a very popular model to parameterize this residual stress to the large scale field:

$$
\tau_{ij} = -2 \nu_T \overline{\mathcal{S}_{ij}} + \frac{1}{3} \delta_{ij} q_{sgs}^2
$$

where $\delta_{ij}$ is Kronecher delta, and $q_{sgs}^2 = \tau_{kk}$ is the subgrid scale energy, $\overline{\mathcal{S}_{ij}} = \frac{1}{2} (\partial \bar{u}_i / \partial x_j + \partial \bar{u}_j / \partial x_i)$ is the large-scale strain-rate tensor, and $\nu_T$ is an eddy viscosity, which, in general, is modelled to correlate to the large-scale flow field. For example,

$$
\nu_T = l^2 \sqrt{2 \overline{\mathcal{S}_{ij} \mathcal{S}_{ij}}}
$$

where $l$ is the length scale related to the grid sizes. The subgrid scale model for scalar quantities can be treated in similar ways.
Figure 2.2: Turbulent Boundary Layer on a Wall (above), Large-scale structure in a turbulent mixing layer (below), Ref. 35
Figure 2.3: Homogeneous Turbulence Behind a Grid, Ref. 35
During the past decade, considerable progress has been made in the large-eddy simulations of inert incompressible turbulent flows. The effort has shed new light on the physics of turbulence. The pioneering work of LES was done by Deardorff [38], who used LES to study the three dimensional turbulent channel flow at large Reynolds numbers. Since then LES method has been successfully used to study the channel flows [39, 40, 41, 42], boundary layer flows [43], mixing layer [44], and transitional channel flows [45, 46]. There is also an example for the LES to have been used in the compressible turbulent boundary study [47]. Deardorff [48] used LES to study the turbulence mixing in an entraining mixed layer.

Schumann is the first to use pure (as compared with LEPDF method) LES for the turbulent reacting flow [49]. He used LES to simulate Convective Boundary Layers (CBL). The effect of turbulence on chemical reactions has been investigated for idealized conditions. It is pointed out that a more realistic chemistry model has yet to be developed. In spite of the large computational effort, such studies appear to be feasible in the near future (after 1989).

For non-reactive flows, large-eddy simulations provide a tractable and affordable alternative to DNS without loosing the accuracy of the DNS method. It is far from clear, however, that LES is a useful approach for turbulent combustion, because it does not overcome the closure problem associated with nonlinear reaction rates. This same problem has already been discussed in the $k$-$\epsilon$ method. The equation for the resolved composition (scalar) $\overline{\psi}_\alpha(x_1, x_2, x_3, t)$ contains the filtered reaction rate $\mathcal{F}_\alpha(x_1, x_2, x_3, t)$. The problem of determining $\mathcal{F}_\alpha$ in LES method is precisely analogous to the problem of determining $\mathcal{F}_\alpha$ in a mean-flow closure in $k$-$\epsilon$ method. As observed by Givi [50], an appropriate evaluation of $\mathcal{F}_\alpha$ has never been attempted in LES.
2.5 LEPDF Method

It is clear that DNS methods is extremely useful for many geometrically-simple flows at low or moderate Reynolds and Damköhler numbers. It has provided much invaluable information to help us to understand the fundamental physics of turbulence, and the turbulence chemistry interactions. But for the flows with higher Reynolds number and Damköhler number in practical devices, DNS is not feasible in the foreseeable future\[57\]. LES has been proven to be a very effective and accurate simulation method for the inert turbulent flows, but it still has the difficulty to cope with the nonlinearity problem in the chemical reaction rate. In the moment method, such as $k - \epsilon$ model, it models all the scales of structures by the gradient-diffusion model, which is considerably inaccurate even for some inert flows \[58\]. Pdf methods overcome the major closure problems and they have been shown to be tractable for complex flows and with realistic finite-rate kinetics. However, the macro-mixing due to the large scale motion is not properly resolved. In the past, it is described by a second-order moment closure. In the the velocity, dissipation and composition joint pdf approach, the turbulence model difficulty is circumvented. However some newly proposed stochastic model is needed to resolve the dissipation rate to get the time and length scales \[59, 60\].

Therefore, it can be concluded that there is not a single numerical approach which can effectively (within today's computer abilities) and accurately resolve the turbulent chemically reactive flows in the practical engineering devices. It is realized that there is a possibility for some new approach to emerge to combine the advantages of all the methods mentioned above, but offset their deficiencies or shortcomings.

Based on the extensive investigation of the current numerical simulation meth-
ods for turbulent reactive flows, Large Eddy Probability Density Function (LEPDF) simulation method is developed in the present study. This method is the combination of the LES method and the PDF approach. It is claimed to be the best for both worlds: accuracy and the efficiency. In this new method, the large scale motion, coherent structure, scalar macro transport are resolved EXACTLY in LES method, the subscale motion tend to be very universal and is taken care of by the subgrid (SGS) model in the LES mode. The molecular mixing, the turbulent mixing, and chemical reaction are well resolved by the PDF mode. The major closure problem related to the chemical reaction rate is finally AVOIDED in the pdf method. The chemical reaction term is resolved exactly without any model involved. The more profound advantage of LEPDF method is that the molecular model and the turbulence model used here are much more accurate than the counterpart in the former pdf method, even the similar model forms may be used for both cases. This is because that the models for molecular mixing and turbulence mixing in the former pdf method model all the scales of the motion, but corresponding models used in the LEPDF method only model the subscale motions.

LEPDF method is a generalization of the existing PDF concept, which was first introduced, without so called, by Pope in a review article in 1985 [62]. To the best of our knowledge, the first simulation done so far, by using the LES method in conjunction with pdf method is the work done by Lin and Pratt in 1987 [63]. They used a similar method (they called it hybrid method) to investigate the turbulent mixing in a spatially-developing, free shear layer with isothermal, fast chemical reactions. In the flow field prediction, large-eddy simulation was conducted by a modified 2-D vortex method with subgrid-scale modeling. In scalar transport, the Monte Carlo method was extended to the simulation of the time-dependent pdf
transport equation. In 1990, Pope [57] proposed to use LES and filtered PDF for turbulent reactive flows. He suggested to use filtered PDF to remedy the chemical reaction closure problem in the LES method. The filtered pdf is defined as:

\[ \mathcal{F}_\phi(\psi, \mathbf{x}, t) = \int \delta(\psi - \phi(y, t)) G(|\mathbf{x} - \mathbf{y}|) dy \]  

(2.8)

where \( \delta(\psi - \phi) \) is written for the delta-function product \( \prod_{\alpha=1}^{\sigma} \delta(\psi_\alpha - \phi_\alpha) \), and \( G \) is the LES filter function, \( \sigma \) is the total number of scalars.

In 1993, Gao and O'Brien [6] developed a general methodology for simulating the complicated reacting flow problem. The method combines the large-eddy simulation technique with the existing probability density function approach for turbulent reacting flows and provides a closed form representation for all terms that are involved in the simulations. Frankel et al [64] used LES to simulate turbulent reactive flows with assumed pdf methods. In their study, simple non-premixed reacting systems involving an isothermal reaction of the type \( A + B \rightarrow \text{Product} \) under both chemical equilibrium conditions are considered. The Smagorinsky closure equation is employed to account for hydrodynamic fluctuations, and the assumed pdf is employed for modelling the effects of scalar fluctuations. They pointed out that at present the assumed pdf methods are somehow "feasible" than the transport equation approach for simulating practical problems. It is encouraged that further research on the pdf modelling is necessary for the pdf transport equation approach.
CHAPTER 3

FORMULATION OF LEPDF METHOD

The state of a reactive flow composed of \( \sigma - 1 \) species is fully described by the species mass fractions \( y_\alpha(x, t)(\alpha = 1,2,\ldots,\sigma - 1) \), the species enthalpy \( h(x, t) \), the pressure \( p(x, t) \), and the three components of velocity \( u = u_1, u_2, u_3 \). The evolution of the reactive flow field is governed by the basic conservation equations of mass, momentum, chemical species and enthalpy [65]. The dimensionless forms of the above equations are:

\[
\frac{\partial u_j}{\partial x_j} = 0 \quad (3.1)
\]

\[
\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j}(u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{1}{R_e} \frac{\partial^2 u_i}{\partial x_j \partial x_j} + g_i * L^2/U_0 \quad (3.2)
\]

where \( U_0 \) and \( L \) are the reference velocity and the length scales. \( g_i \) is for the gravity effect in the \( i \)th direction. \( R_e \) is defined as \( R_e = U_0 * L/\nu \). \( p \) is made dimensionless by \( \rho U_0^2 \).

The scalar \( \psi_\alpha \) (species or enthalpy) conservation equation can be generalized as:

\[
\frac{\partial \psi_\alpha}{\partial t} + u_j \frac{\partial \psi_\alpha}{\partial x_j} = D \nabla^2 \psi_\alpha + S_\alpha[\psi(x, t)] \quad (3.3)
\]

where \( D \) and \( S_\alpha \) are nondimensionized by \( LU_0 \) and \( U_0/L \) respectively.
In this chapter, we are going to develop the general methodology for Large Eddy Probability Density Function (LEPDF) method for turbulent reactive flows. In the LEPDF method, LES method will be employed to resolve the turbulent flow field, while PDF approach will be used to simulate the molecular mixing processes and the chemical reaction effects. For simplicity, we assume that the heat release from the chemical reaction is not very significant, so the density change due to the chemical reaction is negligible. With this assumption, the effect of turbulence on the mixing and chemical reaction processes are studied. The effect of combustion to the turbulent field is neglected. However, the general methodology can be easily extended to the compressible turbulent reactive flows. In the following sections, we will discuss the formulations for turbulent flow field and chemical combustion process in details.

3.1 Velocity Flow Field

3.1.1 Filtered Equations

In large Eddy Probability Density Function (LEPDF), the velocity field and the scalar field are decomposed into a large scale component and a subgrid component by applying a filtering operation. For any variable \( f \), the filtered value \( \mathcal{f} = f - f' \) (\( f' \) is the unresolved part) is defined by

\[
\mathcal{f}(x_1, x_2, x_3) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \prod_{i=1}^{3} G_i(x_i - x'_i) f(x'_1, x'_2, x'_3, t) \, dx'_1 \, dx'_2 \, dx'_3
\]

(3.4)

After applying the filtering operator, the continuity and momentum equations assume the following forms:
\[
\frac{\partial \bar{u}_j}{\partial x_j} = 0 \quad (3.5)
\]

These equations represent the transport of the filtered velocity (corresponding to the resolved length scales) and contain additional terms which quantify the interaction between the grid (resolved) scales and the subgrid (unresolved) scales. The last three nonlinear terms together form the subgrid scale stresses, \( \tau_{ij} \):

\[
\tau_{ij} = - (\bar{u}_i u'_j + u'_i \bar{u}_j + u'_i u'_j) \quad (3.7)
\]

The residual stress can be further decomposed into the cross stress \( C_{ij} \) and the subgrid-scale Reynolds stress \( R_{ij} \), given by

\[
C_{ij} = - (\bar{u}_i u'_j + u'_i \bar{u}_j) \quad (3.8)
\]

\[
R_{ij} = \bar{u}'_i u'_j \quad (3.9)
\]

respectively, in which \( u'_i = u_i - \bar{u}_i \) is the subgrid-scale velocity. In addition, the Leonard stress \( L_{ij} \) is defined as

\[
L_{ij} = -(\bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j). \quad (3.10)
\]

The cross stress \( C_{ij} \) and subgrid scale Reynolds stress \( R_{ij} \) are invariably modelled, while the Leonard stress can be either computed or modelled.
3.1.2 Filter Discussion

For the large-eddy simulation of turbulent flows, the most commonly used filters are the Gaussian filter, the sharp Fourier cutoff filter and the box filter. The Gaussian filter is defined as

\[
G_i(x_i, x'_i) = \left( \frac{6}{\pi \Delta^2_i} \right)^{1/2} \exp\left( -\frac{6(x_i - x'_i)^2}{\Delta^2_i} \right)
\]

where \( \Delta_i \) is the filter width in the \( i \)th direction, usually related to the grid size \( \Delta x_i \).

The sharp Fourier cutoff filter is most conveniently defined in Fourier space:

\[
\hat{G}_i(k_i) = \begin{cases} 
1, & \text{for } k_i < K_{ci}, \\
0, & \text{otherwise}, 
\end{cases}
\]

in which \( \hat{G}_i(k_i) \) is the Fourier coefficient of the filter function \( G_i \) and \( K_{ci} \) is the cutoff wave number in the \( i \)th direction that is related to the filter width by \( K_{ci} = \pi / \Delta_i \).

The variable-width box filter is defined as

\[
G_i(x_i, x'_i) = \begin{cases} 
1/\Delta_i, & \text{for } |x_i - x'_i| \leq \Delta_i/2 \\
0, & \text{otherwise}, 
\end{cases}
\]

When either the Gaussian or the box filter is used, the subgrid scales represent both large and small scales of motions [66], and even resolved scales contribute to the subgrid-scale field. When the cutoff filter is used, on the other hand, the subgrid scales only contain the effect of the structures with wave number larger than the cutoff wave number \( K_{ci} \), and the large scales of motion can be represented in terms of the grid-scale velocity only. At the early stages of transition (normally, the simulation of turbulent reactive flows starts from laminar flows to transitional stage
then to the fully developed turbulence) only large scales of motion (the Tollmien-Schlichting waves) are present: since these structures are resolvable, a large-eddy simulation should give the same results as a direct simulation. Since this requirement cannot be satisfied if the Gaussian filter is used, the cutoff filter is chosen for the present study.

It is also useful to remark that the sum of the cross stress, Leonard stress, and subgrid-scale Reynolds stress is invariant to Galilean transformation, regardless of the filter used [67]. The subgrid scale Reynolds stress $R_{ij}$ has the same property. The Galilean invariance properties of Leonard and cross stresses, however, depend on the type of filter used. If either the Gaussian or the variable-width box filter is employed, neither the Leonard stresses nor the cross stresses are Galilean invariant, but their sum is. On the other hand, if the cutoff filter is used, both Leonard and cross stress are Galilean invariant. It is another reason for us to choose cutoff filter in the present study.

### 3.1.3 Subgrid Scale Modeling

Most of the models currently in use correlate the residual stress with the large-scale strain-rate tensor $\mathcal{S}_{ij}$,

$$\mathcal{S}_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)$$

(3.14)

which, in incompressible flow, is traceless. The trace of the residual stress tensor is, therefore, commonly incorporated into the total pressure, and only the anisotropic part of the residual stress tensor

$$\tau_{ij} = \tau_{ij}^\tau - \frac{1}{3} \tau_{kk} \delta_{ij}$$

(3.15)
(in which $\tau_{kk} \equiv q_{sgs}^{2}$ is the subgrid scale kinetic energy) requires modelling.

The most commonly used residual stress models for large-eddy simulation of turbulent flows are modifications of the Smagorinsky model. As mentioned earlier, the Smagorinsky model is an eddy viscosity mode that relates the modelled residual stress $\tau_{ij}^m$ to the strain-rate tensor $\mathcal{S}_{ij}$ through an eddy viscosity $\nu_T$:

$$
\tau_{ij}^m = -2\nu_T \mathcal{S}_{ij} \tag{3.16}
$$

In which $\nu_T$ is given by

$$
\nu_T = l^2 \sqrt{2\mathcal{S}_{ij} \mathcal{S}_{ij}} \tag{3.17}
$$

and $l$ is a subgrid length scale, which is usually related to the filter width by

$$
l = C_s (\Delta x \Delta y \Delta z)^{1/3} \tag{3.18}
$$

where $C_s$ is the Smagorinsky constant.

The Smagorinsky model is absolutely dissipative. The model is incapable of predicting the reverse cascade regions and overestimates the subgrid-scale dissipation. Part of the problem is due to the fact that the model is only based on large-scale quantities and predicts nonzero residual stresses even in laminar flow. Piomelli et al [68] used the transition stage factor $(H_l - H)/(H_l - H_t)$ to account for the transition effects from laminar to turbulent flow, where $H = \delta^*/\theta$ is the shape factor, $\delta^*$ is the displacement thickness, $\theta$ is the momentum thickness, and subscripts $l$ and $t$ refer, respectively, to laminar and fully developed turbulent flows. Considering the transition effect, the length scale $l$ can be given
In the wall-bounded turbulent flows, the length scale is often multiplied by a Van Driest's damping function \[69\] to account for the fact that the growth of even the large structures is inhibited by the presence of the wall. The length scale \(l\) then becomes

\[
l = C_s \frac{(H_l - H)}{(H_l - H_i)} (\Delta x \Delta y \Delta z)^{1/3}
\]  

(3.19)

where \(y^+\) is the distance from the wall made dimensionless by the shear velocity \(u_r = (\tau_w/\rho)^{1/2}\) (where \(\tau_w\) is the wall stress) and kinematic viscosity \(\nu\).

### 3.2 Passive Scalar Transport

#### 3.2.1 Filtered PDF Equation

As discussed earlier, the scalar transport can best be resolved with PDF method. There are several different methods of deriving pdf transport equations. Pope \[62\] derived the transport equation of pdf by employing the concept of conditional expectation.

Lundgren \[29\] derived the pdf transport equation starting from the expression for the pdf of a delta function. The resulted transport equation for the composition pdf \(f(\phi; x, t)\) is

\[
\frac{\partial f(\phi)}{\partial t} + u_j \frac{\partial f(\phi)}{\partial x_j} = - \frac{\partial}{\partial \phi_\alpha} \left\{ [D \nabla^2 \phi_\alpha + S_\alpha(\psi)] f(\phi) \right\}
\]  

(3.21)

where \(\psi\) are scalar variables and \(\phi\) is the corresponding sample space variables.

Applying the filter on both side of the above equation, we obtain
3.2.2 Modeling for Pdf Transport Equation

In the above pdf transport equation, the convective on the left hand side is expressed explicitly. There is no need of modelling for this term. Moreover, the chemical reaction term on the right hand side is also in explicit form. This is the major advantage of pdf method. The only terms need to be modelled are the molecular mixing and the turbulent mixing. The turbulent mixing term on the right hand side of (3.22) is the subgrid scale contribution, and can be modelled through the eddy diffusivity model.

\[
\frac{\partial \overline{f}(\phi)}{\partial t} + \overline{u_j \frac{\partial \overline{f}(\phi)}{\partial x_j}} = -\frac{\partial}{\partial \phi} \left\{ D(\overline{f(\phi)\nabla^2 \phi}) + S_\alpha(\phi) \overline{f(\phi)} \right\} - \frac{\partial}{\partial x_j} (\overline{u_j f(\phi)} - \overline{u_j \overline{f}(\phi)})
\]  

(3.22)

\[
\overline{u_j f(\phi)} - \overline{u_j \overline{f}(\phi)} = -D_p \frac{\partial \overline{f}(\phi)}{\partial x_j},
\]

(3.23)

It should be realized that the gradient model used here is ONLY FOR SUBGRID SCALE MOTION. It is much more accurate (reasonable) than the counterpart in the \(k - \epsilon\) model. The subgrid motion tends to be isotropic for turbulent flows with high Reynolds numbers. It can be shown [6] that the \(D_p\) is equal to the \(D_s\) in the following eddy-diffusivity-type model:

\[
\overline{u_j \psi_\alpha} - \overline{u_j \overline{\psi}_\alpha} = -D_s \frac{\partial \overline{\psi}_\alpha}{\partial x_j}
\]

(3.24)

The molecular mixing term can be written in a different way:

\[
(\nabla^2 \psi_\alpha \overline{f(\phi)}) = < \nabla^2 \psi_\alpha \phi > \overline{f(\phi)}
\]

(3.25)
where the angle bracket stands for the expectation.

After the above manipulation, the transport equation for the filtered pdf becomes:

\[
\frac{\partial \tilde{f}(\phi)}{\partial t} + \mathbf{u} \cdot \nabla \tilde{f}(\phi) = -\frac{\partial}{\partial \phi_a} \left\{ [D < \nabla^2 \psi_a | \phi > + S_a(\phi)] \tilde{f}(\phi) \right\} - \frac{\partial}{\partial x_j} \left\{ D_p \frac{\partial f(\phi)}{\partial x_j} \right\}
\]

(3.26)

3.2.3 Chemistry Consideration

Until now, we have not mentioned how to determine the chemical reaction rate \( S_a \). In the diffusion (strictly speaking, nonpremixed) flame, the chemical reaction can occur only when the fuel and oxidizer mix well down to the molecular level. So the combustion process is controlled by the macro transport, turbulent mixing, and molecular mixing. The slowest process among them, if there is one, is the "bottle neck" or the controlling process. This argument can be summarized in a dimensionless group, Damkohler number, which is defined as the ratio of turbulent mixing time scale to the chemical reaction time scale. In the limit of infinite Damkohler number, the chemical reaction is extremely faster than the turbulent mixing process, then the combustion is totally controlled by the turbulent process. The conserved scalar method is developed to calculate the combustion process for this case. The species concentrations are equal to those at the equilibrium state. And they are only functions of temperature. In the case of finite rate chemistry, the combustion process is controlled by both the chemical process and the turbulent mixing. Generally, it is very difficult or even impossible to use a single expression for the overall combustion rate calculation. In the present study, we will consider the simplified chemistry, that is
\[ A + B \rightarrow P \] (3.27)

where \( A \) is for oxidizer, \( B \) for fuel, and \( P \) is the only combustion product. The chemical reaction rate for this simplified reaction can be calculated by Arrhenius expression.

The effect of chemical reaction heat release is assumed negligible, which together with the further assumption of a low Mach number flow, results in a constant density formulation. Under these assumptions, the hydrodynamics and the transport of the chemical species and temperature are decoupled.
CHAPTER 4

NUMERICAL SIMULATION TECHNIQUES

The general methodology of LEPDF method developed in the last chapter can be applied for different incompressible turbulent chemically reactive flows. The success for this method to be applied for a specific practical problem depends greatly on whether we can find an appropriate numerical scheme for the problem. With the limitation of current supercomputer resource, to design an efficient numerical code is a crucial factor to decide the solvability of a problem. In this chapter, we will discuss in detail about the numerical schemes, initial condition and boundary conditions, as well as the supercomputing techniques.

4.1 Numerical Scheme

The choice of a numerical scheme for a turbulent flow simulation is determined by many factors, such as the flow geometry, initial conditions, and boundary conditions. The numerical scheme to solve the governing equations developed in last chapter can differ greatly from one flow to another. Sometimes, even a slight change in the boundary conditions may have dramatic effects on a scheme. It could make a scheme which is very efficient for one case, to be very inefficient or even inapplicable in other cases. In this section, the general numerical schemes for turbulent flows will be discussed. And a numerical scheme for spatially developing turbulent reactive...
flows will be developed. As an example of the methodology, the scheme will be applied for the spatially developing turbulent reactive channel flows, in which the oxidizer is fed into the channel in the main stream (streamwise direction) and the fuel is injected through the side walls (Fig. 4.1).

4.1.1 Numerical Schemes for the Velocity Flow Field

4.1.1.1 Spectral Method and Finite Difference Method

The two main techniques used for the spacial discretization in turbulence numerical simulations are spectral methods and finite difference methods. The main advan-
tage of spectral method is the high order accuracy and efficiency with the help of fast Fourier transform (FFT). In the view of the complexity of the numerical solutions, the spectral method could make the solution procedure much simpler. In the simplest “box” case with periodic boundary conditions in all three directions, the spectral method effectively converts the original PDE’s to simple algebraic equations. These kind of simulations are called temporal simulations because only the evolution with time is considered. As contrast, the simulations with spatial development are called spatial simulations. To date most successful direct simulation have been performed with spectral methods because of the very high accuracies of these methods [70]. The principal disadvantage of this method is that they can only be used for the problems with very restricted boundary conditions. The widely used Fourier spectral method can only be used for the flows with periodic boundary conditions. For the flows with non-periodic boundary conditions, Chebyshev spectral method may be used. However, the non-uniformly distributed grid will cause very serious stiffness problem in the numerical solution procedure. Another difficulty with the Chebyshev spectral method is the complication of the resulting matrix in the discretization process. It makes the implicit algorithm, which requires the direct inversion of the matrix, very expansive.

The greatest advantage of finite difference method is that it can be used for complicated geometries and there is not limitation, in general, for the boundary conditions. Moreover, the finite-difference methods are simple to implement and are also the most commonly used methods in current application codes. Another important feature of this method is that the code can be easily modified and applied for different turbulent flow fields. The major shortcoming of currently used finite-difference methods is that their accuracy levels are inadequate. It is claimed
by Browning and Kresis [71], however, that the fourth-order finite difference are sufficient to reduce the spatial error to a size which is totally acceptable.

The spectral element method attempts to retain the high accuracy of spectral methods and the geometric flexibility of finite-difference and finite-element methods, a combination of these two methods are widely used in the turbulent simulation practice. Generally, the spatial method is used in the direction(s) with periodic boundary conditions, while the finite difference method is used in the direction(s) of spatial development. The so-called spectral-element method is one of these methods. To combine the advantages of finite element method and spectral method, Givi and Jou [72] developed spectral-element method to simulate reacting, spatially developing mixing layer. Amon [73] used spectral element method for transitional flows in complex geometries. There have, of course, been numerous incompressible Navier-Stokes computations which used mixed spectral/finite-difference methods. The parallel boundary-layer transition calculations of Wray and Hussaini [74] fall into this category. Moin and Kim [39] used slightly different spectral/finite-difference method in their LES of turbulent channel flow.

In regards to the application of the spatially developing turbulent reactive channel flow simulations, the boundary conditions are not applicable in both streamwise and normal directions of the channel. In the streamwise direction, a suitable inflow and outflow condition must be specified. The details will be discussed in the section of inflow and outflow boundary conditions. In the channel normal direction, the no-slip conditions for streamwise and spanwise velocity components can be enforced, while a specified transpiration (blowing or suction) function will be specified for the normal velocity component. The periodic boundary condition can be used in the spanwise direction for the velocity flow field. According, the Fourier spectral
method can be used in this direction. However, in order to have the flexibility for the code to be used in some other flows without any periodic boundary conditions, such as spatially developing duct flows, we use finite different methods in all three directions.

4.1.1.2 Fractional-Step Algorithm

Recall the filtered continuity and momentum equations, neglecting the gravity force and decomposing the pressure in two parts: the streamwise driven pressure and the pressure fluctuation,

\[
\frac{\partial \bar{u}_j}{\partial x_j} = 0
\]  \hspace{1cm} (4.1)

\[
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \bar{u}_i \bar{u}_j = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left\{ \left( \frac{1}{R_e} + \nu_T \right) \frac{\partial \bar{u}_i}{\partial x_j} \right\} + \frac{\partial}{\partial x_j} \left( \nu_T \frac{\partial \bar{u}_j}{\partial x_i} \right) + C_p \delta_{ij} \]  \hspace{1cm} (4.2)

where \( \partial p/\partial x_i \) and \( C_p \) are the fluctuation and the streamwise driven pressure gradients respectively.

The residual stress model used here are the modified Smagorinsky model with transitional and the near wall Van Dreist’s modifications. That is,

\[
\nu_T = l^2 \sqrt{2 \Sigma_{ij} S_{ij}}
\]  \hspace{1cm} (4.3)

\[
l = C_s \frac{(H_H - H)}{(H_H - H)} \left[ 1 - e^{(-y^+/25)} \right] (\Delta x \Delta y \Delta z)^{1/3}
\]  \hspace{1cm} (4.4)

The filter widths used in x (streamwise), y (normal), and z (spanwise) directions \( (\Delta x, \Delta y, \Delta z) \) are given by
\[ \Delta x = \frac{L_x}{N_x} \]
\[ \Delta y(j) = \frac{(\Delta y_j + \Delta y_{j+1})}{2} \]
\[ \Delta z = \frac{L_z}{N_z} \]

(4.5)

where \( \Delta y_j = y_j - y_{j-1} \), \( L_x, L_z, N_x \), and \( N_z \) are the lengths and grid numbers in the \( x \) and \( z \) directions. For this choice of the filter widths, the value of the Smagorinsky constant \( C_s \) is taken to be 0.1.

The major difficulty in obtaining a time-accurate solution for an incompressible flow arises from the fact that the continuity equation Eq. (4.1) does not contain the time-derivative explicitly. The constraint of mass conservation is achieved by an implicit coupling between the continuity equation and the pressure in the momentum equations Eq. (4.2). We may understand the fact in another way that the pressure adjust itself instantly (infinite transmit velocity) to satisfied the continuity equation. One may attempt to use an explicit time-advancement scheme which obtains the pressure at the current time-step such that the continuity equation at the next step is satisfied. However, for fully implicit or semi-implicit schemes, the aforementioned difficulty prevents the use of the conventional alternating-direction-implicit (ADI) scheme to advance in time as is the case for compressible flows. The difficulty can be avoided by introducing the vorticity equations like the work in Fasel’s group [21].

An alternative approach to avoid the the coupling difficulty is the fractional-step scheme (or called splitting method) discussed in Yanenko [75] and Marchuk [76]. The main ideal for this method is to introduce an “intermediate time step”, in which the pressure effects are not accounted temporally, then the pressure adjust itself in such way that the continuity constrain will be satisfied in the next time step.
Chorin [77] and Temam [78] developed splitting methods for the incompressible Navier-Stokes equations, and more recently, Glowinski [79] has described several such schemes combined with a finite-element spatially discretization. The splitting scheme proposed by Zang and Hussaini [80] uses the staggered grid in y direction, and consists of an advection-diffusion step at \( t_{n+\frac{1}{2}} \) and a pressure correction step at \( t_n \). The pressure step may be viewed as a projection of the velocity field onto a divergence-free space. Kim and Moin [81] developed a fractional-step scheme based on the Chorin [82] fractional-step methods. Here we extend this method to the LEPDF simulations of the spatially developing turbulent reactive channel flows.

Finally, the original coupling system Eq. (4.1 and 4.2) can be decoupled into the following system:

at \( t = t_{n+\frac{1}{2}} \)

\[
\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \tilde{u}_i \tilde{u}_j = + \frac{\partial}{\partial x_j} \left\{ \left( \frac{1}{Re} + \nu_T \right) \frac{\partial \tilde{u}_i}{\partial x_j} \right\} + \frac{\partial}{\partial x_j} \left( \nu_T \frac{\partial \tilde{u}_j}{\partial x_i} \right) + C_p \delta_{ij} \tag{4.6}
\]

at \( t = t_{n+1} \)

\[
\frac{\partial \tilde{u}_i}{\partial t} = - \frac{\partial p}{\partial x_i} \tag{4.7}
\]

\[
\frac{\partial \tilde{u}_j}{\partial x_j} = 0, \tag{4.8}
\]

4.1.1.3 Temporal Discretization

The major restrictions for a temporal discretization method is the accuracy and the stability characteristics. Generally speaking, explicit method is cheaper in terms of computational CPU time, but has poor stability characteristic, which in turn has
very severe requirement for the time step size. However, the implicit method is very stable but quite expensive to solve. If the accuracy is the key restriction for the scheme, a explicit scheme will normally employed. The implicit scheme will be used in the case where the instability restriction for the time step size is more severer than that imposed by the accuracy requirements.

The viscous term in Navier-Stokes equation imposes very severe stability requirement if an explicit scheme is used. This is because that the maximum eigenvalues corresponding to the discretized Laplacian operations are proportional to $N^2$, $N^2$, and $N^4$ for finite-difference, Fourier spectral, and Chebyshev spectral methods respectively [70]. The $N$ is the total number of the grid points in a discretization direction. And the stability requirement demands that the product of the maximum time step and the maximum eigenvalue is less than a prescribed constant.

$$\Delta t |\lambda|_{\text{max}} < C$$  \hspace{1cm} (4.9)

where C depends on the discretization scheme. This situation will be much severer if a stretch grid scheme is used. In the case of channel flow, the grid points are clustered near the wall, then the stability requirement forces the time marching step much smaller than that required by the calculation accuracy. In order to avoid the instability problem associated with the viscous term, an absolutely stable or A-stable scheme must be used. This can be done by employing an implicit scheme for the viscous terms. Crank-Nicholson (CN) method, is almost a standard implicit method used for the viscous term.

For the convection term, many people used second order Adams-Bashforth (AB-2) method. Rain and Moin [83] pointed out that the AB method is unstable for all the Courant-Friedrichs-Lewy (CFL) numbers for convection term. However, the
instability is very weak and the method usually works for CFL number less than 1.0 in the presence of viscous term. The Runge-Kutta methods seem more suitable for the convective terms because of their stability. The low-storage Runge-Kutta methods of Wary [84] have additional advantage that they require the minimum amount of computer run-time memory for this class of schemes.

In this study we used a three-step hybrid Runge-Kutta/Crank-Nicholson scheme developed by Spalart and used by Rai and Moin [83]. That is, the viscous term is treated in Crank-Nicholson scheme, while the rest of the terms are treated in third order Runge-Kutta scheme. This method is second-order accurate in time for the viscous terms and third-order accurate in time for the convective terms, the overall accuracy being second order in time.

After applying the temporal discretization, the three-step Runge-Kutta scheme to solve the Eq. (4.6, 4.7, and 4.8) is given by:

Step 1.

\[ u_i^a = u_i^n + \Delta t \left\{ \gamma_1 H_i(u_i^n) + \alpha_1 \left\{ \frac{1}{R_e} + \nu_T \right\} \right\} \left\{ \frac{\delta^2}{\delta x_1^2} + \frac{\delta^2}{\delta x_2^2} + \frac{\delta^2}{\delta x_3^2} \right\} (u_i^n + u_i^a) \]  
(4.10)

\[ \frac{\ddot{u}_i - u_i^n}{\Delta t} = -G(\gamma_1 \varphi) \]  
(4.11)

\[ D(\ddot{u}_i) = 0 \]  
(4.12)

Step 2.
\[ u_i^b = \tilde{u}_i + \Delta t \left\{ \gamma_2 H_i(\tilde{u}_i) + \xi_1 H_i(u_i^n) + \alpha_2 \left\{ \frac{1}{Re} + < \nu_T > \right\} \left\{ \frac{\delta^2}{\delta x_1^2} + \frac{\delta^2}{\delta x_2^2} + \frac{\delta^2}{\delta x_3^2} \right\} (\tilde{u}_i + u_i^b) \right\} \]  
(4.13)

\[ \frac{\tilde{u}_i - u_i^b}{\Delta t} = -G(\gamma_2 \tilde{\varphi} + \xi_1 \varphi) \]  
(4.14)

\[ D(\tilde{u}_i) = 0 \]  
(4.15)

Step 3.

\[ u_i^c = \tilde{u}_i + \Delta t \left\{ \gamma_3 H_i(\tilde{u}_i) + \xi_2 H_i(\tilde{u}_i) + \alpha_3 \left\{ \frac{1}{Re} + < \nu_T > \right\} \left\{ \frac{\delta^2}{\delta x_1^2} + \frac{\delta^2}{\delta x_2^2} + \frac{\delta^2}{\delta x_3^2} \right\} (\tilde{u}_i + u_i^c) \right\} \]  
(4.16)

\[ \frac{u_i^{n+1} - u_i^c}{\Delta t} = -G(\gamma_3 \tilde{\varphi} + \xi_2 \tilde{\varphi}) \]  
(4.17)

\[ D(u_i^{n+1}) = 0 \]  
(4.18)

where \( G \) and \( D \) are discrete gradient and divergence operators, and \( H_i \) is given by:

\[ H_i = -\frac{\partial}{\partial x_j} (\overline{u_i u_j}) + C_p \delta_{i3} + \frac{\partial}{\partial x_3} \left\{ (\nu_T - < \nu_T >) \frac{\partial \overline{u}_i}{\partial x_3} \right\} \]

\[ + (\nu_T - < \nu_T >) \left\{ \frac{\partial^2 \overline{u}_i}{\partial x_1^2} + \frac{\partial^2 \overline{u}_i}{\partial x_2^2} \right\} + \nu_T \left\{ \frac{\partial \overline{u}_i}{\partial x_1} + \frac{\partial \overline{u}_i}{\partial x_2} \right\} \]

\[ + \frac{\partial \nu_T}{\partial x_2} \left\{ \frac{\partial \overline{u}_i}{\partial x_2} + \frac{\partial \overline{u}_i}{\partial x_3} \right\} + \frac{\partial \nu_T}{\partial x_3} \frac{\partial \overline{u}_i}{\partial x_3} \]  
(4.19)
\( \varphi \) is a scalar to be determined. It is different from the original pressure: in fact,
\[
p = \varphi + (\Delta t/2R_e) \nabla^2 \varphi.
\]

And \( < \nu_T > \) is the average of \( \nu_T \) taken in the entire interior domain at a given instant. Such a use of \( < \nu_T > \) in the discretization of the momentum equations is advantageous from stability considerations. This technique was used by Moin and Kim [39] and Madabhushi and Vanka [85].

The constants used in the Eq. 4.10, to Eq. 4.18, are listed as follows:

\[
\begin{align*}
\alpha_1 & = 4/15 \\
\alpha_2 & = 1/15 \\
\alpha_3 & = 1/6 \\
\gamma_1 & = 8/15 \\
\gamma_2 & = 5/12 \\
\gamma_3 & = 3/4 \\
\xi_1 & = -17/60 \\
\xi_2 & = -5/12
\end{align*}
\]

(4.20)

4.1.1.4 Spatial Discretization

As pointed out by Rai and Moin [83] that the controlling of aliasing error is very important to the turbulent simulation. Use of schemes which do not have a mechanism of controlling aliasing error can result in the decay of the turbulence in a given flow field or an unbounded growth of the solution. One approach to overcoming this problem is to use energy conserving schemes. A second method of controlling aliasing error is to extract and discard at each time step that energy which would otherwise be aliased back. However, current procedures that perform this operation rely on series representations of the dependent variables (such as Fourier represen-
tations), and it is not clear how these procedures can be extended to curvilinear grids.

For the reasons outlined above, the present method uses an upwind differencing technique for the convective terms in the Eq. 4.10, Eq. 4.13, Eq. 4.16. The leading truncation error term of some upwind differences is dissipative in nature and thus damps the higher frequency content. Since only the energy in the upper portion of the spectrum is aliased back, a dissipation of the energy content of this part of the spectrum (due to the natural smoothing of upwind scheme) results in significant control of aliasing errors. The main disadvantage is that the useful information in the upper portion of the spectrum is also lost in the process. The upwind technique (like other finite-difference techniques) also has the advantage that it can be used for curvilinear grids.

First-order accurate upwind differences are extremely dissipative in nature and are hence of little use in practical applications. Second-order accurate upwind methods are considerably less dissipative and are widely used in application codes. However, even second-order accuracy can be insufficient for the turbulence simulations. So, in the present study, we use a fifth-order accurate difference scheme for the convective terms. But it can be shown that 2n+1 grid points are required to produce nth-order accurate upwind differences. This requirement translates into a 11-point stencil in order to produce fifth-order accurate upwind differences. The problem with such large stencils is that many grid points near the computational boundaries cannot longer be treated using the finite differences used in the interior. Hence, finite differences are needed that are as compact as possible subject to the constraint that they have the desirable natural smoothing that controls aliasing errors.

Upwind-biased differences require a much smaller stencil than fully upwind differ-
ences to obtain a given order of accuracy. In addition, the upwind-biased difference
used in the present study have the desired natural dissipation to control aliasing er-
ror. In the LEPDF simulation scheme we develop here, the finite difference scheme
developed by Rai and Moin [83] is directly adopted.

The treatment of the convective terms in the $H_i$ expression can be illustrated by
the following example for the first term in the $u_1$ momentum equation:

if $u_1 > 0,$

$$
\left( u_1 \frac{\partial u_1}{\partial x_1} \right)_i = (u_1)_i \frac{-6(u_1)_{i+2} + 60(u_1)_{i+1} + 40(u_1)_i - 120(u_1)_{i-1} + 30(u_1)_{i-2} - 4(u_1)_{i-3}}{(120\Delta x_1)}
$$

(4.21)

if $u_1 < 0,$

$$
\left( u_1 \frac{\partial u_1}{\partial x_1} \right)_i = (u_1)_i \frac{4(u_1)_{i+3} - 30(u_1)_{i+2} + 120(u_1)_{i+1} - 40(u_1)_i - 60(u_1)_{i-1} + 6(u_1)_{i-2}}{(120\Delta x_1)}
$$

(4.22)

The remaining convective terms are evaluated in a similar manner. The viscous
terms are evaluated using central differences. For stretched meshes, the coefficients
in the difference formulate are evaluated numerically in the code using Lagrange
polynomials so as to retain high-order accuracy. In general, different stencil sizes
will have to be used to obtain the same order of accuracy for the first and sec-
ond derivatives in the integration methods. In the present study a maximum of
seven consecutive grid points are used in the evaluation of the convective and vis-
cous derivatives. With a seven point stencil, the convective and viscous terms are
approximated to fifth- and sixth-order accuracy, respectively.

The staggered grid is used in the discretization. With the staggered mesh, the
Figure 4.2: Staggered Grid Showing Physical Locations at Which the Dependent Variables Are Defined
velocity components are evaluated at the midpoints of the vertical and horizontal sides of each cell. That is, the \( u_1, u_2, \) and \( u_3 \) are evaluated at \((i, j - \frac{1}{2}, k - \frac{1}{2}), (i - \frac{1}{2}, j, k - \frac{1}{2}), \) and \((i - \frac{1}{2}, j - \frac{1}{2}, k)\) respectively if the grid node is defined at \((i,j,k)\). The pressure and the pressure related quantity \( \varphi \) is defined at the cell center, \((i - \frac{1}{2}, j - \frac{1}{2}, k - \frac{1}{2})\). The momentum equations are evaluated at the velocity nodes. The continuity equation is enforced at the midpoint of each cell. The eddy viscosity terms are evaluated according to the momentum equations. One important advantage of using the staggered mesh for incompressible flows is that ad hoc pressure boundary condition are not required. This will be explained in details in next section.

Figure 4.1 shows the two-dimensional counterpart of the three-dimensional staggered grid that was used to obtain the results of this study. The divergence operator is defined at the cell centers, and the spatial derivatives of this operator are defined using a stencil size of four. Thus on an equispaced grid, this operator takes form:

\[
D_{i-\frac{1}{2},j-\frac{1}{2}} = \frac{[-(u_1)_{i+2,j-1/2} + 27(u_1)_{i,j-1/2} - 27(u_1)_{i-1,j-1/2} + (u_1)_{i-1,j-1/2}]}{(24\Delta x_1)} \\
+ \frac{[-(u_2)_{i-1/2,j+2} + 27(u_2)_{i-1/2,j+1} - 27(u_2)_{i-1/2,j} + (u_2)_{i-1/2,j}]}{(24\Delta x_2)}
\]

The gradient operator is defined in a similar manner using four grid points in each direction. Consequently, the Laplacian of \( \varphi \) is defined on a stencil of seven grid points in each spatial direction. As shown in Fig. 4.1, the components of velocity are defined at different physical locations. Considering the \( u_1 \) momentum equation, we see that the convective terms of this equation require the \( u_2 \) and \( u_3 \) velocity components to be defined at the \((i, j - \frac{1}{2}, k - \frac{1}{2})\) locations. A cubic interpolation technique is adopted here (fourth-order accurate) to obtain these velocity components.

For the boundary grid point, a different scheme is developed. For simplicity,
only equispaced boundary grid points are discussed here. For a temporal channel simulations, only the wall boundaries need to be treated specially. In the streamwise and spanwise directions, periodic boundary conditions are used. The boundary points can be treated like the “inner points” after the simple extension of the flow field periodically. For the spatial channel flow simulations, all the boundaries in the directions of non-periodic boundary conditions need to dealt differently. As an example, the treatments for wall boundary points will be discussed in details. If the point \((i - \frac{1}{2}, j - 1)\) in the Fig. 4.1 is considered the boundary point, the divergence operator for the cell \((i - \frac{1}{2}, j - \frac{1}{2})\) is taken to be

\[
D_{i-\frac{1}{2},j-\frac{1}{2}} = \frac{[-(u_1)_{i+1,j-\frac{1}{2}} + 27(u_1)_{i,j-\frac{1}{2}} - 27(u_1)_{i-1,j-\frac{1}{2}} + (u_1)_{i-2,j-\frac{1}{2}}]}{(24 \Delta x_1)} + \frac{[(u_2)_{i-\frac{1}{2},j} - (u_2)_{i-\frac{1}{2},j-1}]}{(\Delta x_2)}
\]

The \(x_1\) component of the gradient operator is computed using the fourth-order accurate finite-difference given as

\[
\left( \frac{\partial \varphi}{\partial x_1} \right)_{i,j-\frac{1}{2}} = \frac{-\varphi_{i+\frac{1}{2},j-\frac{1}{2}} + 27\varphi_{i+\frac{1}{2},j-\frac{1}{2}} - 27\varphi_{i-\frac{1}{2},j-\frac{1}{2}} + \varphi_{i-\frac{1}{2},j-\frac{1}{2}}}{24 \Delta x_1}
\]

\[
\left( \frac{\partial \varphi}{\partial x_2} \right)_{i-\frac{1}{2},j} = \frac{\varphi_{i-\frac{1}{2},j+\frac{1}{2}} - \varphi_{i-\frac{1}{2},j-\frac{1}{2}}}{\Delta x_2}
\]

The corrector step of Eq. 4.11 for the points \((i - 2, j - \frac{1}{2}), (i - 1, j - \frac{1}{2}), (i, j - \frac{1}{2}), (i + 1, j - \frac{3}{2})\), and \((i - \frac{1}{2}, j)\) can be rewritten as

\[
\frac{(\bar{u}_1)_{i-2,j-\frac{1}{2}} - (u_1^2)_{i-2,j-\frac{1}{2}}}{\Delta t} = -\gamma_1 \left( \frac{\partial \varphi}{\partial x_1} \right)_{i-2,j-\frac{1}{2}}
\]
\[
\frac{(\bar{u}_1)_{i-1,j-\frac{1}{2}} - (u^a_1)_{i-1,j-\frac{1}{2}}}{\Delta t} = -\gamma_1 \left( \frac{\partial \varphi}{\partial x_1} \right)_{i-1,j-\frac{1}{2}} \\
\frac{(\bar{u}_1)_{i+1,j-\frac{1}{2}} - (u^a_1)_{i+1,j-\frac{1}{2}}}{\Delta t} = -\gamma_1 \left( \frac{\partial \varphi}{\partial x_1} \right)_{i+1,j-\frac{1}{2}} \\
\frac{(\bar{u}_1)_{i+2,j-\frac{1}{2}} - (u^a_1)_{i+2,j-\frac{1}{2}}}{\Delta t} = -\gamma_1 \left( \frac{\partial \varphi}{\partial x_1} \right)_{i+2,j-\frac{1}{2}} \\
\frac{(\bar{u}_1)_{i-\frac{1}{2},j} - (u^a_1)_{i-\frac{1}{2},j}}{\Delta t} = -\gamma_1 \left( \frac{\partial \varphi}{\partial x_2} \right)_{i-\frac{1}{2},j}
\]

(4.27)

whereas the corrector step for the point \((i - \frac{1}{2}), j\) is given by

\[
\left( \bar{u}_2 \right)_{i-\frac{1}{2},j-1} = \left( u^a_2 \right)_{i-\frac{1}{2},j-1} = v_0
\]

(4.28)

where \(v_0\) is the dimensionless blowing velocity from the wall.

Using the divergence operator defined in Eq. (4.24), Eq. (4.27) and Eq. (4.28) can be combined to yield

\[
\frac{-(u^a_1)_{i+1,j-\frac{1}{2}} + 27(u^a_1)_{i,j-\frac{1}{2}} - 27(u^a_1)_{i-1,j-\frac{1}{2}} + (u^a_1)_{i-2,j-\frac{1}{2}} + (u^a_2)_{i-\frac{1}{2},j} - v_0}{(24\Delta x_1)} \\
= \gamma_1 \Delta t \left\{ \frac{-(\varphi x_1)_{i+1,j-\frac{1}{2}} + 27(\varphi x_1)_{i,j+\frac{1}{2}} - 27(\varphi x_1)_{i-1,j-\frac{1}{2}} + (\varphi x_1)_{i-2,j-\frac{1}{2}}}{(24\Delta x_1)} \\
+ \frac{(\varphi x_2)_{i-\frac{1}{2},j}}{(\Delta x_2)} \right\}
\]

(4.29)

Substituting Eqs. (4.25) and (4.26) for the gradient operator into Eq. (4.29), we obtain the difference equation for \(\varphi\) at the cell center \((i - 1/2, j - 1/2)\). This method of implementing the surface boundary condition does not requires an ad hoc pressure boundary condition.

The predicting step of Eq. (4.10) requires the evaluation of the viscous and inviscid terms. Consider for example the term \(u_2 \partial u_2 / \partial x_2\) of the \(u_2\) momentum
equation at the point \((i, j + \frac{1}{2})\). A seven-point stencil of the type used in Eq. (4.21) and (4.22) cannot be employed because of the approximation of this point to the wall. Hence lower-order accurate finite-difference that require smaller stencils are used in this evaluation as

if \(u_2 > 0\)

\[
\left( u_2 \frac{\partial u_2}{\partial x_2} \right)_{i-\frac{1}{2}, j} = \frac{(u_2)_{i-\frac{1}{2}, j+1} - (u_2)_{i-\frac{1}{2}, j-1}}{2\Delta x_2}
\]

(4.30)

if \(u_2 < 0\)

\[
\left( u_2 \frac{\partial u_2}{\partial x_2} \right)_{i-\frac{1}{2}, j} = (u_2)_{i-\frac{1}{2}, j} \left( \frac{-(u_2)_{i-\frac{1}{2}, j+2} + 6(u_2)_{i-\frac{1}{2}, j+1} - 3(u_2)_{i-\frac{1}{2}, j} - 2(u_2)_{i-\frac{1}{2}, j-1}}{6\Delta x_2} \right)
\]

(4.31)

4.1.1.5 Solution Techniques for Velocity and Pressure Equations

In the implicit numerical method, such as Crank-Nicholson (CN) method, the problems with multi-dimensional nonperiodic boundary conditions is very challenging for the numerical solution of the finite difference equation. If there is only one direction with nonperiodic boundary conditions, the resulting matrix of the finite difference equation will be diagonal matrix. In the numerical scheme developed here, seven points stencil is used for the Laplacian operators in the velocity prediction step and the pressure equation. Therefore, the resulting matrix of the finite difference equation will be a pentadiagonal matrix, which can be directly inverted efficiently. The time complexity of the direct inversion process is of order of \(n\), where \(n\) is the dimension of the matrix. However, for the problems with more than one directions of nonperiodic boundary conditions, the solution process is much more complicated
that the case with one dimensional nonperiodic boundary conditions. The main reason for the complexity is that the resulting matrix of the discretization process is a full matrix. The direct inversion of this kind matrix is very expansive. The time complexity of the direct inversion algorithm is of the order of $n^3$. In turbulent numerical simulations, a algorithm with time complexity of $n^2$ or higher is regarded as an very expensive or unacceptable algorithm.

Because of the reasons mentioned above, it is not wise to solve the prediction step and the pressure Poisson equation in a direct method. Therefore an approximate factorization method is used to solve the prediction equation. The Poisson equation resulting from the corrector steps is solved using transform methods. To illustrate the mechanism of the approximate factorization method, Eq. 4.10 can be rewritten as

$$(1 - A_1 - A_2 - A_3)(u_i^n - u_i^l) = \Delta t \gamma_1 H_i(u_i^n) + 2(A_1 + A_2 + A_3)u_i^n$$  \hspace{1cm} (4.32)

where

$$A_1 = \Delta t \alpha_1 \left( \frac{1}{R_e} + < v_T > \right) \frac{\delta^2}{\delta x_i^2}$$  \hspace{1cm} (4.33)

$$A_2 = \Delta t \alpha_1 \left( \frac{1}{R_e} + < v_T > \right) \frac{\delta^2}{\delta x_2^2}$$  \hspace{1cm} (4.34)

$$A_3 = \Delta t \alpha_1 \left( \frac{1}{R_e} + < v_T > \right) \frac{\delta^2}{\delta x_3^2}$$  \hspace{1cm} (4.35)

The left-hand side of Eq. (4.32) is then approximated by the factorization method as follows:
Equation (4.36) is an $O(\Delta t^3)$ approximation to Eq. (4.32). The biggest advantage of this approximation is the significant reduction in the computing cost and memory. The approximated system only requires inversions of a diagonal matrix.

The pressure related scalar $\varphi$ can be obtained by combined the $\varphi$ equation and the continuity equation. Take the step 1 in the Eq. (4.10) as an example,

\[
(1 - A_1)(1 - A_2)(1 - A_3)(u_i^n - u_i^0) = \Delta t \gamma_i H_i(u_i^n) + 2(A_1 + A_2 + A_3)u_i^n \tag{4.36}
\]

for $i = 2, 3, \ldots, N_l - 1$, $j = 2, 3, \ldots, N_2 - 1$, $k = 2, 3, \ldots, N_3 - 1$.

A solution to Eq. (4.37) and the corresponding boundary conditions can be easily obtained as in [39]. Let

\[
\varphi^{n+1}(i, j, k) = \sum_{l=0}^{N_l-1} \sum_{m=0}^{N_3-1} \varphi(l, j, m) \cos \left( \frac{\pi l}{N_l} \left( i - \frac{1}{2} \right) \right) \cos \left( \frac{\pi m}{N_3} \left( k - \frac{1}{2} \right) \right) \tag{4.38}
\]

for $i = 1, 2, \ldots, N_l$, $j = 1, 2, \ldots, N_2$, $k = 1, 2, \ldots, N_3$. Here $i, j,$ and $k$ are grid index in the streamwise, normal, and spanwise directions of the channel. Substituting Eq. (4.38) and the corresponding expression for $Q$ into (4.37) and (4.36) and using the orthogonality property of cosines, we obtain

\[
\frac{\delta^2 \varphi}{\delta x_2^2} - k'_l \varphi - k'_m \varphi = \hat{Q}(l, j, m), \tag{4.39}
\]

where $k'_l = 2[1 - \cos(\pi l/N_l)]/\Delta x_2^2$ and $k'_m = 2[1 - \cos(\pi m/N_3)]/\Delta x_3^2$ are the modified wave numbers. For each set of wave numbers, the above banded system of
equations can be easily inverted, and \( \tilde{\varphi} \) is obtained from Eq. (4.39). The velocity field \( \tilde{u}_i \) is then obtained from

\[
\tilde{u}_i = u_i^a - \Delta t G(\tilde{\varphi})
\]  

(4.40)

4.1.1.6 Stability Discussion

In the Runge-Kutta/Crank-Nicholson numerical scheme, the CN method is an absolutely stable method. The stability restriction comes from the R-K method. In a LEPDF code, just like in a LES code, it is not possible to treat the terms involving the eddy viscosity implicitly because of the nonlinear dependency of eddy viscosity on the filtered strain stresses. So the eddy viscosity related terms as well as the convection terms must be treated explicitly. There is not much we can do for the convection terms with regards of the stability restriction. However, there is some room for the improvement of the stability requirement for the eddy viscosity terms. It is common practice in LES method to add a constant pseudoviscosity to the implicit term and subtract it from the explicit term. The effect of such pseudoviscosity, \( \nu_v \), on diffusive stability requirement has been studied by Leslie and Gao [86], who have shown that stability is ensured if only if the following condition is satisfied:

\[
(\nu_T - \nu_v)\Delta t \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right) < \frac{1}{4}
\]  

(4.41)

The pseudoviscosity used in the current scheme is \( \nu_t \). The time increment should also satisfy the CFL stability condition for convective terms. The CFL number is given by
\[ CFL = \Delta t \max_{x,y,z} \left( \frac{|\bar{u}|}{\Delta x}, \frac{|\bar{v}|}{\Delta y}, \frac{|\bar{w}|}{\Delta z} \right) \]  

(4.42)

and should be less than \( \sqrt{3} \) for stability. In LES, \( \nu_T \) is directly proportional to the grid resolution and \( < \nu_T > \) is of same order as \( \nu_T \). Therefore, with the present treatment, the viscous stability requirement as given by Eq. (4.41) is less restrictive than the CFL condition.

### 4.1.2 Monte Carlo Method for Scalar Pdf Equation

The pdf method seems to be of little more than academic interest due to the apparent difficulty in obtaining solutions to the pdf evolution solution equations. The difficulty comes from two aspects. Some terms like molecular diffusion effect is not explicitly related to the independent variables. Stochastic modelling is always employed to build a relationship between the unknown terms and the independent variables. The second reason is that the high dimensionality of the pdf evolution equation. The joint pdf of several scalars or the joint pdf of velocity and scalars is a function of many independent variables. Even in constant-property inert (without chemical reaction) flows, the pdf equation is an integro-differential equation in up to seven independent variables (three velocity components, three spatial coordinates, and time). In flows of practical interest, analytic solutions are out of the question, and conventional numerical techniques (such as finite difference and finite element methods) are impracticable. However, it is possible to solve the modelled pdf equation by a Monte Carlo method, which is ideally suited to problems of large dimensionality. The main advantage of Monte Carlo method is because it is a linear algorithm, while most finite difference methods and finite element methods are at least ideally even exponential algorithms. In the Monte Carlo method, the joint
pdf can be represented computationally by the discretization representation, and its evolution can be computed via stochastic models.

4.1.2.1 Stochastic Modelling for Scalar Pdf Evolution Process

In the filtered pdf transport equation (3.26) for turbulent reactive flows, the conditional expectation term regarding the molecular mixing is not explicitly related to the unknowns in the system. Thus the conditional expectation term need to be modelled while the remaining terms are known. Before considering the terms to be modelled, we emphasize again that no modelling is needed for the terms pertaining to reaction and transport in physical space.

For a simple single species diffusion process, the governing equation should be

\[ \rho \frac{D\phi}{Dt} = D \nabla^2 \phi \]  \hspace{1cm} (4.43)

The evolution equation for \( f_\phi(\psi; t) \) can be obtained by integrating the general pdf evolution equation. The equation reads,

\[ \frac{\partial f_\phi}{\partial t} = -\frac{\partial}{\partial \psi}[f_\phi(D/\rho) \nabla^2 \phi | \psi] \]  \hspace{1cm} (4.44)

It may be seen that the evolution of the pdf depends entirely upon the conditional expectation \((D/\rho) \nabla^2 \phi | \psi\) which is to be modelled.

Dopazo suggested the following deterministic model:

\[ \frac{\partial}{\partial \phi}[f_\phi(D/\rho) \nabla^2 \phi | \psi] = -\frac{1}{2} C_\phi (\psi - \overline{\phi}) / \tau \]  \hspace{1cm} (4.45)

where \( \tau = k/\epsilon \) is the decay time scale of the velocity fluctuations, \( C_\phi \) is a proportional constant between the turbulent velocity decay time scale and the turbulent scalar
decay time scale $\tau_\phi$. 

$$\tau_\phi \equiv \frac{1}{2} \phi'^2$$  \hspace{0.5cm} (4.46)  

$$\epsilon_\phi = \frac{D}{\rho} \frac{\partial \phi'}{\partial X_i} \frac{\partial \phi'}{\partial X_i}$$  \hspace{0.5cm} (4.47)  

$$\tau_\phi = \frac{T}{C_\phi}$$  \hspace{0.5cm} (4.48)  

In this model, it is suggested that in composition space the conditional particle move towards the mean at the rate proportional to its distance from the mean. This model is attractive in its simplicity, and it is straight forward to verify that the modelled pdf equation admits the Gaussian solution as it should. However, the model predicts that the shape of the pdf remains unchanged during decay, and consequently, from an arbitrary initial pdf, there is no relaxation to a Gaussian distribution.

A model of scalar dissipation analogous to the Langevin equation is 

$$\Delta_{\delta t} \phi^*(t) = G[\phi^*(t) - \bar{\phi}(t)]\delta t / \tau + [B\phi'^2 / \tau]^{1/2} \Delta_{\delta t} W_t.$$  \hspace{0.5cm} (4.49)  

Here $G$ and $B$ are constants to be determined and $W_t$ is, as always, a Wiener process. The qualitative behavior of the Langevin model is satisfactory in all respects except that there equation also admit negative value for the scalar.

The widely used and accepted model is particle-interaction model, which is also called Curl’s model, the coalescence/dispersion model or simply C/D model. It is the model we are going going to adopt in this study. Consider the discrete representation in which the pdf $f_\phi(\psi)$ is represented by $N$ delta functions:

$$f^{*}_{\phi N}(\psi; t) \equiv \frac{1}{N} \sum_{n=1}^{N} \delta(\psi - \phi^{*(n)}(t))$$  \hspace{0.5cm} (4.50)
The discrete pdf evolves by the N stochastic particles $\phi^{(n)}$ moving in $\psi$ space.

In a small interval of time $\delta t$, there is a small probability that a pair of stochastic particles will "mix". The time $\tau_N$ is defined by

$$\tau_N = \frac{\tau}{C\phi N}$$

(4.51)

where $N$ is the total number of stochastic particles. $\tau$ is a turbulent time scale, as discussed before.

$$\tau = \frac{k}{\epsilon}$$

(4.52)

Then in the time interval $\delta t$, with probability $1 - \delta t/\tau_N$, the compositions of all the stochastic particles do not change: but, with probability $\delta t/\tau_N$, the compositions of a pair of particles change. These two particles (denoted by p and q) are selected at a random without replacement and their values of $\phi^*$ are replaced by their common mean $\frac{1}{2}(\phi^{*(p)} + \phi^{*(q)})$. This stochastic model can be written as:

with probability $1 - \delta t/\tau_N$:

$$\phi^{*(n)}(t + \delta t) = \phi^{*(n)}(t), n = 1, 2, ..., N$$

(4.53)

with probability $\delta t/\tau_N$:

$$\phi^{*(p)}(t + \delta t) = \frac{1}{2}[\phi^{*(p)}(t) + \phi^{*(q)}(t)], \quad \phi^{*(q)}(t + \delta t) = \frac{1}{2}[\phi^{*(p)}(t) + \phi^{*(q)}(t)]$$

(4.54)

and

$$\phi^{*(n)}(t + \delta t) = \phi^{*(n)}(t), n = 1, 2, ..., N, n \neq p, n \neq q.$$  

(4.55)

where * is used to distinguish the stochastic process and the original physical process. The evolution equation for $f^*(\phi; t)$ corresponding to this stochastic model
can be shown to be

\[
\frac{\partial f^*(\phi, t)}{\partial t} = 2C^\phi \left\{ 2^\sigma \int f^*(\phi + \phi')f^*(\phi - \phi')d\phi' - f^*(\phi) \right\} / \tau \tag{4.56}
\]

Pope [62] summarized the six requirements that the modelling must satisfy. Pope also pointed that of all the three models described, the particle-interaction model is the only model to satisfy all the aspects of the requirements. The Dopazo's simple model is not satisfactory in that the shapes obtained are far from Gaussian. The Langevin model is not applicable because it violates the principle of composition. However, it is a good model for the velocities, which we will discuss later.

For the diffusion and convection processes, they are exactly expressed in the pdf equation. There is no need of modelling for these terms with regards to closure of the pdf evolution equation. As mentioned earlier, the complexity of the solution procedure due to the high dimensionality of the pdf equation prevents pdf method as an effective practical method in the turbulent reactive flow research. It is much convenient and effective (will be discussed later) to introduce some stochastic processes to model the original physical processes. The principal difference between the modelling here and the modelling of the molecular diffusion process is that in the former case, the modelled pdf evolves exactly as the original physical process. The essence of the whole modelling process is to construct a system of stochastic particles whose evolution is simply computed and in which the pdf evolves in the same way as the pdf of fluid particles.

Langevin [87] model is adopted here to model the diffusion and turbulent mixing processes, that is,

\[
\Delta \bar{z}^*(t) = D(\bar{z}^*[t], t)\delta t + [R(\bar{z}^*[t], t)]^{1/2}\Delta \bar{W}_t \tag{4.57}
\]
where the coefficients $D$ and $B$ are to be determined and $\mathcal{W}_t$ is an isotropic Weiner process. $D$ and $B$ are called drift and diffusion coefficients respectively [88].

The corresponding evolution equation for $f^*(\phi)$:

$$\frac{\partial f^*(\phi, t)}{\partial t} + \frac{\partial}{\partial x_i} \left[ D_i f^*(\phi) \right] - \frac{1}{2} \frac{\partial^2}{\partial x_i \partial x_i} \left[ B f^*(\phi) \right] = 0$$

(4.58)

In order for the diffusion process Eq. (4.57) to correspond to the spatial transport in the modelled pdf equation, Eq. (4.58) should be same as the corresponding terms in Eq. (3.26). This requires:

$$B = 2D_p$$

(4.59)

$$D = \overline{u} + \nabla D_p$$

(4.60)

Thus, in the solution procedure, spatial transport (during the time interval $\Delta t$) is accounted for by moving each stochastic particle independently by

$$\tilde{z}^*(t + \delta t) = \tilde{z}^*(t) + \delta t \left\{ \overline{u} + \nabla D_p \right\}_{\tilde{z}^*(t)} + \left[ 2\delta t D_p \right]^{\frac{1}{2}} \xi_{\tilde{z}^*(t)}$$

(4.61)

where $\xi$ is a standardized joint normal random vector.

### 4.1.2.2 Fractional-Step Algorithm to Solve Pdf Evolution Equation

We consider the turbulent flow within a three-dimension volume of physical space: the solution domain. At time $t$, pdf $\overline{f}(\phi, z; t)$ is represented by $N(t)$ stochastic particles in a state space. At time $t$, the state of the $n$th stochastic particle is

$$\phi^{*(n)}(t), z^{*(n)}(t), \quad n = 1, 2, ..., N(t)$$

(4.62)
As the time proceeds, the states of the stochastic particles change: some particles may leave the solution domain and some may enter as prescribed by the boundary conditions. Substituting the molecular model Eq. (4.56) and the diffusion Eq. (4.58) model discussed above into the pdf evolution equation, the modelled equation for $\overline{f}(\phi, x; t)$ (for brevity, * for stochastic quantity will be omitted) to be solved is:

$$\frac{\partial \overline{f}(\phi)}{\partial t} = \frac{\partial}{\partial \psi_1} \left\{ S_1(\psi) \overline{f}(\phi) \right\} - \frac{\partial}{\partial x_1} \left\{ (\overline{u_i} + \nabla D_{\phi}) \overline{f}(\phi) \right\} + \frac{1}{2} \frac{\partial^2}{\partial x_i \partial x_j} \left\{ 2D_{\phi} \overline{f}(\phi) \right\}$$

$$+ \frac{2\sigma}{\tau} \int \overline{f}(\phi + \phi') \overline{f}(\phi - \phi') d\phi' - \overline{f}(\phi)$$

(4.63)

The above equation is a differential-integral equation, the solution for this is very hard, especially for high dimension case. Standard techniques such as finite-difference are severely limited because of the large dimensionality of the pdf. For the problems with a large number of independent variables, Monte Carlo methods usually provides a feasible alternative means of obtaining numerical solutions. The basic idea of Monte Carlo method is "to solve a problem by putting in random numbers and getting out random answers". In 1980, Pope [89] introduced the Monte Carlo method to solve pdf equation for turbulent flow. He also pointed out that the error of the Monte Carlo method decreases inversely as square root of the total number of the stochastic particles. The fractional step scheme based on the Monte Carlo method and developed in [62] is adopted here to solve the above pdf equation.

Equation (4.63) can be rewritten

$$\frac{\partial \overline{f}(\phi)}{\partial t} = (P_1 + P_2 + P_3) \overline{f}(\phi)$$

(4.64)

where $P_1$ corresponds to the chemical reaction part, $P_2$ for the molecular mixing,
and $P_3$ for the convective and the diffusion effects. For each time step, the method is defined by the three fractional steps:

$$\begin{align*}
\frac{\partial \tilde{f}_1(\phi)}{\partial t} &\equiv (I + \delta t P_1) \tilde{f}(\phi) \\
\frac{\partial \tilde{f}_2(\phi)}{\partial t} &\equiv (I + \delta t P_1) \tilde{f}_1(\phi) \\
\frac{\partial \tilde{f}_3(\phi)}{\partial t} &\equiv (I + \delta t P_1) \tilde{f}_2(\phi)
\end{align*}$$

(4.65)

It is shown [62] that Eq. (4.65) is first order approximation to the Eq. (4.64).

Then we will examine the details for each of the fractional steps:

First Fractional Step: Chemical Reaction

In the first step only the chemical reaction is included. It is assumed that the stochastic particles stay at the same physical space during the chemical reaction process. The pdf evolution equation corresponding to this step is:

$$\frac{\partial \tilde{f}(\phi)}{\partial t} = -\frac{\partial}{\partial \psi_\alpha} [S_\alpha(\psi) \tilde{f}(\phi)]$$

(4.66)

The solution of the above equation can be simply achieved since Eq. (4.66) is the evolution equation corresponding to the stochastic system

$$\Delta_{\delta t} \phi^*_\alpha = S_\alpha(\phi^*) \delta t$$

$$\Delta_{\delta t} x_i^* = 0$$

(4.67)

Integrating these equations for a time $\delta t$ using the explicit Euler method yields (to first-order in $\delta t$):

$$\phi^*(t + \delta t) = \phi^*(t) + S_\alpha(\phi^*) \delta t$$

$$x_i^*(t + \delta t) = x_i^*$$

(4.68)
Thus in the first fractional step, the states of each of the \( N(t) \) stochastic particles change independently according to Eq. (4.68).

**Second Fraction Step: Stochastic Mixing Model**

In the second fractional step only the compositions may change by mixing while the position of the particle will not change as in the first fractional step.

In the coalescence/dispersion model, in the small interval \( \delta t \), the probability of a pair of particles mixing is

\[
C_\phi N(t)\delta t/\tau
\]

Consequently, the probability of the \( n \)th particle being selected is

\[
2C_\phi \delta t/\tau
\]

since, if mixing takes place, two out of the \( N \) particles are selected. Similarly, for the general inhomogeneous case, in the small time interval \( \Delta t \) the probability of the \( n \)th particle being selected is

\[
P^{(n)} \equiv 2C_\phi \Delta t/\tau(\mathcal{C}^{(n)}[t],t)
\]

Certainly \( \Delta t \) should be chosen to be significantly smaller than \( \tau \).

A simple computational algorithm to chose particles is to generate \( N \) independent random number \( \omega^{(n)}, n = 1, 2, ..., N \), each uniformly distributed between zero and one. If

\[
P^{(n)} + \omega^{(n)} > 1
\]

then the \( n \)th particle is selected for mixing.
Mixing takes place locally in physical space, and this is reflected in the pairing of the selected particles. Each particle selected is close (in physical space) to its partner. A simple algorithm used here to accomplish this local pairing, is to divide physical space into cells, and to pair particles within each cell. That is, for chosen particles $p$ and $q$,

$$
\phi^*(p)(t + \delta t) = \phi^*(p)(t + \delta t) = \frac{1}{2} [\phi^*(p)(t) + \phi^*(q)(t)],
$$

(4.73)

Third Fraction Step : Spatial Transport

In the third step, the stochastic particles will move in the physical space due to the convection and turbulent mixing, but the composition and enthalpy will not change. The corresponding pdf evolution equation for the processes is

$$
\frac{\partial \bar{f}(\phi, t)}{\partial t} + \frac{\partial}{\partial x_i} [D_i \bar{f}(\phi)] - \frac{1}{2} \frac{\partial^2}{\partial x_i \partial x_i} [B \bar{f}(\phi)] = 0
$$

(4.74)

where

$$
B = 2D_p
$$

(4.75)

$$
D = \bar{u} + \nabla D_p
$$

(4.76)

and

$$
\bar{z}^*(t + \Delta t) = \bar{z}^*(t) + \Delta t \left\{ \bar{u} + \nabla D_p \right\}_{\bar{z}^*(t)} + [2 \Delta t D_p]^{\frac{1}{2}} \bar{z}^*(t) \xi
$$

(4.77)

where $\xi$ is a standardized joint normal random vector.
4.2 Initial and Boundary Conditions

4.2.1 Boundary Conditions

Most of the numerical simulations (DNS or LES) are based on the so-called temporal model. In this model, the flow is assumed to be spatially periodic in the streamwise direction so that periodic boundary conditions can be employed at the inflow and the outflow boundaries, i.e., inflow quantities for both the base flow and the disturbance flow are identical at the inflow and outflow boundaries. The spatial periodicity allows efficient use of (pseudo) spectral approximation in the streamwise direction. But for flows with more pronounced streamwise variation, e.g., boundary layers with pressure gradients, and/or local suction or blowing at the wall, the assumptions in the temporal model are no longer justifiable. For such flows, the so-called spatial model should be used for realistic developing simulation. However, the use of the spatial model introduces two major difficulties: 1) a large streamwise integration domain is required; 2) boundary conditions for the inflow and outflow boundaries have to be specified and implemented into the numerical model.

In the present study, there is very strong blowing fuel streams through the side walls. There is significant development of the turbulent flow field from the inlet to the outlet. The streamwise periodicity is no longer a appropriate assumption. In the case of "weak" transpiration channel flows, Piomelli [42] did use temporal simulation to study the transpired turbulent channel flows. Spalart [93], Spalart & Watmuff [94], and Liu & Piomelli [95] used fringe method to avoid the difficulties associated with the treatment of inflow/outflow boundary conditions.

For the laminar to turbulent transition studies, the inflow boundary conditions is normally set to the undisturbed laminar flow [21] [92]. For spatially developing
turbulent flows, the inflow boundary condition can be so specified that the its spectrum is similar to what was measured experimentally. Lee et al [96] developed a method to generate stochastic inflow boundary conditions with a prescribed power spectrum. Rai and Moin [12] added an additional domain before the leading edge of the “interested” domain in order to get prescribed turbulence distribution at the edge of the “interested” domain. Givi and Jou [72] prescribed the inflow boundary condition in their reacting mixing layer by the combination of unperturbed and perturbed velocity profiles.

Rai and Moin [12] are the first to simulate the entire boundary layer spatial development. The simulation starts with inlet free-stream with perturbation in three velocity components. The disturbance in the free-stream is designed in such a way that the turbulence energy spectrum at the end of the first zone or the beginning of the second zone matches the prescribed spectrum. In one of the simulations, the computational zone is 46 inch long, 3 inch high, and π/2 inch in the spanwise direction. The total number of grid points is up to 17,357,664. Even high CFL number is used, a typical simulation uses about 800 hours on a Cray-YMP supercomputer.

The high demand on the computational time is still a concern for us, even though we get access to both CRAY-YMP supercomputers in NASA Jet Propulsion Laboratory and NASA AMES National Aeronautic Simulation research center. What we most interested in this research is the turbulence and combustion interaction in the fully developed turbulence. In fact, of turbulent combustion flows in the practical applications, turbulent flows develops very quick to reach fully developed turbulence because of the heat release of the chemical reaction.

Here, we innovatively combined the temporal simulation and spatial simulation in our turbulent reactive flow simulations. We start with temporal simulations to get
the fully developed turbulent flow field. Then we use the obtained fully developed flow field as the initial condition for the continued spatial simulations with fuel injection through the side walls. Also the inlet boundary conditions is constructed based on the turbulence field obtained through the temporal simulation and a small amplitude random perturbations.

The scalar fields are just the unperturbed part, and they uniformly equal the species fraction and the temperature of the incoming oxidizer flow.

The outflow boundary conditions are very important, but difficult part for the spatially simulations. The outflow boundary condition should be so specified that even the nonperiodic, large-amplitude fluctuations can pass through this boundary without causing UNPHYSICAL upstream effects. Proper physical outflow boundary conditions are not known, and there is still considerable debate over appropriate numerical outflow boundary conditions. As pointed by Kloker et al [92] that completely satisfactory and fairly general outflow boundary conditions which work for different situations, are very difficult to find. One way to bypass the need for proper outflow boundary conditions is to use an integration domain such that the outflow boundary is always ahead of the vorticity disturbance front. Thus the computational time and memory requirements grow nonlinearly when the domain of interest is increased.

The buffer-domain technique for a effective non-reflecting outflow boundary was introduced by Streett and Macaraeg [97]. The technique is based on the recognition that, for incompressible flow, the ellipticity of the Navier-Stokes equations, and thus their potential for upstream feedback, come from two sources: the viscous terms and the pressure field. Examination [98] of earlier unsuccessful attempts at spatial simulations indicated that upstream influence occurs through the interaction of these
two mechanisms; strong local velocity perturbations interact with the condition imposed at the outflow boundary to produce a pressure pulse that is immediately felt everywhere in the domain, especially at the inflow boundary. Therefore both mechanisms for ellipticity have to be treated. To deal with the first source of upstream influence, Joslin et al [98] smoothly reduced the streamwise viscous terms to zero in the buffer domain in their three-dimensional incompressible spatial direct numerical simulation study. They also reduced the effect of pressure field ellipticity by multiplying the source term of the pressure Poisson equation with an attenuation function in the buffer domain. Liu and Liu [22, 99] used buffer domain technique to study instabilities in flat plate boundary layers and channel flow. In the direct numerical simulation of a spatially developing boundary layer, Rai and Moin [12] employed the buffer method for the outflow boundary conditions. In the buffer domain, the grid is gradually coarsened in the streamwise direction (by a factor of 160). This approach has been found to numerically dissipate most of the unsteadiness within the boundary layer and, in addition, eliminates the reflection of high-frequency pressure waves. Kloker et al [92] tried six different techniques for the outflow boundary conditions, and found that the vorticity-suppression zone method evidently succeeded in keeping the disturbance below the nonlinear threshold level necessary for global instability. In the reacting, spatially mixing layer simulation, Givi and Jou [4] [33] assumed either the first Order or the second order of derivatives of the velocity and the scalar fields equal to zero at the outflow boundary.

In our study here we will adopt the zero second order derivative condition on the velocity and the scalar field at the outflow boundary layer.

The wall boundary condition is very straightforward in the DNS method. No-slip condition is always used for the wall boundary. Near a solid surface, however,
all turbulence structures are small and the grid resolution has to be very fine to resolve even the energy-carrying structures. It is claimed by Deardorff [38] that no-slip boundary conditions cannot be employed at the walls, because the grid interval $\Delta y$ is very much larger than the height of the viscosity sublayer. Piomelli et al [100] discussed series of artificial wall boundary conditions. Two new approximate boundary conditions have been applied to the large eddy simulations of channel flows with and without transpiration. These new boundary conditions give more accurate results than those previously in use, and allow significant reduction of the required CPU time over simulation in which no-slip conditions are applied.

For simplicity, the no-slip boundary condition will be used here for the velocity field, and the Dirichlet boundary condition will be used for the species fractions and temperature at the wall.

It is very common practice to use periodic boundary condition in the spanwise direction for both DNS and LES. In the present LEPDF scheme, we just use the periodic boundary conditions in the spanwise direction.

4.2.2 Initial Conditions

To start the LEPDF computation, the computational domain must be initialized with some appropriate velocity and scalar fields. The only absolute requirement is that the numerical scheme must be able to converge from this starting field to the appropriate stationary state. Provided this requirement is met and the process is stationary, then the simulation must succeed. It is still desirable to specify the starting field well, since this will reduce the computing time needed to pass from the initial state to a stationary condition.

In their turbulent channel flow studies, Moin et al [90] used an initial field with
a component from the solution of the Orr-Sommerfeld and superimposed upon it a mean flow and some random perturbations. The Orr-Sommerfeld equation introduces the necessary large structures in the flow. Fasel et al [21] started their transition simulation with a undisturbed flow field, which was obtained by numerical solving the Navier-Stokes equation for steady flow. The disturbance was introduced by localized blowing and suction within a narrow strip. Givi and Jou [91] initialized their spatially developing reacting mixing layer by superposition of mean flow field, most unstable mode of its instability and the subharmonic disturbance of the predominant mode.

It appears that for a mixing layer the initial conditions are more sensitive in determining the subsequent development of the flow, even after a long streamwise distance, than for other turbulent shear flows [14]. Therefore care must be taken not to introduce any artificial modes in the mixing layer simulation studies. In the case of boundary layer, this is happily not too critical. Experiments show that the initial Tollmein-Schlichting disturbances quickly break up into three-dimensional structures. It is therefore likely that even if the initial large structures are unrealistic, they will evolve into their natural modes. However, one constrain in the present study is that the simulation time is much shorter than is needed for this evolution to be fully realized. It follows that the simulation cannot succeed unless the starting field is quite close to reality.

As mentioned above, the initial boundary conditions for the spatial simulations of the turbulent reactive channel flow is based on the fully developed channel flow field obtained through prior temporal simulations. The initial boundary conditions for the temporal simulations is well chosen as follows:
\begin{align*}
    u(x, y, z, t) &= 1 - y^2 + \epsilon_{orr} u_o + \epsilon_{ran} \tilde{u} \\
    v(x, y, z, t) &= \epsilon_{orr} v_o + \epsilon_{ran} \tilde{v} \\
    w(x, y, z, t) &= \epsilon_{orr} w_o + \epsilon_{ran} \tilde{w}
\end{align*}

(4.78)

where \( \tilde{u}, \tilde{v}, \) and \( \tilde{w} \) are obtained from a random generator, \( u_o, v_o, \) and \( w_o \) are the eigenfunctions for the Orr-Sommerfeld equations. \( \epsilon_{orr} \) and \( \epsilon_{ran} \) are the magnitudes for the eigenfunction solution and the random velocity components respectively.

For the initial scalar field, it is simply assumed that all the channel is initially filled with oxidizer. The species concentration and the temperature are uniform inside the channel. There is no disturbance for the initial scalar field.

### 4.3 Supercomputing Techniques

Supercomputing is characterized by two important aspects: memory and speed. Memory is referred to the core memory not the disk memory. The speed is normally represented by the number of operations per unit time, such as MFLOPS (millions of floating point operations per second). Memory size of a computer directly limits the number of grid points of the problems, which therefore restricts the physical size and the spatial precision of the problems. The speed of a supercomputer limits the time complexity of the problem and the temporal accuracy of the simulations. In a real practice, there are always limits for the time and memory for each supercomputer. For example, the maximum size of the memory used in any single job in NASA AMES NAS center is 256 MWs (million words). To improve the supercomputing performance is a task for both the computer engineers and scientists and
computational fluid dynamics scientists. In this section, we will only discuss how to better use the computer resource to improve the supercomputing performance.

Even though the core memory size of a supercomputer is fixed, there is still lots of room for the user to improve the usage of the memory. The simple rule here are only to declare only the necessary arrays in the simulations and try to shear, if possible, the memory among the intermediate variables. The new development of SSD, Solid State Disk, makes it possible to shear arrays among many variables. The idea is to put the contents of some of the variables into a file in SSD and read the contents back at the time when the contents are required. It is realized that this treatment takes some CPU time. There is tradeoff between the CPU time and the memory size utilization. The advantage of SSD is that the memory access time is much shorter than other disks, even it is still slower than core memory [102].

To speed up the computations includes optimization of the code, and parallel processing. To take full advantage of the processing power and speed of the supercomputer, the code needs to be optimized. The most important part of the optimizing code is increasing vector performance. This will make the program execute faster because the supercomputer derives much of its speed from vector processing.

A vectorized DO loop that indexes a one-dimensional array with the DO loop index will fetch that data at an optimal rate when the increment of the DO loop is one. An increment of one provides a stride of one, which causes the memory banks to be used in order, and the original bank is not revisited until all the other banks have been used. This gives the original bank time to recycle and avoids waiting memory. However, if the stride of a vector fetch is greater than one, memory banks are skipped and the original bank may be revisited before it has recycled, causing processing to wait. Because the number of banks is a power of two, a power-of-two
stride of N will return to the original bank N times sooner, which will causes the great
loss of the performance. So it is important for the code designer to avoid a power-
of-two loop stride in any DO loops. Vector accesses of multidimensional arrays can
result in hidden stride problems because these data structures are stored in a linear
manner in physical memory. Fortran stores multidimensional arrays in column major
order, which means the left-most dimensions are incremented more quickly and the
right-most dimensions more slowly. When the elements of consecutive indexes are
accessed, the hidden stride problem may rise. For example if A is defined as A(10,
20, 30), the hidden stride for a consecutive access A(1,1,l) is 10*20=200.

In general, to prevent loss of program performance due to bank conflict, one
should avoids strides divisible by any power-of-two. One way to do it is to index
array along the first dimension of the inner loop. The other way is to define the
array in such a way that the last dimension is odd.

Another important aspect for the vector optimization is that the optimization
only effective for the inner DO loop. Greater efficiency is obtained from longer
vectors for two reasons: the smaller number of instructions required to complete the
loops, and the decreased overhead cost to set up vector operations. It is common
practice to use dummy indexes in the arrays with three dimensions or higher. For
example, a three dimension array A(l, J, K) can be treated as B(I*J, K,l). The
advantage for this changing is that the inner dimension for B is I*J, which is much
higher than I of A. Therefore, the vectorizing process will work on I*J instead of I
as in array A.

Parallel processing is to use more than one CPUs for a single-user program.
The program must be divided into parts to allow for simultaneous execution by
more than one CPU. The objective of parallel processing is to reduce the wall-
clock time required by execution. The CPU time spent will be greater due to the increased system overhead required by the processing. It is encouraged to use parallel processing by the supercomputer center. The free time policy (no matter how many CPUs a user really use, the center only charge at most the four times of the connection time for a job) in NASA AMES NAS center is a evidence of the importance of parallel processing.
CHAPTER 5

LES SPATIAL SIMULATIONS FOR FULLY DEVELOPED TURBULENT CHANNEL FLOWS

The developed LEPDF simulation code for turbulent reactive flows is first applied for spatial simulations of non-reactive turbulent channel flows. The numerical simulation results for fully developed (non-transpired) turbulent channel flows will be presented in this chapter. The simulations for transpired fully developed turbulent channel flows will be discussed in next chapter.

Fully developed turbulent channel flow has been numerically simulated at Reynolds number of 3860 (or 200), based on center-line velocity (or wall shear velocity) and channel half-width. The large-scale flow field has been obtained by directly integrating the filtered, three-dimensional, time-dependent Navier-Stokes equations. The small-scale field motions are taken care of by Subgrid Scale (SGS) model. The numerical scheme is a highly accurate finite difference scheme. Inflow and outflow boundary conditions have been prescribed in the streamwise direction. No-slip condition is used in channel normal direction. Periodic boundary conditions, is applied, as always, in spanwise direction. The simulations were carried out on the Cray Y-MP2E supercomputer at NASA Jet propulsion Laboratory and the Cray Y-MPC90 supercomputer at NASA AMES research center. The maximum grid size is 128*101*128 (1,654,784).
The statistical mean flow and turbulence quantities are extensively compared with the existing Direct Numerical Temporal simulations and experimental data. The computed flow field is also used to study the detailed turbulent structures. The contributions to the Reynolds from different near wall phenomena are studied in details. The correlation between velocity fluctuation and vorticity statistically depicts the roles of vorticity plays in the turbulence production.

5.1 Code Verifications

In order to test the accuracy and robustness of the current code, two test cases have been designed.

The first test case is an exact solution of Navier-Stokes equations. The sizes of computation domain are \([-\pi/2, \pi/2], [-\pi/2, \pi/2], \) and \([-\pi/2, \pi/2] \) in streamwise (x), normal (y), and spanwise (z) directions respectively. The initial and boundary conditions are:

The intial conditions:

\[
\begin{align*}
    u(x, y, z, 0) &= -\cos(y) \cdot \sin(x) \\
    v(x, y, z, 0) &= \sin(y) \cdot \cos(x) \\
    w(x, y, z, 0) &= 0
\end{align*}
\]  

(5.1)  

The boundary conditions:

\[
\begin{align*}
    u(-\pi/2, y, z, 0) &= \cos(y) \cdot e^{-2t} \\
    u(\pi/2, y, z, 0) &= -\cos(y) \cdot e^{-2t}
\end{align*}
\]
\[ v(-\pi/2, y, z, 0) = 0 \]
\[ v(\pi/2, y, z, 0) = 0 \]
\[ w(-\pi/2, y, z, 0) = 0 \]
\[ w(\pi/2, y, z, 0) = 0 \]  \hspace{1cm} (5.2)

and,

\[ u(x, -\pi/2, z, 0) = 0 \]
\[ u(x, \pi/2, z, 0) = 0 \]
\[ v(x, -\pi/2, z, 0) = -\cos(x) * e^{-2t} \]
\[ v(x, \pi/2, z, 0) = \cos(x) * e^{-2t} \]
\[ w(x, -\pi/2, z, 0) = 0 \]
\[ w(x, \pi/2, z, 0) = 0 \]  \hspace{1cm} (5.3)

The exact solutions are:

\[ u(x, y, z, t) = -\cos(y) * \sin(x) * e^{-2t} \]
\[ v(x, y, z, t) = \sin(y) * \cos(x) * e^{-2t} \]
\[ w(x, y, z, t) = 0 \]
\[ p(x, y, z, t) = \frac{1}{4}(\cos(2x) + \cos(2y))e^{-4t} \]  \hspace{1cm} (5.4)

Series of different grid sizes, such as \(16^3\), and \(32^3\) have been tested, the relative error of the computational results is in the order of \(10^{-4}\). At the same time, another test for same flow field but in \(y\) and \(z\) directions has been also tested. The similar accuracy is achieved.
The second test consists of calculating the evolution of small-amplitude disturbances in channel flow. The disturbance is taken to be an eigensolution of the Orr-Sommerfeld equation. The flow is initialized as:

\[
\begin{align*}
    u(x, y, z, t) &= 1 - y^2 + \epsilon \tilde{u} \\
    v(x, y, z, t) &= \epsilon \tilde{v} \\
    w(x, y, z, t) &= 0
\end{align*}
\] (5.5)

where \(\tilde{u}, \tilde{v}\) represent an eigensolution (wave number of 1) and \(\epsilon\) is a very small number to make sure the disturbance is in the linear range. The Reynolds number chosen for the current study is 75,000. The domain sizes are \([0, 2\pi], [-1, 1],\) and \([0, 2\pi]\) in streamwise, normal, and spanwise directions. The energy associated with the disturbance is defined as:

\[
E(t) = \int_{-1}^{1} \int_{0}^{2\pi} (\tilde{u}^2 + \tilde{v}^2) \, dx \, dy
\] (5.6)

It is shown from the linear theory that the energy in the channel \(E(t)\) grows exponentially in time as \(e^{2ct}\). For the Reynolds number we chosen here, the value of \(c\) is 0.002235. The quantity \(E(t)/E(0)\) is monitored to determine the accuracy of the developed code. The computational result agrees very well with the linear theory results.

### 5.2 Generation of Initial and Inflow Conditions

As mentioned in the last chapter, two major difficulties in spatial simulations are 1) a large streamwise integration domain is required; 2) reasonable boundary conditions for the inflow and outflow boundaries have to be specified. Ideally, the inflow and
outflow boundary conditions can be specified from experiment measurements. The turbulence flow field, however, is a time dependent flow field. The time dependent measurements of the instantaneous turbulent flow field are very difficult, if not impossible. Therefore, the turbulent statistical quantities, such as turbulence power spectrum, have been used, eg. [96] and [12], to specified the inflow or outflow boundary conditions.

The primary interest of this study is to investigate the interactions (mixing, combustion, ...) between fully developed turbulent main stream and the secondary injected flow streams through the channel side walls. The reason for us to study fully developed turbulent main stream is that of turbulent combustion flows in the practical applications, turbulent flows develops very quickly to reach fully developed turbulence because of the heat release of the chemical reactions. The basic ideal is to use fully developed turbulent flow field as the initial condition for the our spatial simulation and extract information from the fully developed flow field to prescribe the inflow boundary conditions. The outflow boundary conditions applied here are just to assume the second order of derivatives of all flow field quantities equal to zero. In order to test the feasibility of the scheme, a non-transpired fully developed turbulent channel flow is first simulated. The extensive comparisons among the present spatial simulation, temporal simulations, and experimental data prove that the spatial development even in a non-transpired channel is significant. As compared with the existing temporal simulations, the present spatial simulation is in better agreement with the experimental data.

In order to effectively generate fully developed channel flow database, temporal simulation is used. The temporal simulation is initialized with laminar flow and certain perturbations.
\begin{align}
    u(x, y, z, 0) &= 1 - y^2 + \epsilon_{orr} \bar{u} + \epsilon_{ran} u_r \\
    v(x, y, z, 0) &= \epsilon_{orr} \bar{v} + \epsilon_{ran} v_r \\
    w(x, y, z, 0) &= \epsilon_{ran} w_r
\end{align}

(5.7)

where \( \bar{u} \) and \( \bar{v} \) are the eigenfunctions for the 2-D Orr-Sommerfeld eigenfunction solutions. \( u_r, v_r, \) and \( w_r \) are random perturbations obtained by random generator. \( \epsilon_{orr} \) and \( \epsilon_{ran} \) are the magnitudes for the perturbations. It is found that the magnitude of the perturbation is important for the simulations. Too large perturbation may lead to the perturbation grow unbounded, while too small perturbation will make simulation take very long time for the flow to transfer from laminar flow field to turbulent flow field. \( \epsilon_{orr} \) and \( \epsilon_{ran} \) chosen for the present studies are in the orders of 0.01 and 0.00001 respectively. Periodic boundary conditions are used in both spanwise directions. No-slip condition is applied in the normal direction.

The sizes of the computation domain are \([0, 4\pi], [-1, 1], \) and \([0, 2\pi]\) in streamwise (\(x\)), normal (\(y\)), and spanwise (\(z\)) directions. The grid is equispaced in both streamwise and spanwise directions and stretched in the normal direction. The stretching in the normal direction is based on a geometric progression. Several grid size have been used. The minimum spacing in the normal direction is about 0.5 wall units.

In the early stage of the simulation, coarse grid size \((64*65*64)\) is used. After the simulation reach to a certain point that the turbulent small structure is important, the grid size is transferred to a finer grid size \((128*101*128)\). At the same time, the flow field is interpolated from coarser grid to the finer grid. Then the simulation will continue until the flow field reaches statistically steady state.

The generated temporal simulation database is directly used as the initial con-
ditions for the further spatial simulations. The inlet boundary condition for the further spatial simulation is constructed in such a way that the temporal flow field is assumed to be at the upper stream of the computational domain of the spatial simulations. In other words, the computational domain for the later spatial simulations consists of two sub-domains denoted domain 1 and 2. The first domain is in the upper stream of the second domain. The flow field of the first domain is result of the early temporal simulation. The inflow boundary condition of the second domain is equal to the outlet flow field of the first domain. We further assume that the instantaneous flow quantities in the first domain is convected downstream with a constant velocity.

5.3 Mean-Velocity Profile and Turbulence Statistics

5.3.1 Mean-Velocity Profile

Starting from the initial condition obtained from the above mentioned temporal simulation, the governing equations are integrated forward for several “turnover time” (the turnover time is defined as the time for a inlet disturbance to reach the outlet boundary). The domain is divided into 8 equal size segments for the calculation for statistical quantities. In each segment, all the statistical quantities are averaged in the horizontal plane and time.

Figure 5.1 shows the streamwise mean-velocity profiles from the temporal simulation and spatial simulation. Unless otherwise stated, the spatial simulation results presented in this paper are the results for the sixth segment in the downstream direction. Also shown in the figure are the mean velocity profiles from the experimental result of Eckelmann [103] for \( R_r = 142 \) and result of Wallace et al [104] for \( R_r = 208 \). The law of the wall and the log law are shown in the figure too. In
the near region \((y^+ < 5)\), both the experimental data and the present numerical simulation data follow in the linear law of the wall. In the logarithmic region, the numerical simulation result \((R_t = 200)\) is very close to the the experimental data of \(R_t = 208\).

### 5.3.2 Turbulence Intensity

The streamwise turbulence intensities by the wall-shear velocity are shown in Fig. 5.2.

Shown in the figure are the LES spatial and LES temporal simulations of the present study. Also shown in the figure is the DNS (direct numerical simulation)
temporal simulation results from Kim et al [16] for $R_T = 180$. The experimental data are from Kreplin & Eckelmann [105] for $R_T = 194$. It can be seen that the LES spatial simulations predict better results than DNS temporal simulation even though LES only use only about 27% of the grid points of used in the DNS. In the region corresponding to the maximum turbulence intensity, the LES spatial simulation agree much better with the experimental data than the LES temporal simulation, in terms of the magnitude of the intensity and the position corresponding to the maximum intensity. It is evident that the streamwise evolution of turbulence even in the non-transpired channel is still very important.

The turbulence intensities in normal and spanwise directions are shown in Fig. 5.3 and 5.4. In addition to the experimental data from Kreplin & Ecklemann, the
It is shown that there is not much difference among the simulation results. The experimental data from Kreplin & Ecklemann is much higher than the numerical simulations. The reason for this discrepancy has been discussed by Kim et al [16]. They pointed out that the experimental data of velocity in the wall region measured by the standard hot-wire techniques, especially for the normal component, may contain significant error caused by cross-contamination. The data by Niederschulte is obtained by using advanced LDV technique at a $R_T = 178.6$. In general, all the simulation results agree very well with this experimental data. It is shown in Fig. 5.4 that there is not much difference between LES temporal simulation and LES.
spatial simulation. The LES predict better results than DNS simulations. Again, in the wall region, there is notable discrepancy between numerical simulation and the experimental data.

The Reynolds shear stress (normalized by the wall shear velocity) is shown in Fig. 5.5 based on both the LES temporal and spatial simulations. Shown in the figure are also the experimental data from Eckelmann [103] for $R_r = 142$ and 208. The overall performance of the spatial simulation is much better than that of temporal simulation. The maximum Reynolds stress predicted by temporal simulation is much lower than the experimental data, while the prediction from the spatial simulation is in good agreement with the experimental data ($R_r = 208$). In the region very close to the wall ($y^+ < 30$), there is significant difference between the experimental
data and the numerical results from both temporal and spatial simulations. As pointed by Kim et al [16] that this difference may be attributed to the experimental measurements. The experimental data in the immediate vicinity of wall seems to be too high as compared with the expected $y^3$ behavior in this region.

5.3.3 Turbulence Power Spectra

The one-dimensional energy spectrum functions in streamwise direction:

$$\phi(k) = \frac{E_i(k)}{\langle u_i^2 \rangle},$$

where $\int_0^\infty \phi(k)dK = 1$  \hfill (5.8)
for the three velocity components are shown in figures 5.6, 5.7, and 5.8.

In all these figures, the LES spatial simulation results are for both $y^+ = 5.52$ and $y^+ = 16.2$. The LES temporal simulation for $y^+ = 5.52$ and DNS temporal simulation of Kim et al [16] for $y^+ = 5.39$ are also shown in the figures. The experimental data are from Balint et al [107] for $Re_d = 27,650$ at $y^+ = 18$ and Wei and Willmarth for $Re_{d/2} = 22,776$ at $y^+ = 15.9$. The LES spatial simulation results for all the velocity components indicate that there are more small structures at $y^+ = 16.2$ than at $y^+ = 5.52$. The numerical simulation result agrees well with the experimental data at low wave numbers. At high wave number region, the experimental data is much higher than the numerical simulation results. With the help of turbulence (SGS) model, LES predict much better results than the DNS.
Figure 5.7: Normal Velocity Power Spectrum in Streamwise Direction

Simulations. It is very important to point out that the LES spatial simulation predicts much more accurate results than the temporal simulation. Once again, the comparison between temporal simulation and spatial simulation illustrates that the streamwise evolution of turbulence in the non-transpired channel flow is also important.

Shown in the Fig. 5.9 are the spanwise turbulence spectrum for three velocity components. The DNS simulation for Rai & Moin [83] is also shown in the figure. The simulation results agree well with each other. It is shown that there is not much difference in the spanwise energy spectrum between the simulations with and without consideration of the streamwise turbulence evolution. It is because that the energy at high Kx wave number is at least two generations smaller than that at low
Kx wave numbers. It can be clearly seen that the relationship between the spanwise spectrum and the streamwise spectrum:

\[
\frac{E_i}{\langle (u_i)^2 \rangle} = \int_0^\infty \int_0^\infty \phi(K_x, K_z) d(K_x) d(K_z),
\]

\[
= \int_0^\infty \phi(K_z) d(K_z),
\]

\[
= \int_0^\infty \phi(K_x) d(K_x)
\]

so,

\[
\phi(K_x) = \int_0^\infty \phi(K_z) d(K_z),
\]
5.3.4 Turbulence Structures

Coherent structure of any turbulent flows is the key to understand the local balance of production, transport, and dissipation of turbulence quantities such as kinetic energy and Reynolds stress. In turbulent boundary layer, production is concentrated in the region very close to the wall. Knowledge of the turbulence structure in this region is of special importance. As pointed out by Klint et al [109] that roughly half of the total turbulence energy production occurs within the region very close to the wall. The outer 80% or so of the boundary layer, to the wake, contributes only about 20% to the total production. The study of turbulent coherent structure can

\[ \phi(K_z) = \int_0^{\infty} \phi(K_z) d(K_z) \]  

Figure 5.9: Velocity Power Spectrum in Spanwise Direction

---

\( \int_0^{\infty} \phi(K_z) d(K_z) \)
help us to build up accurate predictive models, to control or make use of turbulent flows, to better understand the statistical properties in associate with the turbulent dynamics.

In the past four decades, there have been enormous efforts to identify and understand the turbulence structure in the boundary layer [110], [111], [112], and [113]. Most of the studies so far are based on experimental observations. Coherent study based on numerical simulation database, such as [40], emerge as an efficient tool to study the details of turbulent structure.

Based on the numerical simulation database generated by our LES spatial simulation technique, we will identify the near wall “streaky structure” and its statistics. The “busting” and “sweep” processes and their contribution to turbulent stresses will be discussed in detailed. Finally, the relationship between the “bursting” and “sweep” processes and the vorticity structure will be studied in this section.

5.3.5 Near Wall Streaky Structure

Beatty, Ferrell, & Richardson [114] are the first to observed the streaky structure when they pumped a dye solution through a pipe and the residual dye was formed into streamwise filaments at the wall after flushing with water. Experiments by Kline & Rundstadler [115] revealed that the regions in the immediate region of the wall dye streaks have low velocities in the streamwise direction and that average spacing between the streaks is about 75 wall units (normalized by wall friction velocity and free stream velocity). Kline et al [109] attempted to find a more objective method for measuring the spanwise spacing of the streaks than counting dye streaks by taking the Fourier transform of instantaneous spatial correlations of streamwise velocity fluctuation. On the basis of these measurements and a re-evaluation of
earlier dye studies, they found the spacing is about $100 \pm 20$ wall units. Gupta et al [116] found the spanwise spacing to increase from 100 to 150 wall units, when the Reynolds number $R_{\infty}$ was increased from 2,200 to 6,500.

Figure 5.10 and 5.11 are typical streamwise and spanwise correlations for velocity fluctuations at $y/h=0.389$ ($y^+ = 78$). Shown in the figure is also the experimental data from Comte-Bellot at $y/h=0.44$ for $R_e = 135,000$ [117]. It is very clear that the each velocity component correlates strongly for a long distance in the streamwise direction. However, the spanwise correlation decrease from one to zero and negative value in a relatively short distance in the spanwise direction. It indicates that corresponding structure in the near region should be “thin” and long streaks.

The spanwise correlation of streamwise velocity component for different horizon-
tal planes are shown in the figure 5.12. The correlation decreases very quickly from 1 at \( r_3 = 0 \). The separation when the spanwise correlation of streamwise velocity reaches a minimum is normally used to estimate the mean separation between the high- and low-speed fluids, e.g. half of the spacing of the streaks. At \( y^+ = 5.52 \), the correlation reaches minimum at \( r_3 = 0.25 \). For the present Reynolds number \( R_r = 200 \), this \( r_3 \) corresponds to 50 wall units. So the spacing at this plane is about 100 wall units, which is in good agreement with experimental data mentioned above. It can be seen that the spacing increases as the plane move away from the wall region to the outer flow field. In fact, in the core region, there is essentially not any streaky structures.

Figure 5.11: Spanwise Correlations for Velocity Fluctuations
5.3.6 Near Wall Events and Their Association with Turbulence Production

The studies by Kim [118] and his co-workers indicated that that the low-speed fluid in the region near the wall occasionally erupts violently into the high-speed outer region of the boundary layer. This process is generally referred as "bursting" or "ejection" process. The entire bursting process is a continuous chain of events leading from a relatively quiescent wall flow to a formation of relative large and relatively chaotic fluctuations. The process, as they observed, is of an on-off or intermittent character. The bursting starts with the lifting of a low-speed streak from the wall. As the low-speed streak move downstream it also gradually moves away from the wall. As a result, the low-speed streak at first move away from the
wall very slowly over a very long streamwise extent. Once the low-speed streak has reached some critical height in the range of $8 < y^+ < 12$, an unstable oscillatory motion of marked fluid lines (time lines) was observed. During the process, the instantaneous velocity profile with an inflexion point, is significantly different from the well-known averaged mean flow profile. As the amplitude of the oscillatory motion of the rising fluid became larger, the pattern 'break up' at a distance from the wall in the range $10 < y^+ < 40$. They also reported that essentially all the turbulence production occurs during bursting times in the zone of $0 < y^+ < 100$.

Corino & Brodkey [119] used a high-speed motion camera to visualize the trajectories of very small particles suspended in the fluid. The camera was mounted on a travelling mechanism so that the motion within the convected flow structure responsible for the bursting process could be kept in the view of the camera. The main sequence of the events they observed began with a local deceleration of the flow over a relatively large extent near the wall. Within the decelerated region, the flow had a very small velocity gradient so that at its edges there were regions of high shear. From further upstream a large-scale fluid mass then entered the field of the view, this mass moved at a higher velocity and began to accelerate the decelerated fluid. Immediately, after the acceleration began there occurred an ejection of fluid from the decelerated region outwards from the wall, and at times more than one injection from the same decelerated region occurred. This was then followed by the higher fluid mass (moving with a velocity usually greater than the mean and parallel to or at a slight angle towards the wall) sweeping the field of the retarded fluid. They also pointed out that the ejection and resulting fluctuations were the most important feature of the wall region. The ejection process is responsible for 70% of turbulence production, while the sweep process balances to make up 100%.
Wallace et al [104] investigated the process of Reynolds stress production by hot-film measurement in a fully-developed channel flow. The signal of Reynolds stress was classified into four categories; the two main ones were that with negative $u$ and positive $v$, which can be associated with the ejection-type motion, and that with positive $u$ and negative $v$, associated with the sweep-type motion. It was founded that over the wall region investigated, $3.5 < y^+ < 100$, these two types of motion give rise to a stress considerably greater than the total Reynolds stress. Two others of motion: $u$ and $v$ negative, $u$ and $v$ positive, were found to accounted for the 'excess' stress produced by the first two categories, which gives contribution of opposite sign.

The quadrant analysis of the Reynolds shear stress provides detailed information regarding the turbulence contribution from various events occurring in the near wall region. Figure 5.13 is the normalized Reynolds stress contribution from different quadrants of $u$ $v$ plane. The first quadrant, $u > 0$ and $v > 0$, corresponds to outward motion with high-speed fluid; the second quadrant, $u < 0$ and $v > 0$, corresponds to the motion ejection motion of low-speed fluid, the third quadrant, $u < 0$ and $v < 0$, corresponds to the inward motion of low-speed fluid; and the fourth quadrant, $u > 0$ and $v < 0$, corresponds to the sweep of the high-speed fluids.

The experimental data from Wallace et al [104] is also shown in the figure. The overall agreement between the numerical simulation and the experimental data is very good. The ejection and sweep are the two dominant events in the wall layer. They are responsible for 120% of the total Reynolds stress in this region. The interactions between the sweep and ejection count for negative 20% of the Reynolds stress. It can be seen from both experimental data and the simulation that the
Towards the wall, the sweep event dominates the turbulence production. The cross point of these distinct region is at about $y^+ = 13.6$ and $14.45$ from the numerical results and the experimental data. In the core region, the total Reynolds stress is essential close to zero, so the relative quadrant quantities are very large.

To further understand the relationship between the near wall turbulent events and the turbulence production, we include the skewness for both $u$ and $v$ in Fig. 5.14. Shown in the figure are the present numerical simulations and the experimental data from Barlow & Johnson [120] and Kreplin & Eckelmann [105]. It is shown that the spatial simulation is much better than the temporal counterpart. For the skewness
of u, the simulation agree with Kreplin et al's data very well. For v skewness, the agreement between simulation and Barlow et al’s data is good in the close wall region. In the core region, there is significant difference between the simulation results and the experimental data.

As compared with the Reynolds stress quadrant distribution, the $S(u)$ distribution is in a reasonable shape. $S(u)$ decreases from positive at the immediate vicinity of the wall to negative in the major of the wall layer. The location corresponding to zero $S(u) \ (y^+ = 11.06)$ is approximately equal to the cross point in Fig. 5.13. So it can be understood that beyond the cross point, the ejection is dominant, while in the immediate vicinity of the wall, the sweep is the prevailing event.

However, there is not such a direct correspondence between $S(v)$ and Reynolds stress distribution. According to the $S(v)$ distribution, the wall layer can be divided into three different regions. In the first region ($y^+ < 10$), both $s(v)$ and $s(u)$ are positive, but sweep contributes most to the turbulence production. According to Corino & Brodkey's visual investigation [119] that in the sublayer $y^+ < 5$, there are only very small disturbance. It is observed that a few elements with particularly strong deviating velocities do escape outward. Combining the visual observation and the results in Fig. 5.13 5.14, the event in the sublayer can be summarized as follows: even through the outward motion is not violent in the sublayer, the inward motion from outer layer is even less violent; the inward motion carry high-speed fluids so that the inward motion contributes most to the turbulent production. According to the Corino & Brodkey's observation, this region is the position of origin of the majority of the fluid ejection. From the experimental data and simulation result in Fig. 5.13 the contribution to turbulence production from ejection is less significant than the sweep process. It is clear that there is some high-speed fluid, which carries
Figure 5.14: Skewness Coefficients for $u$ and $v$
great amount of momentum move inward from outer layer to this region.

In the second region, \((10 < y^+ < 30)\), both \(S(u)\) and \(S(v)\) negative, and ejection contributes more to Reynolds stress than sweep process. According to the Corino & Brodkey’s observation, this region corresponds to the decelerated zone. The velocity of the fluid in the decelerated zone is much smaller than the local mean velocity. Kline et al [109] indicated that during the low-speed streaks lifting process, the instantaneous velocity is greatly retarded, and there even exists a inflexion point in the velocity profile. Based on these experimental results and the statistical results in Fig. 5.13, the relationship between the fluid event and the turbulence production in this region can be explained as follows: 1) there are lots of ejection and sweep event and their interactions in this region; 2) the outward ejection process causes the some fluid elements have lower velocity than the local mean velocity; 3) when the fluid moves inward from outer region (A of Fig. 5.15 ) to a certain point (B), the momentum increase at B associated with this motion is denoted by \(\delta I\) is much smaller than the momentum decrease, denoted by \(\delta D\), caused by the motion of a low-speed fluid move outward from inner region (C) to B; 4) even though the inward motion is stronger than the outward motion (corresponding to the negative \(S(v)\)), the resulting net exchange of the momentum with the u velocity will still be negative; and 5) it is clear that the ejection process will contribute more to the Reynolds stress than the sweep (inward) process.

In the outer region, \((y^+ > 30)\), \(S(u)\) is negative and \(S(v)\) is positive. It can be understood that there is stronger ejection event than sweep event in this region. According, the ejection process dominates the turbulence production.
5.3.7 Streamwise Vorticity Associated with the Ejection Phenomenon

In 1952 Theodorsen [121] characterized turbulent boundary layer as being composed of large-scale horseshoe-shape vortexes which are responsible for turbulent transport. The motion picture by Kline et al [109] suggested that the slow streak lift-up is a result of the streamwise vorticity. Willmarth & Lu [122] studied the correlation between streamwise velocity fluctuation at a fixed point at wall and streamwise vorticity at a point at wall and the streamwise vorticity at another point in downstream direction. They suggested that the positive streamwise vorticity component is associated with the burst phenomena.

Blackwelder & Eckelmann [123] have found evidence for counter-rotating pairs of vortices using combination of hot-film sensors in the flow and flush with the wall.
of an oil channel at low Reynolds number with a viscous sublayer. The low-speed streak is created by the counter-rotating vortex pair which are separated by the half streak wavelength and which “pump” the low-speed fluid away from the wall.

Shown in the Fig. 5.16 is the correlation between streamwise velocity and vorticity. The symmetry between positive and negative vorticity is an evidence of the existence of the counter-rotating vortex. That is, for each horizontal plane parallel to the solid wall, the positive (or negative) streamwise velocity fluctuation has almost equal possibility with positive and negative vorticities. However, for either positive or negative vorticity, there is significant difference (about 25%) between the possibilities to be with positive and negative streamwise velocities. It can be summarized that even though the counter-rotating vortex is mainly responsible for the turbulent events in the boundary layer, there will be some other mechanism(s) to be responsible about 20% of this events.

5.4 summary

Through the extensive comparison among spatial simulation, temporal simulation and experimental data, it can be concluded that:

1. The new large eddy spatial simulation code is very accurate, robust, and efficient.

2. The spatial development of turbulent channel flow is very important even for non-transpired channel flows. The LES spatial simulation predicts much more accurate results than DNS temporal simulation, because smaller turbulence structure can be accurately caught in the LES spatial simulation.
3. Ejection and sweep are two dominant events in the wall region of the channel flows. They are responsible for about 120% of the total turbulence production. Their interactions have negative contribution to the turbulence production, thereby keeping the total 100%.

4. Counter-rotating vortex mechanism is mainly responsible for the turbulent production in the near wall region of channel flows. However, some other mechanism(s) will contribute about 25% of the total turbulence production.
CHAPTER 6

NUMERICAL SIMULATIONS FOR TRANSPIERED TURBULENT CHANNEL FLOWS

6.1 Background

The turbulent boundary layer with non-zero normal velocity at the wall, $v_w$, is of considerable practical interest. Injection of fluid at a surface is frequently used for thermal protection; and suction is used for boundary-layer control. The basic combustion phenomenon in hybrid rocket is turbulent boundary layer combustion, in which the oxidizer is fed through the main stream while fuel comes from solid fuel vaporization from the side walls.

Between 1967 and 1975 many experimental investigations were carried out on the characteristics of transpiration on boundary layer. Extensive measurements of mean velocity profiles, skin friction coefficients and Reynolds stresses in transpired boundary layers, have been done by Simpson et al [124], Julien et al [125], and Andersen et al [126].

In this chapter, the developed LES spatial simulation code, used for non-transpired fully developed turbulent channel flow in the last chapter, is applied for transpired fully developed turbulent channel flow.

The predicted mean velocities for different blowing and suction rates agree very well with experimental data [126]. The boundary thickness increases with the increase of the injection rate, and it decreases with the increase of the suction rate.
The predicted streamwise turbulence energy agrees well with the experimental data [126]. Both show that the streamwise turbulent energy decreases with the increase of the blowing rate. However, there is a significant difference between experimental data and predicted results of the normal and spanwise velocity fluctuations. It is not clear yet whether the difference of the pressure gradient and Reynolds number between experimental condition and numerical simulation are the reason for the discrepancy. The predicted wall friction coefficients for series of different injection and suction rates match very well with the experimental data. They indicate that the friction coefficient increases with the suction rate, and decreases with the injection rate.

The study of different turbulent structure related parameters for different injection and suction velocities, such as correlation of streamwise velocity component and streamwise vorticity for different injection and suction velocities, skewness, and quadrant Reynolds stress distributions, indicates that there is not significant effect of injection or suction on turbulent structures.

6.2 Results and Discussion

For the discussion of the fully developed channel flows, fluid is injected or removed from both upper and lower walls at same same rate. A relative transpiration rate, \( F = v_w / U_\infty \) is used to define the transpiration rate. Seven different transpiration rates (\( F = -0.004, -0.002, -0.00134, 0, 0.00134, 0.002, 0.004 \)) have been employed in the present study.

The computational domain is the same as the one used in the last chapter, that is, \([0, 4\pi] \times [-1, 1] \times [0, 2\pi]\) in x, y, and z direction. The grid size is 128*101*128. The grids are uniformly distributed in x and z directions. The same kind of stretched grid
as in the last chapter is used here. The initial conditions and boundary conditions are the same as used in the last chapter, except that the wall normal velocities are specified according to the different injection or suction rates.

The mean velocity profiles normalized by the local wall velocity are shown in Figure 6.1. The experimental data for transpiration is from Andersen et al [126], the one for non-transpiration from Kreplin & Eckelmann [105]. The overall agreement between experimental data and present numerical simulations is very good. The Reynolds number, \( R_r \)'s, (with channel half width, wall friction velocity, and kinematic viscosity) for non-transpiration case are 208 and 200 for the experimental data and numerical simulation. In the experiments, \( R_\theta \) (based on the momentum thickness and free stream velocity) for both \( F=0.004 \) and \(-0.002 \) are 6870 and 2226. The counter-parts in the numerical simulation are 2407 for both \( F \)'s.

The predicted wall friction coefficient associated with the experimental data are shown in Figure 6.2. The experimental data is from Simpson et al [124]. It is shown that the numerical prediction agrees well with the experimental data. The wall friction increases with the suction rate and decreases with the injection rate.

Shown in the Figure 6.3 is turbulent streamwise velocity fluctuation normalized by wall shear velocity. The experimental data are from the same source as in Figure 6.1. The Reynolds number \( R_\theta \) for experiment for \( F=-0.004 \) is 1258, while ones for numerical simulation are 2407. The agreement between experimental data and numerical prediction for \( F = \pm0.0014, 0 \) are very good in the near wall region. In the region \( y^+ > 40 \) the experimental data are substantial higher than numerical simulation. The differences are due, at least in part, to the different Reynolds number. For \( F=-0.004 \), the shape of the numerical profile is in good agreement with that of experimental profile, even though the numerically predicted intensity
Figure 6.1: Mean-Velocity Profile From LES Spatial Simulation and Experimental Data

is much higher than experimentally measured intensity.

The normal direction and spanwise turbulent intensities and normalized Reynolds Stress are shown in the Figure 6.4, 6.5 and 6.6. Shown in the figures are also the experimental data from Kreplin & Eckelmann [105]. From the above three figures, it can be seen that the normalized turbulent intensities and Reynolds stress increase with the injection rate, decrease with the suction rate. The main reason for this trend is due to the wall shear velocity decrease with the increase of the injection rate.

The predicted one dimension normalized streamwise turbulent power spectrum is shown in Figure 6.7. It is shown that the streamwise velocity power spectrum does
not change much as the injection (suction) rate changes. The turbulence energy for spanwise and normal direction velocity components increase as suction rate increase in low wave number region. They decreases as suction rate increases in the high wave number region.

Shown in Figure 6.9 and 6.10 are the streamwise and spanwise two point correlations for three velocity components for three different injection rate \((F = \pm 0.004\) and \(0\)) at \(y/h = 0.922\) and \(y/h=0.026\). The experimental data for \(F=0\) is from Comte-bellot [117]. The comparison among the results for these three different injection rates indicates that the injection rate does not have much effect on the turbulent structure.

Shown in the Figure 6.11 are the quadrant Reynolds stress distribution for differ-
ent injection (suction) rates. The experimental data for $F=0$. are from Eckelmann [103]. It is shown that the injection does not have much effect on the Reynolds stress distributions. The ejection ($u < 0$ and $v > 0$) and sweep ($u > 0$ and $v < 0$) are two major events responsible for turbulence production. The contribute more than 120% of the entire Reynolds stress, while the interaction between ejection and sweep ($u > 0$ and $v > 0, u < 0$ and $v < 0$) have negative contribution to the Reynolds stress, and cancel out some of the ejection and sweep contribution. In the inner region, sweep has greater contribution than ejection. In the outer region, the contribution from ejection is greater than the contribution from sweep.

The skewness factor for streamwise, normal direction, and spanwise velocity components are shown in the Figure 6.11. Shown in the figure is also the experimental
Figure 6.4: Normal Velocity Turbulent Intensity Normalized by Wall Shear Velocity data for F=0. from Kreplin & Eckelmann [105] and Barlon & Johnson for S(u) and S(v) respectively. From S(v), it is clear that the injection pulls the v velocity distribution towards the standard Gaussian distribution in the inner region, while pushes it even further away from the Gaussian distribution. In associated with the quadrant Reynolds stress distribution in Figure 6.10, It can be understood that the injection cancels out part the sweep effect in the immediate wall region, and enhances the ejection effect in the outer region. From the S(u) distribution, it can be seen that the injection pushes the u velocity distribution away from the Gaussian distribution in the whole wall layer; and suction pulls it back to towards to the Gaussian distribution in the entire wall layer. There is not much difference for S(w) distribution for different injection and suction rates.
Finally, the correlations between streamwise velocity and vorticity are shown in the Figure 6.13. It is shown that transpiration rate does not have much effects on the correlations. Accordingly, the transpiration does not have much effects on the turbulent structures.

6.3 Summary

Through the extensive comparison between numerical prediction and experimental data, it can be concluded that:

1. The new code can accurately predict turbulent flow statistical quantities, such as mean flow velocity, turbulent intensities, and wall friction coefficients for
transpired turbulent channel flows.

2. Injection from the side walls increases the boundary layer thickness and turbulence intensity, but decreases the wall friction and heat transfer rate. Suction, however, has opposite effects.

3. Injection reduces the sweep event at the immediate vicinity of the wall, and enhances the eject event in the outer wall layer. The suction has opposite effect on the ejection and sweep events.

4. The transpiration does not have much effect on the turbulent structure in the near wall region, in the transpiration rate range of present study.
Figure 6.7: Streamwise Turbulent Power Spectrum
Figure 6.8: Spanwise Turbulent Power Spectrum
Figure 6.9: Streamwise Two Point Correlations
Figure 6.10: Spanwise Two Point Correlations
Figure 6.11: Reynolds Stress Quadrant Analysis For Different Transpiration Rates
Figure 6.12: Skewness Factors for Velocity Components
Figure 6.13: Correlation Between Streamwise Velocity and Vorticity
CHAPTER 7

INTRODUCTION TO HYBRIDS

Our plans for space missions and space operations are contingent upon transportation to space. This access to space has frequently been tacitly assumed to either exist or be available when necessary. Practically all of the space missions so far have relied upon two conventional rocket propulsion systems; solid rockets and liquid rockets, or called solids and liquids. There exists a third alternative, the hybrid rocket, or hybrids. In a solid rocket, oxidizer and fuel are in a solid state. In a liquid rocket, both oxidizer and fuel are in a liquid state. In a hybrid rocket, one of the two components, oxidizer or fuel, is in a liquid state, while the other component is in a solid state. The configuration of the general hybrid rocket engine (liquid oxidizer and solid fuel) is basically similar to that of a solid propellant rocket, except the former uses solid fuels instead of solid propellant. Inverse hybrids use solid oxidizer and liquid fuel. In the general hybrid rocket, the oxidizer, stored in a tank in liquid form, is fed to the combustion chamber either by turbopump or stored high pressure inert gas. When the solid fuel is heated, it will evaporate. Then the fuel vapor mixes and reacts with gas oxidizer from the main stream. The schematic structure of a general hybrid rocket is shown in Figure 7.1.

The virtue of high-performance as a single-minded engineering goal has passed. Safety, reliability, affordability, and environmental compatibility form a new attribute
set for all space propulsion systems. The hybrid rocket is potentially important because it has the promise of combining many of the advantages of both liquid and solid rockets. The separation of fuel and oxidizer introduces remarkable advantages in the above attribute set, besides being controllable. It is very instructive, to compare solids, liquids, and hybrids in terms of the new attribute set for space propulsion system.

7.1 Hybrids Are Better Than Solids and Liquids

7.1.1 Safety Comparison

The safety characteristic of a chemical propulsion system comes from the chemical properties of the fuel and oxidizer components. In solid rockets, the commonly used
propellant can be classified into three groups: double base propellant, composite propellant, and composite double base propellant. Composite propellants have played a dominating role in solid rocket propulsion with their high energy density advantage. Due to this reason, we will only discuss composite propellant solid rockets. The three main components in composite propellants are solid oxidizer particles, solid metal particles, and liquid resin. AP (Ammonium Perchlorate) is commonly used as oxidizer, HTPB (Hydroxylterminated Polybutadiene) or PBAN (Polybutadiene Acylic Acid Acrylonitrile) are two most common resins. The functions of resin are twofold. It mechanically combines all the components together in solid state. It also reacts with the oxidizer to produce high temperature, high pressure combustion gas which produces high thrust. In most composite propellant, metallic particles, such as aluminum particles, are widely used not only because of the high heat release when they react with oxidizer and fuel vapor but also due to its ability to restrain combustion instability. Among the above mentioned three major components, AP oxidizer and metallic particles are very explosion sensitive material. AP particles can act as mono-propellant, which can cause many serious safety problems.

The safety issue comes with the solid rocket from the very beginning of the manufacturing preparation process to the very end of the launch processes. Even in the beginning of manufacture, precautions must be brought to care in the dealing with AP material and metallic particles. During the propellant manufacturing (mixing, casting, and curing) processes, any small spark can easily cause a catastrophic explosion, which has happened many times in the history of solid rocket industry. Therefore heavy protective explosion-proof manufacturing units and remote operation systems are necessary for the manufacture of solid propellants.

Very serious safety issue of solid rockets transfers to the very strict requirements
to the manufacturing quality. The quality of the solid rocket propellant and the solid rocket motor are the key elements for the solid rocket propulsion system. The principal failure mode for a solid rocket is abrupt pressure increase resulting from a crack developing in the fuel grain. Any crack in the grain will be followed by quick expansion, thus increasing the burning area, chamber pressure, and causing an explosion.

In the transportation and flight preparation process, special care must be given to prevent any chance of sparks or any other ignition source. To make the safety problem for solid rocket propulsion system even worse is that the solid rocket combustion is not controllable. If some unexpected phenomenon happens, there is not any way to stop the abnormal combustion in the solid rocket.

The main failure mode for a liquid rocket is the leakage of liquid fuels and oxidizer. Normally, the liquid fuel is some kind of liquid hydrocarbon chemicals, which are of very high flammability. Liquid hydrogen (LH) has been widely used in liquid rocket propulsion systems. Even a small concentration (about 4%) of hydrogen, $H_2$, could react with oxygen in the surroundings, and cause fire or explosion. On the other hand, there is a possibility of an on-pad or in-flight accident, which can cause a complete loss of propellant tankage structural integrity, leading almost surely to a catastrophic failure.

As compared with solids and liquids, hybrids are much safer due to the structure of the hybrid rocket. The most fundamental difference is that there is not any explosive material like AP as in the fuel grain nor liquid explosive like LH (liquid hydrogen) as in the liquid rocket. The safety problem does not come to the hybrid rocket until launch and flight phases. The fuel crack failure mode of a solid rocket is intrinsically avoided in the hybrid rocket because a small crack in its fuel grain will
cause extremely fuel-rich flow, with hardly any widening of gas flow path (hybrid combustion occurs along a well oxidizer ventilated surface only). In the latter phase, a hybrid rocket is subject to liquid oxygen leakage and its promotion of local combustion. This would tend to be a low-level energy-release problem in the absence of large quantities of liquid fuels. The liquid-bipropellant failure mode in the liquid rocket is eliminated in the hybrid rocket. It can be concluded that hybrids are much safer than liquids or solids.

7.1.2 Cost Comparison

The cost of a rocket includes the acquisition cost, overall life cycle cost, shelf-life cost and the cost of waste management. Obviously, the safety advantage of a hybrid will transfer a great advantage in the cost of manufacture, transportation, etc, as compared with a solid rocket and liquid rocket. An estimation by Lo & Dargies [127] has shown that the cost of a hybrid can be one thirtieth (1/30) of that of comparable solid rocket. The national Space Propulsion Synergy Group [128] has pointed out that a hybrid propulsion system will have significantly lower life-cycle costs (LCC) than a solids or liquid system. While neither of the conventional systems are better than hybrids in initial research and development, system procurement, and operation and support, hybrids are seen to be markedly superior to liquids in terms of RDT&E (Research Development Test & Evaluation) costs, and to solids in both procurement and operation and support costs. Hybrids are believed to be distinctly superior to the two conventional rocket-propulsion systems in terms of total LCC costs. In a recent study by Ramohalli et al [129], it was shown that the cost of environmental impact during processing, end use, and disposal of waste for a hybrid rocket is likely to be only 3% of the cost of comparable solid propellant
rocket.

7.1.3 Performance Comparison

The rocket motor's performance is characterized by both the specific impulse (achieved impulse delivered by unit mass of propellant) and the rocket mass fraction (the ratio of propellant mass to the total mass of the rocket motor). It is pointed out by National Space Propulsion Synergy Group [128] that the specific impulse achievable in HTPB/LOX (liquid oxygen) hybrid rocket is expected to closely approach that of an equivalent liquid rocket engine (same chamber/exit pressure condition). However, the liquid system probably has a design-point propellant mass fraction advantage over an equivalent hybrid unit. The theoretical results of Ramohalli et al [129] show hybrids can reach a performance level higher than solid rockets. But solids provide a higher propellant mass fraction and good propellant utilization. The concise comparison among solids, liquids, and hybrids is shown in Table 1.
Table 1. Comparison of Solid, Liquid, and Hybrid Rockets

<table>
<thead>
<tr>
<th>TRAIT</th>
<th>SOLIDS</th>
<th>LIQUIDS</th>
<th>HYBRIDS</th>
</tr>
</thead>
<tbody>
<tr>
<td>SPECIFIC IMPULSE</td>
<td>LOW</td>
<td>HIGH</td>
<td>LOW</td>
</tr>
<tr>
<td>COST</td>
<td>LOW</td>
<td>HIGH</td>
<td>N/A (V. LOW)</td>
</tr>
<tr>
<td>FAILURE MODE</td>
<td>SERIOUS</td>
<td>BENIGN</td>
<td>BENIGN</td>
</tr>
<tr>
<td>SHUTDOWN/RESTART</td>
<td>NO</td>
<td>YES</td>
<td>YES</td>
</tr>
<tr>
<td>ACTIVE REDUNDANCY</td>
<td>NO</td>
<td>YES</td>
<td>YES</td>
</tr>
<tr>
<td>FUNCTIONAL TEST</td>
<td>NO</td>
<td>YES</td>
<td>YES</td>
</tr>
<tr>
<td>ENVIRONMENTAL</td>
<td>Cl₂Al₂O₇</td>
<td>BENIGN</td>
<td>BENIGN</td>
</tr>
<tr>
<td>HANDLING/STOREABILITY</td>
<td>HAZARD</td>
<td>HAZARD</td>
<td>ROBUST</td>
</tr>
<tr>
<td>SIMPLICITY</td>
<td>YES</td>
<td>NO</td>
<td>YES</td>
</tr>
<tr>
<td>REUSABILITY</td>
<td>YES</td>
<td>NO</td>
<td>YES</td>
</tr>
<tr>
<td>PROPELLANT DENSITY</td>
<td>HIGH</td>
<td>LOW</td>
<td>HIGH</td>
</tr>
</tbody>
</table>

The advantages of safety, environmental compatibility, operability, and high performance have made the hybrid rocket a very important potential candidate for future space propulsion systems. In 1992, National Research Council (NRC) [130] recommended that in the consideration of the transportation from Earth to Orbit, hybrids need to be given serious consideration as a strap-on booster for lower stages. The private company group lead by American Rocket Company (AMROC), has been designing, constructing, and testing the world largest hybrid rockets [131, 132, 133, 134]. The designed thrust of their H-1800 hybrid rocket motor is 250,000 pound. JIRAD, the combined efforts among many NASA centers and private companies,
is doing the fundamental research about the hybrid rocket combustion. Since our group as the first university research group started the hybrid rocket research, many other universities have established hybrid rocket research teams.

### 7.2 Unsolved Hybrids Problems

Considering all of these advantages, it is instructive to investigate why the hybrid has not yet made it into the mainstream. The reasons are several and complex, varying from pure technical to rather vague. Lack of commitment to its development during the time when intensive developments were made in large solid and liquid rockets is one reason. No "real" large hybrid rocket has ever been tested, let alone flight-proven in space. Another main reason is technical development: there is not a satisfactory theory to follow in the hybrid rocket motor design and production. The fundamental combustion phenomenon is turbulent boundary combustion. As mentioned in Part I, the study of turbulent combustion is on-going research. Hence, there is some distance between the research achievements and the practical application. In fact, this is the principal motivation for the present research. The big picture for the unsolved hybrids problem is shown in Fig. 7.2.

We define the main unsolved hybrid rocket problems are: 1) the low-combustion efficiency, 2) low-regression rate (or burning rate) of the hybrid rocket fuel, 3) the scale-up principal (the relationship of the performance among different sizes of hybrid rockets). The National Space Propulsion Synergy Group [128] stated that there are two as yet unsolved and somewhat unique hybrid rocket performance-degrading problems (which normally would be addressed in any further development efforts). The first one is that the overall combustion efficiencies achieved to date are relatively low, and the second one is that the solid fuel is not fully burned. The low combustion
Figure 7.2: Unsolved Hybrids Problems
efficiency is due to the “poor mixing and incomplete combustion” inside the combustion zone. The fuel vapor and the incoming oxidizer can only react when they are well mixed. In the practical hybrid rocket combustion, there is great amount of fuel vapor escapes through the nozzle without burned. Also some oxidizer remaining in the main stream flows out of the nozzle before it gets a chance to mix and react with fuel vapor in the rocket chamber. There were some tentative solutions, such as disturbing the main oxidizer stream of the rocket chamber downstream close to the nozzle [135] and after-burner [127]. These solutions need more hardware and seriously impact the simplicity and mass fraction of hybrid rocket. The combustion inefficiency reduces the delivered specific impulse, thus significantly penalizing the attainable hybrid performance level.

7.3 Present Advancements

Our ability to solve the above problems depends mainly on understanding the key physical and chemical processes. The key processes are the fuel degradation processes and the turbulent boundary layer combustion processes (including mixing processes) between the incoming oxidizer in the main stream and the evaporating fuel stream.

The general picture of hybrid propellant rocket combustion is similar to that of a turbulent diffusion flame, where the flame zone is established within the turbulent boundary layer (Figure 7.2). In the classical hybrid rocket, the fuel is in a solid state and the oxidizer is in a liquid or gaseous state. The oxidizer is fed into the rocket chamber by a high pressure tank or by a turbopump. The ignition system is then fired to produce the initial heat to start combustion. The heat of ignition provides the initial energy to cause sublimation or degradation (pyrolysis) of the solid fuel.
This evaporated fuel will mix with the oxidizer flow and ignite the mixture, once a suitable mixture ratio of fuel and oxidizer has been reached. From this point on, the combustion is self-perpetuating until the oxidizer flow is shut off.

The purpose of the present research is to clearly delineate the specific unsolved problems that must be studied and solved before the hybrid can compete with solids and liquids. Specifically, the goal is to find a practical way(s) to improve the overall combustion efficiency through a better understanding of the combustion and mixing processes inside the turbulent boundary layer and to investigate the internal ballistics in order to develop the scale-up principles (to predict performance of a larger hybrid rocket with the known performance(s) of smaller hybrids). In Part I, we have already developed the general methodology for the turbulent reactive flow
numerical simulations. The results for the channel turbulent reactive flow can be applied directly in the hybrid rocket turbulent boundary layer research. We have the tool and knowledge to understand the details of the physical and chemical processes inside the hybrid rocket. In this part, we will develop a fuel degradation model to predict the regression rate of different kinds of rocket fuels. The experimental research results can be used to help us to built and to verify the overall hybrid rocket combustion model. The relationship among the provision steps will be depicted in the “Big Picture for Research of Hybrid Rockets” (Fig. 7.3).

In summary, the achievements of the preset research will be summarized as follows:

1. A state-of-the-art hybrid rocket research laboratory has been established. Two
generations of experimental hybrid rockets and testing facilities have been designed and constructed. Rocket testing facilities for the routine measurements (pressure, thrust, temperature) and some advanced combustion diagnosis, such as infrared image technique and gas chromatography, are well developed and utilized in the hybrid rocket experimental research. A computerized data acquisition/control system has been designed and built. A entire hybrid rocket fuel manufacturing set-up and procedure are established. We have reached the point of manufacturing high quality hybrid rocket fuel in any desired geometries and compositions.

2. The numerical simulation tool established in the first six chapters is applied to understand the details of the mixing and combustion process inside the turbulent boundary layer. The controlling processes to affect the overall combustion efficiency are sorted out. A series of different catalysts have been tested in order to improve the regression rate of the hybrid rocket fuel. A new $Cu^{++}$ based catalyst is identified which can improve the burning rate of the general HTPB based hybrid rocket fuel by 15%.

3. Hybrid rocket performance dependency on the rocket geometry is studied. Scale-up principles are developed through a series of experimental testing on different sizes of hybrid rockets.

4. A fuel degradation model with consideration of catalytic effects of small concentration of oxidizer near fuel surface is developed. The numerical predictions for the conditions with and without oxidizer in the environment are in very good agreements with the experimental results. From this model, the pressure dependency of the regression rate of hybrid rocket fuel can be explained
satisfactorily.

5. Hybrid rocket simulations technology has been developed. A hybrid rocket fuel formulation has been proposed and tested. The hybrid fuel combustion properties can match that of The Solid Rocket Booster of the Space Shuttle over 98%. The combustion properties include the combustion temperature, specific impulse, combustion production composition, and the nozzle erosion property.

6. A wide variety of hybrid rockets has been investigated to illustrate that the hybrid rocket can reach at least the same energy level as typical solid rockets with much cleaner combustion exhausts. It is concluded through the detailed comparison that the hybrid rocket is much cheaper than solid rocket in terms of the costs of production and waste management of unburned fuel.
CHAPTER 8

REVIEW OF HYBRID ROCKET COMBUSTION INVESTIGATIONS

Nowadays for new space missions, an increased safety awareness has led to a renewed interest in hybrid propulsion. Many research teams ranging from government NASA centers to private companies and university research groups are conducting theoretical and experimental investigations. Large hybrid rockets have been designed, built, and tested. Plans have been made to produce even larger hybrids. It will be helpful to summarize the previous theoretical and experimental research before we come to our specific topic.

Research in hybrid rockets can be traced back to the early 1930s when the California Rocket Society designed and fired a hybrid rocket. Around the same time, work was performed in Germany on a liquid-graphite rocket. The Pacific Rocket Society followed up with a significant experimental investigation in the 1940s and launched a missile to an altitude of 30,000 ft in 1951. Hybrid research was dormant until it became a subject of interest again in the 1960s. During the 1960s, extensive experimental and theoretical work was accomplished. The research focus of this period was to understand the internal ballistics of hybrid rockets, to predict the regression rate variation principle(s) along the fuel tube and at different working conditions. In the early 1970s there was some research on the fundamentals of hybrid rocket combustion.
8.1 Experimental Investigations

In the introductory remarks about hybrid studies, Green Jr. [136] reviewed and summarized the hybrid researches before 1964. The hybrid research started with experimental studies by Noeggerath [137] in 1937. He used a stack of multiple perforated cylindrical disks of coal as solid fuel, through which flowed gaseous nitrous oxide. As reported later by Lutz [138] in 1945, the rapid development of uniform burning through the length of the motor was promoted by lining each of the disk perforations with celluloid. The ignition is accomplished by a small initiation charge of gunpowder and a booster charge of granulated coal.

During approximately the same time (1938 - 1941), unreported experiments using a fluted carbon bar as a fuel grain for gaseous oxygen was conducted by the California Rocket Society. The Isp (specific impulse per unit of propellant mass) reached 160 seconds in the pressure range of 100 - 300 Psi.

In 1964, Houser & Peck [139] studied the combustion of solid polymeric fuels in a stream of gaseous oxygen. The fuels were made in the shape of a rectangle with a cylindrical hole. The regression rates were measured as a function of time, axial distance, and oxygen flow rate (note, not flux).

In the middle 70's, Smoot & Price [141, 142, 143] experimentally investigated the solid fuel regression rate dependency for metalized and non-metalized solid fuels, in which pure oxygen or gas mixture oxygen was used as an oxidizer for both cases. The fuel grain was in a tubular shape. The burning rate of solid fuel was found to be proportional to the power of the oxidizer flux in the range of low oxidizer fluxes and high pressure. But the oxidizer flux dependence decreases with the increase of the flux. There is a strong pressure dependence of regression rate.
Wooldridge & Muzzy [144], in 1965, and Jones et al [145], in 1971, made detailed measures of species, velocity, and sensible enthalpy distribution in a turbulence wind tunnel with mass addition, with or without combustion. It was found that the flame zone occupied approximately 10% of the total boundary layer thickness. The profiles of normalized velocity, sensible enthalpy, and species (oxygen) were similar. All of the profiles exhibited some degree of inflection near the flame zone, which indicated the presence of combustion altered the local transport processes in the turbulent boundary layer. A significant static pressure gradient normal to the wall was also measured.

Recently, Strand [146] at JPL (Jet Propulsion Laboratory) experimentally investigated the regression rate dependency of the oxidizer flux and Aluminum particle content in the fuel. It is found that the molten layer on the HTPB/Al fuel is mainly due to the HTPB itself instead of the Al particle accumulation. The thickness of the molten layer decreases with the increasing of oxidizer flux.

Goldberg & Cook [147] reported the preliminary results of a NASA/industry hybrid propulsion program. The conducted firings indicated the presence of combustion instability in hybrid rockets. The oscillation source is from the combustion itself instead of the liquid feed system. AMROC (American Rocket Company) has already built and tested the largest hybrids in the world. Its H-1800 hybrid is designed to deliver 250,000 pound of thrust.

A more concise summary of the experimental hybrid rocket research is shown in Table 2.
<table>
<thead>
<tr>
<th>INVESTIGATOR OR REPORTER</th>
<th>FUEL</th>
<th>OXIDIZER</th>
</tr>
</thead>
<tbody>
<tr>
<td>NOEGGERATH (1937)</td>
<td>COAL</td>
<td>( N_2O )</td>
</tr>
<tr>
<td>LUTZ (1943)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SMITH (1938-1941)</td>
<td>CARBON</td>
<td>( O_2 )</td>
</tr>
<tr>
<td>BARTEL &amp; RANINE (1946)</td>
<td>CARBON</td>
<td>AIR</td>
</tr>
</tbody>
</table>
| DEMBROW & POMPA (1952)   | NAPHTHA | \( KClO_4, \)  
|                          |      | \( NH_4ClO_4, \) |
|                          |      | \( NH_4NO_3 \) |
| MOORE & BERMAN (1956)    | POLYETHYLENE | \( H_2O_2 \) |
| ORDAHL (1959)            | PRESS METAL | HALOGEN COMPOUNDS |
|                          | SOLID PROPELLANT |          |
| MOUTET & BARRERE (1960)  | ORGANIC PLASTIC | \( HNO_3 \) |
| ADELMAN (1961)           | RUBBER & ALUMINUM | \( N_2O_4 \) |
| BRUNETTI (1961)          | RUBBER | \( N_2O_4 \) |
| MATZLER et al (1960-1963)| PLEXIGLAS POLYETHYLENE POLYSTYRENE ALUMINUM | \( O_2 \) |
Table 2. Experimental Hybrid Combustion Investigations (Continued)

<table>
<thead>
<tr>
<th>INVESTIGATOR</th>
<th>FUEL</th>
<th>OXIDIZER</th>
</tr>
</thead>
<tbody>
<tr>
<td>MARXMAN &amp; GILBERT (1963)</td>
<td>PLEXIGLAS</td>
<td>$O_2$</td>
</tr>
<tr>
<td>HOUSER &amp; PECK (1964)</td>
<td>POLYMER</td>
<td>$O_2$</td>
</tr>
<tr>
<td>WOOLDRIDGE &amp; MUZZY (1965)</td>
<td>POROUS PLATE ($H_2/N_2$)</td>
<td>AIR</td>
</tr>
<tr>
<td>RAMOHALLI &amp; STICKLER (1970)</td>
<td>POROUS PLATE</td>
<td>$O_2/N_2$</td>
</tr>
<tr>
<td>JONES et al (1971)</td>
<td>POROUS PLATE ($H_2/N_2$)</td>
<td>AIR</td>
</tr>
<tr>
<td>BLAZOWSKI et al (1982)</td>
<td>POLYMERS</td>
<td>$O_2$</td>
</tr>
<tr>
<td>KORTING et al (1987)</td>
<td>PMMA</td>
<td>$O_2/N_2$</td>
</tr>
<tr>
<td>VOVELLE et al (1987)</td>
<td>PMMA</td>
<td>AIR</td>
</tr>
<tr>
<td>GOLDBERG &amp; COOK (1992)</td>
<td>HTPB</td>
<td>$O_2$</td>
</tr>
<tr>
<td>RAMOHALLI &amp; YI (1990)</td>
<td>PMMA/PBAN/HTPB</td>
<td>$O_2/N_2/Al$</td>
</tr>
</tbody>
</table>

8.2 Theoretical Investigations

As discussed earlier, the basic combustion phenomenon of hybrid rocket combustion is a turbulent combustion boundary layer. The fuel vapor reacts with a gaseous oxidizer from the main stream. Because of the fuel vapor transpiration and the chemical reaction, the boundary on the solid fuel surface is normally a turbulent boundary. The chemical reactions inside the turbulent boundary generate high
temperature and high pressure gas mixture which produces the thrust for the hybrid rocket. At the same time, part of the combustion heat release is fed back to the solid fuel surface. This heat feed back maintains the solid fuel degradation. The chemical reaction is confined mainly in a very narrow domain, which is called “combustion zone.” The slowest process, if there is one, among the chemical reaction inside the combustion zone, the heat transfer from gas phase to the solid fuel surface, and the solid fuel degradation process will be the controlling process for the overall hybrid rocket combustion.

The hybrid rocket combustion theories can be classified as gas theory and condensed phase theory according to the assumed controlling process. These theories will be discussed in detail in the rest of this chapter.

8.2.1 Gas Phase Theory

The gas phase theory is built on the basis of the mixing, combustion inside the turbulent combustion zone, and the heat transfer to the solid phase. The general picture is already shown in the figure 7.1. Such a recapitulation produces the basic framework for hybrid rocket turbulent boundary layer combustion analysis. In the hybrid rocket turbulent boundary layer combustion model, it is assumed that the oxidizer will diffuse towards the solid fuel surface, while the solid fuel will evaporate towards the gas oxidizer. The oxidizer and fuel will meet in the boundary layer and will react if suitable fuel and oxidizer ratio is reached in the boundary layer. The oxidizer distribution in the turbulent boundary layer will be similar to the distribution of velocity, but the fuel is just the opposite. Most of the chemical reactions will occur in the very thin combustion zone. This descriptive picture is consistent with the experimental investigations.
The pioneer theoretical study by Bartel & Rannie in 1946 [148] considered the essential features of hybrid combustion problems. They studied the hybrid rocket combustion with tubular fuel and turbulent incoming oxidizer flow. It was suggested that the diffusion and transport of oxygen through the gas film to the fuel surface was the rate-controlling factor. Penner [149] simplified the hybrid combustion to a Burke-Schuman diffusion problem. He did not make formal distinction between laminar and turbulent flows. The governing equation reads

\[
\frac{\partial K_0}{\partial X} = \frac{D}{U} \left( \frac{\partial^2 K_0}{\partial r^2} + \frac{1}{r} \frac{\partial K_0}{\partial r} \right) \quad \text{for} \ 0 \leq r < R - \delta(X) \quad (8.1)
\]

where \( K_0 \) is the mass fraction of oxygen; \( D \) diffusivity of oxygen in product mixture; \( U \) average axial velocity; \( \delta(x) \) thickness of boundary layer. And the boundary conditions are:

\[
\begin{align*}
\frac{\partial K_0}{\partial r} &= 0, \quad atr = 0 \\
K_0 &= K_{0,0}, \quad atX = 0 \\
K_0 &= 0, \quad atr = R - \delta
\end{align*} \quad (8.2)
\]

Marxman & Gilbert [150] and Marxman [151, 135] proposed a heat-transfer limited model. In the model, it is proposed that the heat transfer from combustion zone to the solid surface is the key process to control the solid fuel degradation. The regression rate of solid fuel is proportional to the amount of the heat transfer, that is,

\[
\rho_f \dot{r} = (\rho v)_w = \frac{\dot{Q}_w}{\Delta H} \quad (8.3)
\]

where \( \rho_f \) = density of the solid fuel, \( \dot{r} \) = linear regression rate of the fuel surface, \( (\rho v)_w \) = mass flux evaporating from the solid surface, \( \Delta H \) = total energy required to gasify a unit mass of solid fuel originally at the internal temperature of a solid
grain, and $Q_w = \text{heat transferred from the gas to the solid fuel surface.}$

A comprehensive account of the understanding of convective heat transfer through the reacting boundary layer with mass addition was given by Lees [152]. It is believed that the hybrid process is in the general category of heat transfer problems. If the Reynolds' Analogy is assumed valid for turbulent boundary layer, an important simplification is possible. The heat flux is then independent of both the transport mechanism and the magnitudes of reaction rates in the gas. Then it can be described by an equation formally identical to that for a pure, inert gas:

$$\dot{Q} = -\frac{K}{C_p} \frac{\partial h}{\partial y}$$

Recall the definition of Stanton number, the heat flux at the solid fuel surface is

$$\dot{Q}_w = StG(h_{cs} - H_{wg})$$

where $St = \text{Stanton number, } G = \text{mass flux in boundary layer and } G = (\rho_c U_c), h_{cs}$ specific enthalpy at combustion zone, and $h_{wg}$ specific enthalpy at gas side of solid fuel surface.

Combining these two equations,

$$\dot{Q} = -\frac{K}{C_p} \frac{\partial h}{\partial y}$$

$$= St\rho_c U_c(h_{cs} - H_{wg})$$

$$= St_0 \frac{St}{St_0} \rho_c U_c(h_{cs} - H_{wg})$$

where $St_0$ is Stanton number in the case of without surface blowing, and $St/St_0$ will reflect the effect of the surface ablation. For a turbulent boundary layer, surface
Ablation can result in a value as low as about 0.2 for $St/St_0$. $St_0$ can be determined by some empirical boundary layer theory for the case of laminar and turbulent flows.

If the Reynolds' analogy is valid with chemical reaction and blowing, the following will hold:

\[- \frac{\dot{Q}}{\partial h_s / \partial y} = \frac{\tau}{\partial u / \partial y} \quad (8.7)\]

where $Q =$ heat flux, and $\tau =$ shear stress. There is a relationship between the Stanton number and the friction coefficient. For hybrid combustion case, this relationship can be obtained by:

\[\frac{\dot{Q}}{Q_w} = \frac{\tau}{\tau_w} \quad (8.8)\]

or in the integral form:

\[\frac{\dot{Q}}{\rho_c U_c (h_{cs} - h_{ug})} = \frac{\tau_w}{\rho_c U_c^2} \quad (8.9)\]

and

\[St = \frac{1}{2} C_f \frac{\rho_e U_e^2}{\rho_c U_c^2} \quad (8.10)\]

where $St$ is defined in the above way. $C_f$ is local skin-friction coefficient as $\tau_w/(\rho_c U_c^2)/2$.

For the boundary layer without blowing or chemical reaction, the friction coefficient is given by the empirical formula:

\[\frac{St_0}{2} = C R_e X^n P_r^{n_2} \quad (8.11)\]

For laminar boundary layer:

\[C = 0.332 \quad (8.12)\]
For Turbulent boundary layer:

\[ n1 = -0.5 \]
\[ n2 = -2/3 \]

For hybrid combustion, Pr is assumed equal to 1. So,

\[ C_{f0} = 2CRe X^{n1} \quad (8.14) \]

then,

\[ St_0 = CRe X^{-n1} \frac{\rho_e}{\rho_c} \left( \frac{U_e}{U_c} \right)^2 \quad (8.15) \]

Equations (8.5) and (8.6) together describe the convective heat transfer for the flame to the fuel surface. Normally this is the expected primary mechanism of heat transfer. Backing to Eq. (8.4), it is given that

\[ \dot{\bar{r}} = CG \frac{Rc X^{-0.2}}{\rho_f S_{t0}} \frac{s_t}{U_c} \frac{h_{cs} - h_{wg}}{\Delta H} \quad (8.16) \]

8.2.2 Condensed Phase Theory

Unlike the gas-phase theory, the solid-phase theory considers the fuel regression process in the view of the solid fuel. The basic idea is that the solid fuel degradation depends on the amount of energy to reach the solid surface, regardless of the type
of the energy source or the way of the energy transfer. Once the heat flux is known, the regression for a given polymer will be determined.

In 1965, Rabinovitch [153] proposed a kinetics model of polymer degradation. He assumed the degradation takes place in the bulk fuel, remote from the burning surface. By the nature of the C-C bonds in the polymer back-bond, the average degree of polymerization will steadily decrease. It is further assumed that when the fragment reaches a small-enough size that its cohesive energy is less than the bond energy within the back-bond, it will evaporate. The size of a fragment is called the critical fragment size (c.f.s) and defined as

\[ c.f.s = \frac{C - C \text{ Bond Energy}}{\text{Heat of Evaporation of Monomer}} \]  

(8.17)

For hybrid rocket combustion, the degradation process is going on in a plane parallel to the burning surface, and the polymer reaches c.f.s at the fuel surface. For a steady state, assuming the fuel temperature far from the surface is \( T_0 \), and the burning rate \( \dot{r} \) is constant. The governing equation for this case is:

\[ \dot{r} \frac{\partial T}{\partial X} = -\kappa \frac{\partial^2 T}{\partial X^2} \]  

(8.18)

where \( \kappa = \frac{K}{C_p} \) is thermal diffusivity of the polymer, \( K \) the conductivity of the polymer, \( C_p \) specific heat of polymer, and \( \rho \) density of the polymer. The boundary conditions will be:

\[ atX = \infty, T = T_0 \]  

(8.19)

\[ X = 0, T = T_s \]
The equation (8.18) with the boundary conditions 8.20 are not enough to determine the burning rate. The other restriction for the degradation process is that for a certain polymer the size of a fragment at the fuel surface is a strong function of the chemical/physical properties of the polymer and the other surface conditions. Rabinovitch [153] assumed the c.f.s is determined by the polymer's properties only. By looking at back-bond numbers, the degradation process can be described as a first-order rate process, such that:

\[
\frac{dn}{dt} = kn
\]  

(8.20)

where \( n \) is the number of breakable bonds in unvolatilized polymer backbone bond, \( k \) is chemical reaction constant and

\[
k = B \exp\left(-\frac{E_a}{RT}\right)
\]  

(8.21)

The above two equations and boundary conditions of temperature and bond number \( n \) will uniquely determine the regression rate of a solid fuel.

In this simple model, the heat release related to the degradation in a solid is not included. However, relatively little degradation needs to go on in order to prepare the polymer for volatilization. Houser & Peck [139] showed that, the heat of reaction makes less than 50°C difference to the temperature profile.

In the above mentioned model, the fuel degradation process is “isolated” in the solid state only, which does not depend on the combustion in the gas field. However, this is not the case in hybrid rocket combustion. There is much evidence [144, 140] that the degradation of polymer depends on the surface environmental condition, especially the small concentration of oxygen (about 2%). The polymer degradation
process should include an oxidizer term, carbon dioxide, carbon monoxide, or other radical chain degradation initiators.

In order to make up this shortcoming of the above model, Kumar (Ramohalli) and Stickler [156] developed a pressure-sensitive model of hybrid combustion. They proposed that the solid fuel is depolymerized into small fragments, instead of monomers, thereby theorizing the concept of fragment size vaporizing (FSV). FSV is determined by:

\[
FSV = \frac{32.8}{M} P^{-0.2615} \exp\left(\frac{3.67T_w}{1000}\right)
\]  

where \( M \) is the molecular weight of the monomer, \( P \) is the pressure near the fuel surface, and \( T_w \) is the wall temperature. Based on the solid phase energy equation and the fragment size equation, the regression rate was obtained. The pressure dependency of the regression rate is reflected in the pressure dependency of FSV and the concentration of the oxidizer at the surface (wall). The summary of the theoretical investigations can be shown in Table 3.
<table>
<thead>
<tr>
<th>INVESTIGATOR</th>
<th>FLOW MODEL</th>
<th>FLOW CONDITIONS</th>
<th>EFFECT OF MASS ADDITION</th>
</tr>
</thead>
<tbody>
<tr>
<td>BARTEL &amp; RANNEI</td>
<td>CYLINDRICAL</td>
<td>TURBULENT</td>
<td>NOT CONSIDERED</td>
</tr>
<tr>
<td>(1964)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>PENNER (1960,1962)</td>
<td>CYLINDRICAL</td>
<td>LAMINAR</td>
<td>NOT CONSIDERED</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MOUTET &amp; BARRERE (1961)</td>
<td>FLAT</td>
<td>LAMINAR</td>
<td>NOT CONSIDERED</td>
</tr>
<tr>
<td>FINEMAN (1962)</td>
<td>CYLINDRICAL</td>
<td>LAMINAR</td>
<td>NOT CONSIDERED</td>
</tr>
<tr>
<td></td>
<td>TURBULENT</td>
<td></td>
<td>PARTIALLY CONSIDERED</td>
</tr>
<tr>
<td>MARXMAN &amp; GILBERT (1963)</td>
<td>FLAT PLATE</td>
<td>TURBULENT</td>
<td>PARTIALLY CONSIDERED</td>
</tr>
<tr>
<td>RABINOVITCH (1965)</td>
<td>FLAT PLATE</td>
<td>TURBULENT</td>
<td>NOT CONSIDERED</td>
</tr>
<tr>
<td>RAMOHALLI &amp; STICKLER (1971)</td>
<td>POROUS PLATE</td>
<td>TURBULENT</td>
<td>CONSIDERED</td>
</tr>
<tr>
<td>RAMOHALLI &amp; YI (1991)</td>
<td>CYLINDRICAL</td>
<td>TURBULENT</td>
<td>CONSIDERED</td>
</tr>
<tr>
<td></td>
<td>DUCT</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Neither gas phase model nor solid phase model can satisfactorily explain all the aspects of the hybrid rocket fuel regression rate variation principle. The gas phase model explains the oxidizer flux dependency of the regression rate but the pressure dependency cannot be understood. Moreover, in the gas phase model the detailed chemical and physical properties, such as solid fuel pyrolysis activation energy, does not play much role in the determination of the regression rate. In most solid phase models, the regression rate is determined as a function of the fuel surface temperature which is directly dependent on the incoming heat flux to the fuel surface. In these models, the detailed chemical/physical processes in the degradation process are studied. However, the chemical and physical processes in gas phase and the pressure dependency of the regression rate is still not considered.

The deficiencies of gas phase and solid phase models have been recognized for a long time. House & Peck [139] realized that the degradation of unfilled (no oxidizer in the fuel) polymer fuel, as is found in the experimental motor, is not governed by a pyrolytic process, but must include an oxidative term, brought about by the presence of oxygen, carbon dioxide, carbon monoxide, or other radical chain-degradation initiators. Smoot, et al [142] pointed out that the pressure dependence of the regression rate can be attributed to the occurrence of a finite-rate, heterogeneous attack
of oxidizer on the surface of the fuel grain. Ramohalli & Stickler [156] discovered mismatch between the inert polymer degradation experimental regression rate and the real hybrid rocket experimental regression rate. They postulated that fuel surface oxidative depolymerization aids surface thermal degradation in accounting the higher regression rate in the hybrid rocket combustion.

Hirschler [158] studied the effect of oxygen on the thermal decomposition of poly(vinylidene fluoride). Thermogravimetric studies have been made of successive stages of the thermal decomposition of the polymer during programmed heating, at low and high heating rates in nitrogen, air, and oxygen. It is concluded that the presence of oxygen in atmosphere drastically changes behavior of the pyrolysis reaction. Kashiwagi and Ohlemiller [157] experimentally investigated the rate of gasification of PE and PMMA polymers under transient, nonflaming heating by thermal radiation. Five different ambient gas mixtures with different combination of oxygen and nitrogen were used. They concluded that the rate of transient gasification cannot be described simply as a function of surface temperature or proportional to energy input. A model for predicting the rate of transient gasification should include condensed phase oxidative chemical reactions, in-depth thermal decomposition, mass transfer in the sample (diffusive and bubble-induced), changes in molecular weight and thus in viscosity of the molten layer, and changes in the in-depth absorption characteristics of the sample layer.

In this chapter, a polymer oxidative degradation model is developed. In this model, the energy transfer process, oxidizer diffusion (from fuel surface to the inside of the fuel) process, and oxidative pyrolysis process are considered. It is assumed, based on the experimental observation, the fuel surface can be divided into “wet” and “dry” portions. The “wet” part is covered by a thin liquid layer. The details
of the liquid layer evaporation process is studied. It is further assumed that the regression rate is controlled by both the liquid film evaporation and the degradation from the "dry" area. The model is applied in both inert and oxidative polymer degradation. The predictions are in good agreement with experimental data.

9.1 Kinetics of Polymer Oxidative Degradation

This section will describe the oxidative polymer degradation model. The model considers a unsteady heat conduction, backbone bond oxidative depolymerization, and oxidizer diffusion process. In the model, the spatial coordinate is fixed, the initial thickness of the fuel is a constant $L$. The surface position is denoted as $S'$. The oxidizer concentration near the fuel surface is assumed to be a constant during the degradation process. The schematic structure is shown in Fig. 9.1.

The heat conduction equation inside the fuel reads

$$\rho C \frac{\partial T}{\partial t} = K \frac{\partial^2 T}{\partial X^2} - \dot{q}_p$$

(9.1)

where $\rho$ is the density of the fuel, $C$ the specific heat of the fuel, $K$ for the conductivity, and $\dot{q}_p$ is the heat consumption rate of the pyrolysis process. The determination of $\dot{q}_p$ will discussed later.

The initial and boundary conditions are:

$$T(X,0) = T_0$$

$$T(L,t) = T_0$$

$$-K \frac{\partial T(S',t)}{\partial X} = \dot{Q}$$

(9.2)

The oxidizer diffusion process inside the solid fuel can be described in a similar equation.
where $D$ is diffusivity of the solid fuel. The consumption of the oxidizer inside the solid fuel is not counted, because the oxidizer is only as an initiator of the oxidative pyrolysis process. The oxidizer consumption rate is negligible.

The initial and boundary conditions are:

$$C_{ox}(X, 0) = 0$$

$$C_{ox}(S^t, t) = C_{ox}$$
The oxidative degradation of polymers is a free chain reaction. The typical steps for this process are initiation, radical conversion, chain propagation, degenerate chain branching, and termination. A simplified steps for the hybrid fuel oxidative degradation (low concentration of oxidizer) are [159]:

I. Initiation:

\[ RH + O_2 \xrightarrow{K_{i1}} 2R^\cdot + H_2O_2 \]  \hspace{1cm} (9.5)

\[ Initiator + (2f'RH) O_2 \xrightarrow{K_{i2}} 2f'R^\cdot + 2f'R'H \]  \hspace{1cm} (9.6)

II. Radical propagation:

\[ R^\cdot + O_2 \xrightarrow{K_{i3}} RO_2^\cdot \]  \hspace{1cm} (9.7)

III. Chain propagation:

\[ RO_2^\cdot + RH \xrightarrow{K_{i4}} R^\cdot + RO_2H \]  \hspace{1cm} (9.8)

\[ RO_2^\cdot + RH \xrightarrow{K_{i5}} R^\cdot + products \]  \hspace{1cm} (9.9)

IV. Degenerate chain branching:

\[ RO_2H( + 2fRH) \xrightarrow{K_{i6}} 2fR^\cdot + fROH + H_2O \]  \hspace{1cm} (9.10)

V. Termination:

\[ R^\cdot \xrightarrow{K_{i7}} \text{product} \]  \hspace{1cm} (9.11)

\[ RO_2^\cdot \xrightarrow{K_{i8}} \text{product} \]  \hspace{1cm} (9.12)

\[ R^\cdot + R^\cdot \xrightarrow{K_{i9}} \text{product} \]  \hspace{1cm} (9.13)

\[ R^\cdot + RO_2^\cdot \xrightarrow{K_{i10}} \text{product} \]  \hspace{1cm} (9.14)

\[ RO_2^\cdot + RO_2^\cdot \xrightarrow{K_{i11}} \text{product} \]  \hspace{1cm} (9.15)
where R is for the polymer radicals.

Let

\[ [R] = R \]
\[ [RO_2'] = X \]
\[ [RO_2H] = Y \]
\[ [O_2] = Z \]
\[ [RH] = M \]
\[ [O_2] = O \]
\[ [Initiator] = I \]

where \([\ )\] means the concentration.

The reaction rate for each step can be written as:

\[
\begin{align*}
\omega_{11} &= K_{11} MO \\
\omega_{12} &= K_{12} I \\
\omega_2 &= K_2 RO \\
\omega_{31} &= K_{31} MX \\
\omega_{32} &= K_{32} MX \\
\omega_4 &= K_4 Y \\
\omega_{51} &= K_{51} R \\
\omega_{52} &= K_{52} X \\
\omega_{53} &= K_{53} R^2 \\
\omega_{54} &= K_{54} RX
\end{align*}
\]
\[ \omega_{55} = K_{55}X^2 \]

Then,
\[
\begin{align*}
\frac{dR}{dt} &= 2\omega_{11} - \omega_2 + \omega_{31} + \omega_{32} + 2f\omega_4 - \omega_{51} \\
\frac{dX}{dt} &= \omega_2 - \omega_{31} - \omega_{32} - \omega_{52} \\
\frac{dY}{dt} &= \omega_{31} - \omega_4 \\
\frac{dZ}{dt} &= \omega_{11} + \omega_2 \\
\frac{dM}{dt} &= -(\omega_{11} + \omega_{31} + \omega_{32} + 2f\omega_{12} + 2f\omega_4) 
\end{align*}
\] (9.18)

Under steady-state condition, \( \frac{dR}{dt}, \frac{dX}{dt}, \text{and} \frac{dY}{dt} \) are nearly equal to zero. From the above equations, we get:
\[
\frac{dM}{dt} = -\left(K_{11}MO + K_{31}MO^2 + K_{32}MO^2 + 2f'K_{12}I + 2fK_4MO^2\right) 
\] (9.19)

with further assumption that I is very small, the kinetics of the oxidizer polymer degradation process can be simplified as:
\[
\frac{dM}{dt} = -(K^1 + K^2[O])M[O] 
\] (9.20)

We understand that in the inert degradation (without the presence of oxygen), the degradation kinetics is:
\[
\frac{dM}{dt} = -(K^3)M 
\] (9.21)

Combining the above two equations, the kinetics of oxidative degradation process reads:
\[
\frac{dM}{dt} = -(K^1[O] + K^2[O]^2 + K^3)M 
\] (9.22)
and

$$\frac{dm_t}{dt} = -(K^1[O] + K^2[O]^2 + K^3)m_t$$  \hspace{2cm} (9.23)

$m_t$ is the undegraded mass at the time $t$.

If we define the new variable "degree of degradation", $\xi$,

$$\xi = \frac{m}{m_0}$$  \hspace{2cm} (9.24)

where $m$ is the mass in unit volume of the degraded polymer, $m_0$ is the initial mass of the polymer before any degradation. Then

$$1 - \xi = \frac{m_t}{m_0}$$  \hspace{2cm} (9.25)

The final governing for $\xi$ is:

$$\frac{d\xi}{dt} = (K^1[O] + K^2[O]^2 + K^3)(1 - \xi)$$  \hspace{2cm} (9.26)

The $\dot{q}_p$ in the Equation 9.1 can be calculated by the above correlation:

$$\dot{q}_p = D\rho \frac{d\xi}{dt}$$  \hspace{2cm} (9.27)

where $D$ is the heat consumption for per unit of the polymer.

### 9.2 Surface Regression Correlation

From our experimental experience, the fuel surface is covered by a very thin liquid film, to a different extent. The phenomenon was discussed by many other researches. Ramohalli & Stickler [156] discuss the liquid film in the explanation of the low regression rate of the hybrid rocket fuel. In the present study, it is assumed that the solid fuel surface can be divided into "wet" and "dry" portions. The "wet" part is
covered by a thin liquid layer. The regression rate is the "surface weighted average" of the "wet" and "dry" portions. According, the regression rate is controlled by both the liquid film evaporation and the degradation from the "dry" area.

From the "dry" surface, the general energy balance is applied to account for the correlation of the regression rate and the input heat flux, that is,

\[ \dot{Q} = \rho \dot{r} \left( C_p(T_w - T_0) + D\xi \right) \]  \hspace{1cm} (9.28)

Here, \( \dot{r} \) is the regression rate of the fuel, and \( \xi \) is the degree of degradation at the wall surface. So,

\[ \dot{r} = \frac{\dot{Q}}{\rho(C_p(T_w - T_0) + D\xi)} \]  \hspace{1cm} (9.29)

As mentioned early, D is the depolymerization energy to convert unit mass of polymer to same amount of monomer. However, in experimental determination, the depolymerization energy measured is the energy to convert unit mass of polymer to a certain size of fragment which is small enough to leave the fuel surface. For this reason, we absorb \( \xi \) into D, then Equation 9.29 reads:

\[ \dot{r}_d = \frac{\dot{Q}}{\rho C_p(T_w - T_0) + D} \]  \hspace{1cm} (9.30)

For the "wet" part, the vaporization and condensation processes are considered. To explore this question in detail, one must consider the liquid-vapor interface at the molecular level. Starting from the very basic Maxwell molecular velocity distribution in kinetic theory of gases [160], Silver & Simpson [161] suggested the following equation for the interfacial mass flux:
\[
\dot{m}_w = \left\{ \frac{2\hat{\sigma}}{2 - \delta} \right\} \left( \frac{\overline{M}}{2\pi \overline{R}} \right)^{\frac{1}{2}} \left( \frac{P_l}{T_l^{1/2}} - \frac{P_v}{T_v^{1/2}} \right)
\]  

(9.31)

where \( \hat{\sigma} \) is a material property constant, \( \overline{R} \) a university gas constant, \( \overline{M} \) molecular weight, \( P_v \) and \( T_v \) are for vapor pressure and temperature, \( P_l \) and \( T_l \) are pressure and temperature of the liquid film. In our case, we chose the partial pressure of the oxidizer at the fuel surface as \( P_v \), the surface temperature as \( T_l \) and \( T_v \). \( P_l \) is taken as the saturated pressure for a given fuel vapor at temperature \( P_l \) and molecule weight \( M \).

If the area fractions for the "wet surface" and "dry surface" are denoted \( A_w \) and \( A_d \) \((A_w + A_d = 1)\), then the area weighted regression rate can be expressed as:

\[
\dot{r} = A_w \frac{\dot{m}_w}{\rho} + A_d \dot{r}_d
\]

(9.32)

So far, we have finished the description of the polymer oxidative degradation model. In this model, the incoming oxidizer specific flux dependency, such as \( G^{0.8} \) law, is accounted by the heat transfer flux from the gas phase to the solid fuel. The near surface oxidizer affects the regression rate through the oxidative depolymerization in the deep solid and the near fuel surface. The chamber pressure will affect the regression rate through oxidizer concentration near the surface and the partial pressure in the consideration of the liquid film evaporation process. The detailed physical and chemical properties play their roles through the heat and oxidizer conduction and diffusion processes and the backbone bond breaking process. It is prominent in this polymer oxidative degradation model to understand the pressure dependency of the regression rate, oxidizer concentration effects, the dependency of specific mass flow rate of the incoming oxidizer flow, and the physical/chemical
properties of the fuel. In next section, this model is applied in the case of inert polymer degradation and the degradation in reactive environment. The numerical predictions are in good agreement with experimental results.

### 9.3 Results and Discussions

As examples of the application of the above developed polymer oxidative degradation model, the model is applied in inert degradation of both linear polymer and cross-linked polymer and degradation in reactive atmosphere. In order to simplify the solution procedure, a new spatial independent variable $y$ is introduced.

\[
y = \frac{X - S^t}{L - S^t}
\]  

(9.33)

The meanings of $X$, $S^t$, and $L$ were discussed in the first section of this chapter. By introducing the new set of variables $y$, and $t$, the governing equations become:

\[
\rho C_p \left\{ \frac{\partial T}{\partial t} + \frac{y - 1}{L - S^t} \frac{\partial T}{\partial y} \right\} = \frac{K}{(L - S^t)^2} \frac{\partial^2 T}{\partial y^2} - \rho D (1 - \xi)(K^1[O] + K^2[O]^2 + K^3)(1 - \xi)
\]  

(9.34)

\[
\left\{ \frac{\partial C_{ox}}{\partial t} + \frac{y - 1}{L - S^t} \frac{\partial C_{ox}}{\partial y} \right\} = \frac{K}{(L - S^t)^2} \frac{\partial^2 C_{ox}}{\partial y^2}
\]  

(9.35)

\[
\frac{\partial \xi}{\partial t} + \frac{y - 1}{L - S^t} \frac{\partial \xi}{\partial y} = (1 - \xi)(K^1[O] + K^2[O]^2 + K^3)(1 - \xi)
\]  

(9.36)

The initial and boundary conditions are:

\[
T(y, t = 0) = T_0
\]
\[ T(y=1,t) = T_0 \]
\[ -K \frac{\partial T(y=1,t)}{\partial y} = \dot{Q} \]
\[ C_{ox}(y,t=0) = 0 \]
\[ C_{ox}(y=1,t) = 0 \]
\[ C_{ox}(y=0,t) = C_{oxw} \]
\[ \xi(y,t=0) = 0 \]
\[ \xi(y=0,t) = 0 \]  \[(9.37)\]

In addition, the regression rate correlation will keep the original form:

\[ \dot{r} = A_w \frac{\dot{m}_w}{\rho} + A_d \dot{r}_d \]  \[(9.38)\]

### 9.3.1 Polymer Inert Degradation

In the numerical integration, the Crank-Nicholson scheme is used to integrate both the heat conduction and oxidizer diffusion equations. Fourth order Runge-Kutta method is used to integral the depolymerization kinetics equation, while central difference scheme is employed in the spatial derivatives. For a given incoming heat flux from gas phase to solid surface, the numerical simulation starts with an initial field and \( \dot{r} = 0 \). For a small time increment \( \Delta t \), the temperature, oxidizer concentration, and degree of the depolymerization filed can be determined by integrating the above governing equation. The regression rate correlation in Equation (9.32) will determine the regression rate. As long as the time step \( \Delta t \) is small enough, there iteration is not necessary. This new \( \dot{r} \) can be carried in the determination of the fields for next time step. The calculation will continue until a stable temperature \( T(y=0,t) \) is reached.
The inert degradation of linear and cross-linked PMMA (polymethylmethacrylate) are calculated using the above mentioned model and the numerical scheme. The used physical and chemical properties are:

\begin{align*}
B_3 &= 3 \times 10^9 \text{sec}^{-1} \\
C &= 31.5 \times 10^3 \text{cal/mole} \\
\rho &= 1.19 \text{g/cm}^3 \\
C_p &= 0.35 \text{cal/g} \text{C}^0 \\
D &= 280 \text{cal/g} \\
K &= 5 \times 10^{-4} \text{cal/cmsecC}^0 \\
P_v &= 10^5 \text{N/m}^2 \tag{9.39}
\end{align*}

And $B_i$ and $E_i$ are chemical reaction constant and activation energy for $K_i$, that is,

\begin{equation}
K_i = B_i \exp \left( \frac{E_i}{RT} \right) \tag{9.40}
\end{equation}

The activation energy $E_3$ for the linear and cross-linked PMMA are 31 and 42 kcal/mole respectively. The surface area fraction $A_w$ and $A_d$ normally depends on the imposed heat flux $\dot{Q}$. At the time of this study, the experimental information about them is not available. For the sake of simplicity, we assume $A_w$ and $A_d$ are all constant.

\begin{align*}
A_w &= 0.15A_D = 0.85 \tag{9.41}
\end{align*}

The numerical prediction and experimental results for both linear and cross-linked PMMA are shown in Fig. 9.3.1. The experimental data are from the work
of Chaiken et al [154]. It can be seen that for wide range of imposed incoming heat flux, the numerical predictions are in very good agreement with the experimental data for both linear and cross-linked PMMA.

9.3.2 Polymer Oxidative Degradation

There is not much experimental data for polymer oxidative degradation. The only available experimental data is those by Kashiwagi & Ohlemiller [157]. The experiments were performed with PMMA polymer. The reactive environment is established by small concentration of oxygen. The difficulty for the numerical prediction is that the chemical kinetics parameters are not available. Based on our knowledge for the similar process, the activation energy and reaction constants for $K_1$, $K_2$ and $K_3$ ($B_3$ is shown before) are taken as:

\[
\begin{align*}
B_1 & = 7.47 \times 10^9 \text{sec}^{-1} \\
B_2 & = 7.47 \times 10^9 \text{sec}^{-1} \\
E_1 & = 36 \text{kcal/mole} \\
E_2 & = 36 \text{kcal/mole} \\
E_3 & = 31 \text{kcal/mole} \\
\end{align*}
\]

(9.42)

In the numerical prediction, the heat flux corresponding to the experiment has been modified to consider the heat loss from the polymer surface to the surroundings. By using the formula given by Vovelle et al [155], the net heat flux to the fuel surface is 3.819 $W/cm^2$ for the applied heat flux of 4$W/cm^2$. The numerical predictions and the experimental data are compared in Fig. 9.3.2. The numerical predictions for oxygen concentrations of 20% and 40%, the numerical predictions are
PMMA regression rates for different wall temperatures

Chaiken et al Linear PMMA
Chaiken et al Cross-linked PMMA
Numerical Linear PMMA
Numerical Cross-linked PMMA

Figure 9.2: Numerical Predictions and Experimental Results for Linear and Cross-linked PMMA
exactly same with the experimental data. In the inert degradation case, the numerical result is very close to the experimental data. However, there is big difference for between numerical result and experimental data in the case of oxygen concentration of 10lt can be concluded that the overall agreement between the numerical results and experimental data is excellent. It is not unsafe to say that the proposed oxidative model catches the important aspects of the oxidative depolymerization process. There is still a need to refine the current model, especially in the area of of more accurate oxidative kinetics.
Figure 9.3: Numerical Predictions and Experimental Data for PMMA Oxidative Degradation
CHAPTER 10

SOLID ROCKET COMBUSTION SIMULATOR AND
ENVIRONMENTAL IMPACT OF HYBRIDS

10.1 Solid Rocket Combustion Simulator

Solid propellant rockets have carved a niche for themselves in practically all launch vehicle applications. It is desired to improve our understanding of the solid rockets in order to introduce higher cost effectiveness through better predictability and elimination or minimization of known deficiencies. It is very important and necessary to develop a capability to have solid rockets that are controllable, restartable and flexible. Conventional state-of-the-art solid rockets do not meet these requirements.

It is well known that the materials used in solid rockets must undertake very serious environmental conditions, such as high temperature up to about 3000K, high pressure up to 600 psi, and erosive combustion products. Any misunderstanding or mistakes about the usage of the materials could cause a big disaster. The explosion of “challenger” space shuttle, unfortunately, in January 28 of 1986 is the direct result of misconception of an “O” ring used in the solid booster. The idea of solid rocket combustion simulator (SRCS) is to use hybrid rocket technology to simulate the solid rocket combustion. The importance of building such a hybrid rocket has gained wide attention and financial support from the government (NASA). As mentioned in the position paper of Nation Space Propulsion Synergy Group [128], with consultation
with key JPL (Jet Propulsion Laboratory) and MSFC (NASA Marshall Space Flight Center) hybrid-involved personnel, the decision has been made to support a key graduate student who is completing work on hybrid propulsion at the University of Arizona.

More specifically, the purpose of solid rocket combustion simulation is to develop new hybrid rockets which can simulate the advanced solid rocket in energy property, combustion temperature, nozzle erosion property, even the combustion products. It is very challenging to simulate the entire combustion of solid rocket, which contains some special explosive material such as AP (Ammonia Perchlorate), without losing the safety, controllability, restartability, and flexibility of hybrid rockets.

The SRB (Solid Rocket Booster), in particular, is used as the target for this simulation technique. The SRB propellant is composed of high percentage of AP, Al particles, and HTPB resin. From the view point of combustion products, the elements of Al, O, N, Cl, C, H should be included in the new hybrid rocket fuel and oxidizer. The hybrid rocket to simulate combustion of SRB will use mixture of oxygen and nitrogen as the incoming oxidizer. HTPB resin, Al particles, and some AP substitute will be used as the hybrid fuel. The question is which component or components should be used to replace AP of solid propellant. Extensive computational experiments have been performed for different substitutes for AP, $(NH_4ClO_4)$. It is realized that $NH_4$ and Cl must be present in the hybrid rocket fuel (O can be substituted in the incoming oxidizer stream). The considered substitutions are combinations of $MoCl_6$ & $NH_4I$, $NH_4I$ & $KClO_4$, $NH_4I$ & $FeCl_2$, $NH_4I$ & $AlCl_3$, etc. It was found that the best among these formulas is the combination of $MoCl_6$ and $NH_4I$. The problem with this formula is the possibility of manufacturing. We found, however, that it is almost impossible to mix $MoCl_6$ and $NH_4I$ with HTPB
GAS TEMPERATURE COMPARISON BETWEEN SRB AND HYBRIDS

for fuel composition b

Figure 10.1: Comparison of Chamber Temperatures Between Hybrids and SRB

and Al together due to the strong reactivity of Mo and Cl. Also there is a serious
limit for the combustion properties matching due to the inclusion of the elements
of I and Mo, which are not present in the SRB. The best matching of the Isp, com-
bustion products, and combustion temperature between this hybrid rocket formula
and SRB does not exceed 85%.

After reviewing the AP properties, the safety information, and the cost, $NH_4Cl$
was finally chosen as the substitute for AP. With the substitute of $NH_4Cl$ for AP,
computational calculations show that there is a 99.7% matching of Isp between
hybrid rocket and SRB and a 99.5% matching chamber combustion temperature,
97.0% matching of the molar concentration of the hybrid combustion products and
SRB's. The results are shown in Figure 10.1 to Figure 10.3.
Almost all the parts of solid rockets are subject to high temperature, high pressure working condition. A malfunction of any parts will cause very serious even catastrophic result. To fully understand the material properties of the parts is very crucial to the solid rocket design. Unfortunately, the material test in the "real" solid rocket is very difficult and expensive, if possible. It has long been desired to develop a test bed to test the solid rocket material properties. The test bed is required to simulate the combustion of solid rocket but is controllable.

Nozzle is one of the most important parts of the solid rocket, whose erosion property is a key factor to the stabilizing of the chamber pressure, burning rate, and the impulse. The water gas reaction
![Combustion Product Comparison Between ISP and Hybrids](image)

**Figure 10.3: Comparison of Combustion Products Between Hybrids and SRB**

\[
C(s) + H_2O \rightarrow CO + H_2 \quad (10.1)
\]

is the key to understanding the chemical mechanism of the nozzle erosion process.

As an example to illustrate the "combustion similarity" between solid rockets and hybrid rockets, the nozzle erosion properties of the proposed hybrid and SRB are compared. It is shown that the chemical characteristics of the nozzle erosion process between the hybrid and SRB are very similar. The results are shown in Fig. 10.4.
10.2 Hybrids As An Environmental Solution for Solids

As is well known that the solid rocket has the disadvantages of pollution of plume and the waste management of unburned fuel. Hybrid rocket can be used to overcome this disadvantage of solid rocket because the hybrids get rid of the toxic elements in the fuel and oxidizer. Hybrid rocket can be free of explosive elements such as AP so that the disposal of unburned hybrid fuel is equivalent to that of rubber tire of a car. It will be shown that the waste management of hybrid fuel is one-order-of-magnitude easier than that of solid rocket.

Through extensive computational calculations, it is found that hybrid formula HP-121 to HP-131 can deliver at least as much specific impulse as solid rocket with at most half toxin of solid rocket. The detailed formulas of HP-121 to HP-131 are
Figure 10.5: Isp for Different Hybrid Rockets and SRB

listed in Table 10.1. In HP-121 to HP-123 $N_2O_4$ is used for energy property. In HP-124 to HP-128 aluminum particle is used to reach high combustion temperature. Likely, magnesium particle is used in HP-129, and both aluminum and zirconium are used in HP-130 and HP-131. The specific impulse from these different hybrid rockets are shown in Figure 10.5.

From the results shown in the above Fig. 10.5, it can be seen that most hybrid rocket can deliver higher specific impulse than SRB. The higher specific impulse of hybrid rocket is gained by higher concentration of oxygen present in the time of combustion. The toxin fraction, which is summation of mass fractions of toxic species like $NO_x$, $CO$, $Al_2O_3$, $HCl$, ..., of a hybrid rocket and SRB are shown in Fig. 10.6. The toxin mass fraction of hybrid rocket is about half of that in SRB. More
important message sent by this result is that there is not any HCl in hybrid rocket which can bring most serious environmental problems for solid rockets. The toxin fraction in the plume can be reduced further by increasing oxygen flow rate but sacrificing a little bit of the energy property, Isp (Fig. 10.6 and Fig. 10.7). Beyond some value of oxidizer flux, the higher the oxidizer flux is, the more benign the plume will be, but the lower the Isp will be.

<table>
<thead>
<tr>
<th>NAME</th>
<th>HTPB</th>
<th>Al</th>
<th>(NH_4ClO_4)</th>
<th>(N_2O_4)</th>
<th>Mg</th>
<th>Zr</th>
<th>O2</th>
</tr>
</thead>
<tbody>
<tr>
<td>SRB</td>
<td>14%</td>
<td>16%</td>
<td>70%</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HP-121</td>
<td>21%</td>
<td></td>
<td>38.6%</td>
<td>40.4%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HP-122</td>
<td>28.7%</td>
<td></td>
<td>52.9%</td>
<td>18.4%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HP-123</td>
<td>24.3%</td>
<td></td>
<td>44.7%</td>
<td>31%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HP-124</td>
<td>18.6%</td>
<td>10.0%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HP-125</td>
<td>17.5%</td>
<td>9.5%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HP-126</td>
<td>16.6%</td>
<td>8.9%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HP-127</td>
<td>15.8%</td>
<td>8.5%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HP-128</td>
<td>15.0%</td>
<td>8.1%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HP-129</td>
<td>15.1%</td>
<td></td>
<td>7.4%</td>
<td>77.5%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HP-130</td>
<td>13.7%</td>
<td>3.7%</td>
<td></td>
<td>12.5%</td>
<td></td>
<td>70.1%</td>
<td></td>
</tr>
<tr>
<td>HP-131</td>
<td>15.0%</td>
<td>4.0%</td>
<td></td>
<td>13.7%</td>
<td></td>
<td>67.3%</td>
<td></td>
</tr>
</tbody>
</table>

Based on the above observation, we proposed to use specific toxin fraction of plume to measure the environmental property of rocket. The specific toxin fraction is defined as

\[
specific\ toxin\ fraction = \frac{toxin\ fraction}{specific\ impulse} \tag{10.2}
\]
This is well defined parameter. The meaning of the newly defined specific toxin fraction is better understood as total amount of toxin species in the plume per unit of impulse. For a given mission, the total impulse is fixed. So the specific toxin fraction is a measurement of the amount of toxin out of rocket exhaust for a given mission. The specific toxin fractions of hybrid fuel rocket and SRB are shown in Fig. 10.8. It is clear that all the hybrid rockets considered here deliver lower specific toxin fraction than SRB. The best one, HP-128, delivers only about 2.6% of specific toxin fraction of SRB.
SPECIFIC IMPULSE OF HTPB/Al/O2 HYBRID PROPPELLANTS
EXPANSION RATIO = 1/100

Figure 10.7: Specific Impulse for Hybrid Fuels with Different Oxygen Fluxes
Figure 10.8: Toxin Fractions for Fuels with Different Oxygen Fluxes
Figure 10.9: Specific Toxin Fractions for Different Hybrid Rockets
CHAPTER 11

HYBRID ROCKET INTERNAL BALLISTICS
INVESTIGATIONS

11.1 Regression Rate Variation Along Fuel Grain

Different oxidizer mixture (100/0, 90/10, 60/40 of Oxygen/Nitrogen) have been tried to verify the wide combustibility of the new fuels. Experiments have been conducted for four different oxidizer mass flow rates (0.005 to 0.20 lbm/sec/in²), and 2 different aluminum contents in the solid fuel (27% and 5%) for different working chamber pressures (30 psi to 90 psi). A typical rocket pressure trace is shown in Fig. 11.1. The regression rate variation for different fuel is shown in Figure 11.2. It is shown that the regression rates of the new fuels are about five time as high as the PMMA’s. It is seen that the regression rate at nozzle end is higher than that of rest of fuel grain. It is because that the combustion product of upstream enhances the combustion downstream, then increase the heat transfer rate from the combustion zone to the solid fuel surface.

11.2 Experimental Investigation of Scale-up Principles

To investigate the oxidizer specific mass flux dependency and the geometry dependency of the hybrid fuel regression rate, a series of oxidizer specific mass fluxes and different initial diameters of rocket fuels are employed in the experiments. The
regressions are plotted in Fig. 11.3. It is shown that the regression rate of solid fuel is a power function of oxygen flux, but the variation principles are not same for different sizes of fuel tubes. The exponent of the function increases with the tube size. For same oxidizer specific flux, the regression rate increase with the inner diameter of the fuel tube. With these limited experimental data, a reasonable scale-up correlation has not obtained yet. It seems that there is not much question that the geometry of the rocket do affect the regression rate.
11.3 Catalytic Combustion of Metallized Fuel

11.3.1 HTPB Degradation Kinetics

In this section, TGA (thermogravimetric analysis) results of HTPB fuels will be discussed to exploit the kinetics of the degradation process. We are aware of the limitations of low heating rate TGA studies and of the prevailing thoughts on the very applicability of these to solid rocket combustion environments. But these TGA studies do provide valuable insight into some very basic degradation mechanism which are relevant to hybrids. Figure 11.4 is one of a series of TGA experiments for HTPB samples under small concentration of oxygen (1.5% O2, bal N2). It is apparent that the maximum rate of weight-loss occurs at 400°C, which is the typical surface temperature of the HTPB fuel (600-700 K). It is pointed out by Stivala et al...
Figure 11.3: Regression Rates as Function of Oxidizer Flux and Fuel Geometry

[163] that the degradation process of Polybutadiene can be divided into two stages. During the first stage, the fuel degrades by about 10% of the original mass. The major products of the first stage are butadiene and the dimer 4-vinylcyclohexene (VC), plus minor amounts of other unidentified hydrocarbons. Most of the fuel degrades in the second stage. At the start of the second stage, significant butadiene is still observed but the VC content is very low. At the maximum rate of the second stage, there is little butadiene or VC but there is a complex mixture of many hydrocarbons. From the proceeding, depolymerization is the primary process during the first stage of degradation. Our TGA experiments are conducted at a high heating rate which is close to the hybrid rocket combustion environment.
11.3.2 Oxidative Degradation of Metallized Fuel

The effect of copper on the degradation of rubber was studied by Miller [164] in 1865 from the point of view of an aging process. Chovin [165] in 1942 reported the effect of copper on the oxidation of rubber with his kinetic measurements. Villain [166] then showed that most copper compounds possessed the same catalytic activity.

The primary reaction is the chain formation of the hydroperoxide in which the catalyst both starts and stops the reaction chain. The subsequent reaction is the unimolecular decomposition of the hydroperoxide via a "heavy metal catalyst hydroperoxide" complex to give the ketone. The equations proposed by Robertson & Waters [167] on the reaction between hydroperoxide and metallic ions have formed the basis for many later kinetic studies.
$M^{n+} + ROOH \rightarrow M^{(n+1)^+} + RO^- + OH^-$ \hspace{1cm} (11.1)

$M^{(n+1)^+} + ROOH \rightarrow ROO^- + H^+ + M^{n+}$ \hspace{1cm} (11.2)

Where M stands for metallic iron, ROOH for the radical of the polymer. The sum of these two equations gives the same products as in bimolecular thermal decomposition:

$$2ROOH \rightarrow RO^- + RO_2^- + H_2O^-$$ \hspace{1cm} (11.3)

It has been shown that the metallic ions affect the rate of initiation and the rate of propagation. Kochi and Rust [168] reported that the metallic ions could affect the rate of termination if the metallic ions come from complex with the R. radicals.

During the early stage of autoxidation, it has been suggested that the metallic ions might oxidize the hydrocarbon directly. Uri [169] suggested the three possibilities: (1) reduction of activation of traces of hydroperoxide already present in the system; (2) direct reaction of a metal ion with oxygen; and (3) complex formation of metal compounds with oxygen and subsequent formation of $H_2O^-$ radical.

It is pointed out by Lee et al [170] that as in the case of the gas-phase oxidation of hydrocarbons, not all metals posses the same catalytic activities in a given medium. In general, for a polybutadiene polymer, according to the induction time, $Co^{2+}$ and $Mn^{2+}$ ions were the strongest. The activities could be arranged as follows: $Co^{2+} = Mn^{2+} > Cu^{2+} > Fe^{3+} > Pb^{2+} > Ce^{4+}$. The rates followed a slightly different order: $Co^{2+} > Fe^{3+} > Cu^{2+} > Mn^{2+} > Pb^{2+} > Ce^{4+}$. 
11.3.3 Experimental Test Matrix

The experimental test matrix was set up to evaluate the effectiveness of adding metallic ion catalysts to the "baseline" fuel in an effort to increase the burning rate. Initially it was imperative to obtain a solid baseline curve of the fuel burning rate versus oxidizer flux. The "baseline" information will help us to identify the heat transfer controlling zone and the degradation controlling zone for the hybrid combustion. This would be accomplished by a total of 10 rocket firings over a oxidizer flux range of 0.05 - 0.25 lbm/in²sec. The metallic ion catalysts that were chosen where aluminum oxide, $Al_2O_3$, cupric oxide, CuO, cobalt oxide, $Co_3O_4$, and copper chromite, $2CuO Cr_2O_3$. These catalysts were added in the amount of 1% of the total fuel mass. These fuels were fired in the oxidizer flux range from 0.01 to 0.15 lbm/in²sec. Because of its positive effect on the regression rate, additional tests were performed on the catalyst CuO to determine the influence of metal ion concentration on regression rate. The concentrations chosen here are 1%, 3%, 5%, 8%, and 13%.

TGA experiments were also conducted. The main purposes of the experiments are (1) to observe the detailed degradation behavior of HTPB with different kinds of catalysts, and (2) to see the oxygen effects on the HTPB degradation properties. The TGA experimental setup was designed and assembled in the Chemical Engineering Department at the University of Arizona. The system mainly consists of the furnace, reactor, gas-fed system, temperature control system, and temperature and mass recording systems.

In order to get a stabilized temperature, the furnace was preheated for about 1-2 hrs. The certified gas flowed through the reactor for 2-3 hrs to make sure the ambient
gas condition in the reactor was exactly the gas employed for each experiment run. The HTPB fuel samples were shaped in a cube about 0.25" x 0.35" x 0.15". The flow rate of the certified gas was 100 cc/min.

In the HTPB TGA experiments, the samples were held in a metal net suspended in the air of the reactor. The reactor was kept at the desired temperature. The certified gas mixture of $O_2$ and $N_2$ was cycled from the top of the reactor to the bottom. Six degradation experiments of HTPB with three different compositions were conducted. Figure 11.4 and 11.5 are the TGA results for HTPB fuel with additive of pyrogallic acid and calcium compound respectively.

Figure 11.5: HTPB/Pyrogallic Acid Fuel TGA Results
Figure 11.6: HTPB/Calcium Compound Fuel TGA Results

11.3.4 Results And Discussion

In Fig. 11.3, 11.4 and 11.5, there are different TGA results for three different catalysts in the HTPB fuel. It is clear that the HTPB degradation can be divided into two stages. In the first stage, the fuel degrades very slowly. In the second stage, the fuel samples degrade very quickly once they reach a high temperature. From this observation, we can propose that in hybrid combustion, keeping fuel surface temperature above this cutoff temperature will improve the degradation greatly. The additives of pyrogallic acid and the calcium compound will not improve the pyrolysis properties of HTPB fuel.

The experimental regression rates for the fuels with different metallic additives under a series of specific oxidizer fluxes are shown in figure 11.6. There are two
conclusion that can be drawn from these. First of all, the metallic ions affect the HTPB degradation only in the degradation controlling regime. Secondly, there is a significant difference of the catalytic effects among all the catalysts tested so far. Of the four metal containing compounds tested as catalysts, the cupric oxide and copper chromite showed the best improvement in regression rate (Figure 11.6). It was decided that the cupric oxide would undergo more testing to determine the dependence of regression rate on metal ion concentration. Copper Chromite was identified as a candidate for later testing.

The results of the testing using Cupric Oxide are shown in figure 11.7. The concentrations tested were 1, 3, 5, 8, and 13% of the total fuel weight. It can be seen that the burning rate does increase with increasing metals concentration,
reaching an apparent limit near a metal concentration of around 10%. This limit corresponded to approximately 10% improvement in the regression rate. It should be noted that a 5% increase was observed with only 1% addition of the metal compound.
CHAPTER 12

PRESENT ADVANCEMENTS

12.1 Present Advancements

The achievements of the present computational and experimental research can be summarized as follows:

1. A new numerical simulation methodology, Large Eddy Probability Density Function (LEPDF), and corresponding numerical code have been developed for turbulent reactive flow systems.

2. The present turbulent spatial simulation code has been successfully applied in the simulations of transpired and non-transpired fully developed turbulent channel flows. The present simulation code more accurately predicts turbulent channel flows than the existing temporal simulation code with only 27% of the grid size of the temporal simulation code.

3. "Ejection" and "Sweep" are two dominant events in the wall region of turbulent channel flows. They are responsible for about 120% of the total turbulent production. Their interactions have negative contributions to the turbulent production, thereby keeping the total 100%. Counter-rotating vortex is a major mechanism responsible for turbulent production in boundary layer. However, there are some other mechanisms to account for about 25% of the total turbulent production.
4. It is the first time that simulations for turbulent transpired channel flows have been accomplished with the consideration of spatial development of turbulent flow fields. Injection increases the boundary layer thickness and turbulence intensities, but decreases the wall friction and heat transfer. Suction has opposite effect. Transpiration does not have much effect on turbulence structures in the transpiration rate range of present study.

5. A state-of-the-art hybrid rocket research laboratory has been established. Two generations of experimental hybrid rockets and testing facilities have been designed and constructed. Rocket testing facilities for routine measurements (pressure, thrust, temperature) and some advanced combustion diagnosis, such as infrared image technique and gas chromatography, are well developed and utilized in the hybrid rocket experimental research. A computerized data acquisition/control system has been designed and built. A entire hybrid rocket fuel manufacturing set-up and procedure are established. We have reached the point of manufacturing high quality hybrid rocket fuel in any desired geometries and compositions.

6. The numerical simulation tool established in the Part I is applied to understand the details of the mixing and combustion process inside the turbulent boundary layer. The controlling processes to affect the overall combustion efficiency are sorted out. A series of different catalysts have been tested in order to improve the regression rate of the hybrid rocket fuel. A new $Cu^{++}$ based catalyst is identified which can improve the burning rate of the general HTPB based hybrid rocket fuel by 15%. 
7. Hybrid rocket performance dependency on the rocket geometry is studied. Scale-up principles are developed through a series of experimental testing on different sizes of hybrid rockets.

8. A fuel degradation model with consideration of catalytic effects of small concentration of oxidizer near fuel surface is developed. The numerical predictions for the conditions with and without oxidizer in the environment are in very good agreements with the experimental results. From this model, the pressure dependency of the regression rate of hybrid rocket fuel can be explained successfully.

9. Hybrid rocket simulation technology has been developed. A hybrid rocket fuel formulation has been proposed and tested. The hybrid fuel combustion properties can match those of The Solid Rocket Booster of the Space Shuttle over 98%. The combustion properties include the combustion temperature, specific impulse, combustion production composition, and the nozzle erosion property.

10. A wide variety of hybrid rockets have been investigated to illustrate that the hybrid rocket can reach at least the same energy level as typical solid rockets with much cleaner combustion exhausts. It is concluded through the detailed comparison that the hybrid rocket is much cheaper than solid rocket in terms of the costs of production and waste management of unburned fuel.
The detailed flow analysis is carried out for the oxidizer feed system, the rocket combustion chamber and the nozzle. The flow in the oxidizer feed duct is described as an adiabatic frictional flow with constant duct area; the flow in the combustion chamber is simplified as an adiabatic frictional flow with mass addition and constant area. The ordinary isentropic flow analysis is used for the flow in the nozzle. It is found that the flow properties such as the Mach number, the pressure variation and the mass flux depend on the fuel tube-throat area ratio instead of the fuel tube area. Moreover, the more interesting result is that the system’s maximum oxidizer delivery capability is proportional to the chamber pressure. This analysis can be used as the guidance for the hybrid rocket design and operation.

In this analysis, the hybrid rocket is divided into three components: oxidizer feed duct, combustion chamber and nozzle. The detailed flow analysis is accomplished for each of the components. The schematic of the hybrid rocket system is shown in the figure A.1.

The section 1 stands for the section just after flow meter, or the head end of the oxidizer delivery duct; section 2’ for the aft end of the oxidizer feed duct; section 2 for the head end of the hybrid fuel tube; section 3 for the aft end of the hybrid
fuel tube and section 4 for the throat of the nozzle. Each of the following sections is dedicated to the detailed analysis for each of the components.

A.1 Flow Analysis for Nozzle

The Flow in the nozzle can be simplified as one dimensional isentropic flow. For the normal hybrid rocket working conditions, the rocket will reach choked condition, that is, the Mach number at the nozzle throat is equal to one. Then the Mach number at the inlet port of the nozzle, i.e., at the aft end of the fuel tube will be determined uniquely by the area ratio of the fuel aft end and the throat. This dependency can be expressed as [162]:

Figure A.1: The Schematic of Hybrid Rocket Systems
Figure A.2: Differential Element of The Combustion Chamber

\[ \frac{A}{A^*} = \frac{1}{M_3} \left\{ \left( \frac{2}{\gamma + 1} \right) \left( 1 + \frac{\gamma - 1}{2} M_3^2 \right) \right\}^{\frac{\gamma+1}{2(\gamma-1)}} \] (A.1)

**A.2 Flow Analysis for Combustion Chamber**

The flow inside the rocket chamber can be simplified as an adiabatic frictional flow with constant duct area and mass addition. The combined effects of mass addition and friction on the flow properties are studied in details in this section from the basic principles.

Starting from the momentum balance:

\[ \text{Mom}(x + \Delta x) - \text{Mom}(x) = (\rho VA|x + \dot{M} dx)(V + dV) - \rho V^2 A \] (A.2)
where Mom for momentum, $\rho$ for fluid density, $V$ for velocity, $A$ for cross area, and $\dot{M}$ is defined as the mass addition rate per unit length of the side wall.

\[ \dot{M} = \pi D \dot{r} \rho_p \quad (A.3) \]

where $\rho_p$ is the density of the hybrid fuel.

\[ PA - (P + dP)A - \tau_f A_s dx = (\rho VA_x + \dot{M})dV - \rho V^2 A \quad (A.4) \]

where $A_s$ is the wetted perimeter of the duct, and $A_s$ is defined in terms of the "hydraulic diameter" $D$ of the duct:

\[ A_s = \frac{4A}{D} \quad (A.5) \]

and $\tau_f$ is the shear stress at the walls of the duct. The friction factor $f$ is related to the shear stress in the flow direction $\tau_f$ in the following way:

\[ f = \frac{\tau_f}{\frac{1}{2}\rho V^2} \quad (A.6) \]

where $\frac{1}{2}\rho V^2$ is the dynamic pressure of the stream.

Then,

\[ -dP - 2\rho V^2 f \frac{dx}{D} = \rho V dV + \frac{\dot{M}V}{A} dx \quad (A.7) \]

\[ \frac{dP}{P} + 2\gamma M^2 f \frac{dx}{D} + \gamma M^2 \frac{dV}{V} + \frac{\dot{M} \gamma}{\rho VA} M^2 dx = 0 \quad (A.8) \]

Using the equation of state, the Mach number definition and the continuity equation:

\[ \frac{dP}{P} = \frac{d\rho}{\rho} + \frac{dT}{T} \quad (A.9) \]

\[ \frac{dM}{M} = \frac{dV}{V} - \frac{1}{2} \frac{dT}{T} \quad (A.10) \]
\[ \rho dV + Vd\rho = \frac{\dot{M}}{A} dx \]  

(A.11)

so,

\[ \frac{dP}{P} = \frac{d\rho}{\rho} + \frac{dT}{T} = \frac{\dot{M}}{\rho VA} dx - \frac{dV}{V} + \frac{dT}{T} \]  

(A.12)

Plugging equation (A.12) into equation (A.8), we get,

\[ \frac{\dot{M}}{\rho VA} dx - \frac{dV}{V} + \frac{dT}{T} + 2\gamma M^2 \frac{d_x}{D} + \gamma M^2 \frac{dV}{V} + \frac{\dot{M}}{\rho VA} M^2 dx = 0 \]  

(A.13)

or

\[ (\gamma M^2 - 1) \frac{dV}{V} + \frac{dT}{T} + (\gamma M^2 + 1) \frac{\dot{M}}{\rho VA} dx + 2\gamma M^2 \frac{d_x}{D} = 0 \]  

(A.14)

for an adiabatic flow,

\[ T(1 + \frac{\gamma - 1}{2} M^2) = T_0 = \text{constant} \]  

(A.15)

\[ \frac{dT}{T} + (\gamma - 1) M \frac{dM}{1 + \frac{\gamma - 1}{2} M^2} = 0 \]  

(A.16)

Plugging equation (A.10) into equation (A.14), the governing equation for the flow inside the rocket chamber becomes:

\[ (\gamma M^2 - 1)(\frac{dM}{M} + \frac{1}{2} \frac{dT}{T}) + \frac{dT}{T} + (\gamma M^2 + 1) \frac{\dot{M}}{\rho VA} dx + 2\gamma M^2 \frac{d_x}{D} = 0 \]  

(A.17)

or,

\[ \left(\frac{\gamma M^2}{2} + \frac{1}{2}\right) \frac{dT}{T} + (\gamma M^2 - 1) \frac{dM}{M} + (\gamma M^2 + 1) \frac{\dot{M}}{\rho VA} + 2\gamma M^2 \frac{d_x}{D} = 0 \]  

(A.18)

Using equation (A.16), the equation (A.18) will be:

\[ (1 - M^2) \left(1 + \frac{\gamma - 1}{2} M^2\right) \frac{dM}{M} = \left[2\gamma M^2 f + (1 + \gamma M^2) \frac{\dot{M}D}{\rho VA}\right] \frac{dx}{D} \]  

(A.19)
let \( M_2, M_3 \) stand for the Mach numbers at the head and aft ends of the fuel tube, and \( L \) for the length of the fuel tube, \( K \) for the length/diameter of the fuel tube:

\[
\int_{M_2}^{M_3} (1 - M^2) \left(1 + \frac{\gamma - 1}{2} M^2\right) \frac{dM}{M} = \int_0^L \left(2\gamma M^2 f + (1 + \gamma M^2) \frac{MD}{\rho VA}\right) \frac{dx}{D} \quad (A.20)
\]

considering the definition of \( \dot{M} \),

\[
\frac{\dot{M}D}{\rho VA} = \frac{\pi D^2 \dot{\rho}_p}{M_{ox} + \pi D \rho_p \dot{\rho} X} \quad (A.21)
\]

defining:

\[
\dot{M}_{ox} = GA = G \frac{\pi D^2}{4} \quad (A.22)
\]

Here, we assume the burning rate of the hybrid fuel can be calculated by 0.8 law[150],

\[
\dot{\rho} = aG^{0.8} \quad (A.23)
\]

the constant \( a \) is a function of the fuel properties.

\[
\frac{\dot{M}D}{\rho VA} = \frac{a \rho_p G^{-0.2}}{\frac{1}{4} + \rho_p a G^{-0.2} \frac{X}{D}} \quad (A.24)
\]

The dependency of the right hand side of equation (A.24) on \( G \) is very weak. When \( G \) varies from 0.1 to 1.0 lbm/in\(^2\)sec (70.37 Kg/m\(^2\)sec to 703.7 Kg/m\(^2\)sec), \( G^{-0.2} \) changes from 0.42 to 0.26 only. So we may take a constant here to represent \( G^{-0.2} \), in order to make equation (A.24) independent of \( G \). Then the equation (A.20) becomes:

\[
\int_{M_2}^{M_3} (1 - M^2) \left(1 + \frac{\gamma - 1}{2} M^2\right) \frac{dM}{M} = \int_0^K \left[2\gamma M^2 f + (1 + \gamma M^2) \frac{ab \rho p}{\frac{1}{4} + ab \rho p K}\right] d\xi \quad (A.25)
\]

and

\[
\xi = \frac{X}{D} \quad (A.26)
\]

From the above integration, \( M_2 \) can be obtained once \( M_3 \) is known for different \( K \).
A.3 Flow Analysis for Oxidizer Feed Duct

The oxidizer feed duct consists of two parts: section 1-2', section 2'-2. The Flow analysis for the part 1-2' is very similar to that in the combustion chamber except that there is no mass addition effect in the feed duct. So,

\[
\int_{M_1}^{M_2} (1 - M^2) \left(1 + \frac{\gamma - 1}{2} M^2\right) \frac{dM}{M} = \int_0^{L_1} \left[2\gamma M^2 f\right] \frac{dx}{D} \tag{A.27}
\]

where \(L_1\) is the length of the oxidizer feed duct.

For the part from the section 2' to the section 2, incoming oxidizer expands from port area \(A_d\) to \(A_f\). It is well known that the expansion process is an adiabatic process. If we further assume that the flow static temperature does not change much, then the Mach number will remain unchanged (from equation (A.15)).

That is:

\[M_2 = M_{2'}\] \(\quad\) \(\text{(A.28)}\)

It can be summarized that for given length/diameter of the fuel tube and the given fuel/throat area ratio \(\frac{A_f}{A_t}\), the Mach numbers \(M_3, M_2, M_1\) can be definitely determined. The oxidizer flux can be expressed as a function of local Mach number and pressure. The pressure is a function of the local mach number and the total pressure. According to the equation (3.23) of the reference [162],

\[
G = \frac{P_0}{\sqrt{T_0}} \sqrt{\frac{\gamma}{R}} \frac{M}{\left(1 + \frac{\gamma - 1}{2} M^2\right)^{\frac{\gamma + 1}{2(\gamma - 1)}}} \tag{A.29}
\]

\[
\frac{P_0}{P} = \left(1 + \frac{\gamma - 1}{2} M^2\right)^{\frac{\gamma - 1}{\gamma - 1}} \tag{A.30}
\]

so,

\[
G = \frac{P}{\sqrt{T_0}} \sqrt{\frac{\gamma}{R}} M \left(1 + \frac{\gamma - 1}{2} M^2\right)^{1/2} \tag{A.31}
\]
or,
\[
\frac{G}{P} = \frac{1}{\sqrt{T_0}} \sqrt{\frac{T}{R}} M \left(1 + \frac{\gamma - 1}{2} M^2\right)^{1/2}
\]  
(A.32)

If we apply the equation (A.32) at section 2 (head end of fuel tube), we see that the mass flux in the system is proportional to the rocket chamber pressure \(P_c\).

According to the equation (5.30) of the reference [162],
\[
\frac{P}{P^*} = \frac{1}{M} \sqrt{\frac{\gamma + 1}{2 + (\gamma - 1)M^2}}
\]  
(A.33)

where * stands for the critical condition (\(M=1\)). Then,
\[
\frac{P_1}{P_{2'}} = \frac{M_{2'}}{M_1} \sqrt{\frac{2 + (\gamma - 1)M_{2'}^2}{2 + (\gamma - 1)M_1^2}}
\]  
(A.34)

In the sudden expansion from section 2' to section 2, there is pressure head loss. Here we make some further assumptions to simplify the analysis. As mentioned before, we will get,
\[
M_{2'} = M_2
\]  
(A.35)

Combining the continuity condition
\[
(GA)_1 = (GA)_{2'} = (GA)_2
\]  
(A.36)

and equation (A.29), we can get,
\[
P_{02'}A_d = P_{02}A_f
\]  
(A.37)

From equation (A.30), \(\frac{P_2}{\overline{P}}\) is a function of Mach number only. By using equation (A.35),
\[
\frac{P_{02'}}{P_{2'}} = \frac{P_{02}}{P_2}
\]  
(A.38)

Combining equation (A.37) and equation (A.38), we can get
\[
\frac{P_{2'}}{P_2} = \frac{P_{02'}}{P_{02}} = \frac{A_f}{A_d}
\]  
(A.39)
From equation (A.34) and equation (A.39), we can get

\[
\frac{P_1}{P_2} = \frac{P_1 P_2}{P_2^2} = \frac{A_f M_2}{A_d M_1} \sqrt{\frac{2 + (\gamma - 1)M_2^2}{2 + (\gamma - 1)M_1^2}} \tag{A.40}
\]

or,

\[
\frac{P_1}{P_2} \cdot \frac{A_d}{A_f} = \frac{M_2}{M_1} \sqrt{\frac{2 + (\gamma - 1)M_2^2}{2 + (\gamma - 1)M_1^2}} \tag{A.41}
\]

where,

\[
P_2 = P_c \tag{A.42}
\]

### A.4 Results and Discussion

Before we start the calculation, the constant \(a\), \(b\) in the equation (A.25) and the friction factors \(f\) for both the combustion chamber and the oxidizer feed duct must be determined. The regression rate coefficient \(a\) can be evaluated from the rocket experiment conducted before. The experiment showed that the regression rate is equal to 0.5 mm/sec for \(G = 70.37\) Kg/\(M^2\) sec (0.1 lbm/in^2 sec). So \(a\) is equal to 1.67e-5. It is shown before that for \(G\) varying from 70.37 to 703.7 Kg/M^2 sec, \(b\) only changes from 0.42 to 0.26. Here we take \(b\) equals 0.40.

The friction factor \(f\) is a function of the Reynolds number of the flow and the roughness at the boundaries. The Reynolds number is calculated on the basis of the hydraulic diameter of the duct. The relationship among \(f\), the Reynolds number \(Re\) and the relative roughness \(\delta\) is experimentally determined and plotted in Fig. 5.2 of reference [162].

For both the combustion chamber and oxidizer duct, the Reynolds number will be approximately taken as 10000. The friction factor, \(4f\) for combustion chamber is approximately equal to 0.75. And 0.045 for feed duct.
Figure A.3: Friction Factor (df) vs. Re. (Fig 5.2 of Ref. [162])
The calculation is carried out for series of Length/Diameter ratios of the hybrid fuel, series of fuel/throat area ratios and series of $4f \frac{L}{D}$'s of the feed duct. The results are shown in the Fig. A.4. to Fig. A.8.

All the flow properties, $M_1$, $M_2$, $M_3$, $\frac{G}{P_c}$ and $\frac{P_1}{P_c \cdot \frac{A_f}{A_d}}$ exhibit very similar behavior. With the fuel throat diameter ratio ($\frac{D_f}{D_t}$) increasing, $M_3$, decreases, then $M_2, M_1$ decrease too. The mass flux of the entire system will decrease. For a fixed fuel throat diameter ratio, these flow properties will decrease as the fuel length/diameter increase. This is because the friction and mass addition effect increase. From the Fig. A.8, it can be concluded that the pressure ratio $\frac{P_1}{P_2}$ increases with the increase of the Mach number at the head end of the fuel tube. And it increases with the increase of the friction effect $4f \frac{L}{D}$ of the oxidizer feed duct for a given $M_2$. For the fixed friction effect of the oxidizer feed duct and the Mach number at the head end of the fuel tube, the pressure ratio $\frac{P_1}{P_2}$ will increase as the expansion ratio $\frac{A_f}{A_d}$ increases.

In the rocket design or operation, once the chamber pressure $P_c$ is prescribed, the oxidizer flux $G_{ox}$ can be found from the figure A.7. Then the reservoir pressure can be looked up from the figure A.8.
Figure A.4: \( M_3 \) vs. \( \frac{A_f}{A_t} \) for any L/D
Figure A.5: $M_2$ vs. $\frac{A_f}{A_t}$
Figure A.6: $M_1$ vs. $M_2$
Figure A.7: \( \frac{G}{P_c} \) vs. \( \frac{A_f}{A_t} \)
Figure A.8: \( \frac{P_1 A_d}{P_2 A_f} \) vs. \( M_2 \)
APPENDIX B

DESIGN OF HYBRID ROCKETS AND EXPERIMENTAL SET-UP

The schematic structure of experimental hybrid rocket is shown in Fig. B.1. The firing hybrid rocket is shown in Fig. B.2. The rocket case is made of stainless steel and the fuel is placed inside of the case. The head-plate and end-plate are used to support the rocket case. The ignition system is built in the head plate, the nozzle is connected to the end-plate. The nozzle assembly is made of two parts, the nozzle holder and nozzle insert. The nozzle throat diameter can change from 0.1" to 1.5", by simply changing the insert, for a prescribed chamber pressure. The rocket is ignited by the mixture of oxygen and methane and a multi-spark ignition unit. At early time of the project, a general car spark plug was used to ignite the mixture of oxygen and methane. The problem associated with this design is that the time duration between two sparks is not long enough. And the spark is not "strong" enough (too short) to ensure a quick and reliable ignition. The modified ignition system used multi-spark plug which is custom-made from a general sport car spark plug. Since the change of the ignition system, the rocket does not have any problem with ignition system.

In the hybrid rocket, a mixture of, or pure, oxygen is used as an oxidizer, PMMA (Polymethymethycreate), HTPB and PBAN based fuel with and without addition of
Figure B.1: Schematic Structure of Experimental Hybrid Rocket

Al particles and C powder are used as solid fuel. In order to minimize the injection effect, a long induction duct is placed at the head-end of rocket to get uniform oxidizer flow. The diameter and length of the fuel tube (or rocket) can change in a very wide range. Two generations of hybrid rockets were constructed and used in experiments. The length of the hybrid rocket can change from 6" to 36". The diameter can vary from 0.5" to 4". The wide range of hybrid rocket size transfers to a wide range of experimental spectrum. The hybrid rockets have been tested in different pressures (up to 300 psi), a series of incoming oxidizer specific mass flow rates (0.01 to 0.4 lbm/in² sec).

The advanced infrared imaging technique and gas-chromatography were used to monitor the nozzle temperature profile and the exhaust compositions.
Figure B.2: A Firing Experimental Hybrid Rocket

Hybrid rocket experimental set-up

Hybrid rocket firing

Figure B.2: A Firing Experimental Hybrid Rocket
APPENDIX C

HYBRID ROCKET FUEL MANUFACTURE TECHNOLOGY

The Space Technologies Laboratory at the University of Arizona is the only university laboratory to have the ability to manufacture "industry standard hybrid rocket fuel". The solid fuel is made of HTPB as resin, aluminum particles, and ammonium chloride particles. The aluminum particle size is about 15 micrometers which can be directly used in the manufacturing of the fuel. The store bought ammonium chloride ($\text{NH}_4\text{Cl}$) particle is very coarse (about 300 micrometers) even in the form of agglomerate. So pretreatment is necessary for the ammonium chloride.

In order to decrease its viscosity, HTPB is heated to 160°F for 30 minutes before any particles will be added into the batch of Baker-Perkins planetary mixer (Fig. C.1). The ammonium chloride particles are added to the batch in two separate times which are 30 minutes apart. After all the aluminum particles and ammonia chloride particles are put into batch, the fuel will be mixed under vacuum for three hours.

The well mixed fuel will then be cast into the rocket mold, which has already been placed in the transparent vacuum unit. It is found from many trials that the fuel after being cast into mold had better be kept in the vacuum unit for at least 12 hours in order to eliminate the bubbles in the fuel. Even through the bubbles
will not cause any serious explosion problem as in the solid rocket, the existence of the bubbles will affect the uniformity and the fuel density. The cast fuel will cure in oven at the temperature of 110°F for 3 days. Because the hybrid fuel does not contain any explosive material (like AP), its manufacture can be conducted in an ordinary industrial mixer without any expensive explosion-proof processing equipment or automated facility. The whole manufacture process can be depicted in the flowing flow chart.

A key process of fuel manufacturing is to chose right cure agent and with appropriate amount. The cure agent we select to cure HTPB is MDI (isocyanate). The appropriate amount of MDI to cure HTPB depends on the structures of HTPB and MDI. The essential chemical reaction between HTPB and MDI is the reaction
of NCO radicals of MDI and OH radicals of HTPB. There is a little of variation of radical concentration of HTPB and MDI from time to time, which needs to be considered in the fuel manufacturing design. From one failure of the fuel mixing, we find the moisture is a big factor for the fuel quality. The reason is that there is plenty of OH radical in water. After realizing this fact, we dry all the solid particles (Al, C,..) before they are put into mixer.

If the solid particles are not included in the hybrid fuel, the manufacture process is much simpler. In the manufacturing of fuel HTPB/C powder, the fuel only need to mix half an hour. The pretreatment of HTPB is not necessary, because the viscosity of HTPB is low enough to ensure "smooth" casting. The cast fuel does not need to be kept in vacuum because the bubbles can easily pop out from the fuel.
The fuel will cure in less than 12 hours in room temperature not necessary in oven.
REFERENCES


[61] K. Ramohalli and F. A. Williams, private conversation, May, 1993


[106] M. A. Niederschulte, Ph.D. dissertation, Department of Chemical Engineering, University of Illinois at Urbana-Champaign, 1989


[120] R. S. Barlow & J. P. Johnson, “Structure of Turbulent Boundary Layers on a concave Surface,” Rep, MD-47, Department of Mechanical Engineering, Stanford University, Stanford, California, USA

[121] T. Theodosen, “Mechanism of turbulence,” In proc. 2nd Midwestern Conf. on fluid mech., 1952, Ohio State University, Columbus, Ohio


[137] W. Noeggerath, private communication with Green Jr., L., 1937, referred to the above citation


