In compliance with the
Canadian Privacy Legislation
some supporting forms
may have been removed from
this dissertation.

While these forms may be included
in the document page count,
their removal does not represent
any loss of content from the dissertation.

CFD Simulation of a Gas Turbine Combustor

by

Chok Nam Ng

B.Eng. (Aerospace)

A thesis submitted to
the Faculty of Graduate Studies and Research
in partial fulfillment of the requirements
for the degree of

Master of Applied Science

in

Aerospace Engineering

Ottawa-Carleton Institute For
Mechanical and Aerospace Engineering

Department of Mechanical and Aerospace Engineering
Carleton University
Ottawa, Ontario, Canada
May 2003

© 2003
Chok Nam Ng

National Library
of Canada

Bibliothèque nationale
du Canada

Acquisitions and
Bibliographic Services

Acquisitions et
services bibliographiques

395 Wellington Street
Ottawa ON K1A 0N4
Canada

395, rue Wellington
Ottawa ON K1A 0N4
Canada

Your file Votre référence

ISBN: 0-612-88891-6

Our file Notre référence

ISBN: 0-612-88891-6

The author has granted a non-exclusive licence allowing the National Library of Canada to reproduce, loan, distribute or sell copies of this thesis in microform, paper or electronic formats.

L'auteur a accordé une licence non exclusive permettant à la Bibliothèque nationale du Canada de reproduire, prêter, distribuer ou vendre des copies de cette thèse sous la forme de microfiche/film, de reproduction sur papier ou sur format électronique.

The author retains ownership of the copyright in this thesis. Neither the thesis nor substantial extracts from it may be printed or otherwise reproduced without the author's permission.

L'auteur conserve la propriété du droit d'auteur qui protège cette thèse. Ni la thèse ni des extraits substantiels de celle-ci ne doivent être imprimés ou autrement reproduits sans son autorisation.

Canada

Abstract

Advances in CFD modeling and the availability of a gas turbine engine have motivated the simulation of its non-premixed combustor burning diesel fuel. The simulations were conducted with a 3D detailed geometry model with unstructured grids based on the upwind finite volume method and SIMPLE algorithm. Both the $k-\varepsilon$ and RSM turbulence models in conjunction with the Eddy Dissipation and presumed β -PDF combustion models were used for the simulations. The injection of the liquid fuel was modeled with Lagrangian discrete phase model.

The simulations were validated against the results from the literature, and this study confirmed the validities of CFD modeling for the current combustor. Through this study, the advantages and limitations of the models employed are evaluated. Recommendations for future research are suggested based on the recently available computing resources and soon to-be-available combustor test rig.

Acknowledgements

I would first like to thank my supervisor, Professor J.E.D. Gauthier, for his continuous support and invaluable guidance throughout my Master's study, and for giving me the opportunity to work under his supervision.

Special thanks to the staff of the Department of Mechanical and Aerospace Engineering for their valuable assistance.

I would also like to thank my colleagues Mohamed Mehanna and Sylvain Graveline for fruitful discussions about CFD.

Finally, I would like to express my deep appreciation and thanks to my parents for their endless supports.

Table of Contents

Abstract.....	iii
Acknowledgements.....	iv
Table of Contents.....	v
List of Figures.....	vii
List of Tables.....	ix
Nomenclature.....	x
Chapter 1 Introduction.....	1
1.1 Gas Turbine Combustor.....	2
1.2 Computational Fluid Dynamic Combustion Simulation.....	4
1.3 Thesis Overview.....	6
Chapter 2 Theoretical and Literature Reviews.....	7
2.1 CFD Combustion Modeling.....	8
2.2 Governing Equations in Turbulent Reacting Flow.....	10
2.3 Modeling Turbulence.....	12
2.3.1 Limitations of DNS in CFD Combustion Simulation.....	12
2.3.2 RANS Turbulence Models.....	13
2.3.3 Reynolds Stress Model.....	16
2.3.4 Large Eddy Simulation.....	17
2.4 Turbulence Combustion Modeling.....	18
2.4.1 Finite-Rate Chemical Kinetics.....	19
2.4.2 Eddy-Break-Up and Eddy Dissipation Model.....	20
2.4.3 Mixture Fraction Conserved Scalar Approach.....	21
2.4.4 Laminar Flamelet Model.....	23
2.4.5 PDF Transport Model.....	24
2.4.6 Comparisons between Different Combustion Models.....	26
2.5 Discrete Phase Model.....	30
2.6 NO_x Predictions.....	32
2.7 Radiation Heat Transfer.....	34
2.8 Numerical Schemes.....	35
2.9 Basis for Current Combustion Simulation.....	37
Chapter 3 Roll-Royce Allison 250 GT Engine.....	39
3.1 Allison 250 Engine Specifications.....	40
3.2 Engine Configuration and Combustion System.....	41
3.3 Combustor Liner Geometry.....	43
Chapter 4 Combustor Solid Model and Grid Generation.....	45
4.1 Simplified Solid Model.....	46
4.2 Unstructured Grid Generation.....	51

Chapter 5 Boundary Conditions Specification	53
5.1 Discrete Phase Model Boundary Condition.....	54
5.1.1 Liquid Fuel Properties.....	54
5.1.2 Discrete Phase Injection Initial Point Properties	55
5.2 Continuous Flow Boundary Conditions	57
5.2.1 Combustor Interior Fluid Properties	57
5.2.2 Estimations of Continuous Flow Boundary Conditions	59
5.2.2.1 Dome Swirled Flow Prediction.....	59
5.2.2.2 Liner Flow Distribution	62
5.3 Summary of Continuous Phase Boundary Conditions.....	65
Chapter 6 CFD Combustion Simulations and Discussions.....	67
6.1 Grid Independent Study	69
6.2 Turbulence Specification	71
6.3 Combustion Flow Modeling	74
6.3.1 Eddy Dissipation Combustion Model.....	74
6.3.2 Conserved Scalar Approach with Prescribed PDF Combustion Model ..	75
6.3.3 Velocity Flowfield	76
6.3.4 Kerosene and Diesel Combustion.....	78
6.3.5 Temperature Distribution in Combustor.....	80
6.3.6 Temperature Distributions Predicted with Different Combustion Models	82
6.4 Fuel Injection Trajectory and Interaction with Continuous Phase.....	87
6.5 RSM and $k-\varepsilon$ Turbulence Models	90
6.6 Numerical Schemes and Convergence Difficulties	92
6.7 Computational Efficiency with Parallel Processing	95
6.8 Liner Wall Temperature Estimation with Convective Heat Transfer.....	97
6.9 NO_x Emission Estimation	100
Chapter 7 Conclusions and Recommendations for Future Work	102
7.1 Introduction.....	102
7.2 Conclusions.....	103
7.3 Recommendations for Future Work.....	105
References.....	106
Appendix A Liner Geometry	113
Appendix B Lookup Table Preparation	116
Appendix C Convective Heat Transfer Coefficient of Liner Walls	117
Appendix D NO_x Prediction Conversions	119

List of Figures

Figure 1.1. Gas Turbine Engine (Adapted from Anonym 1986).....	2
Figure 1.2. Gas Turbine Combustors (Adapted from Lefebvre 1983)	3
Figure 1.3. Gas Turbine Combustor Terminology (Adapted from Mellor 1990).....	3
Figure 1.4. General Structure of CFD modeling.....	4
Figure 2.1. Lookup Table Concept (Anonym 2003).....	23
Figure 2.2. Coupling between Discrete Phase and Continuous Phase (Anonym 2003) ...	31
Figure 3.1. Allison 250 Engine Airflow (Adapted from Anonym 1999)	42
Figure 3.2. Allison 250 Gas Turbine Engine Combustion Liner	44
Figure 4.1. Dome-Swirlers Holes Distribution and Swirled Flow Direction	47
Figure 4.2. Dome-Swirlers Louver Plates	47
Figure 4.3. Preliminary Combustor Solid Model.....	48
Figure 4.4. Simplified 3D Combustion Solid Model.....	49
Figure 4.5. Turbine Disk Shield at Combustor Outlet.....	49
Figure 4.6. Meshing of Combustor Solid Model: A. Line Mesh, B. Face Mesh.....	52
Figure 4.7. Final Mesh of the Combustor Solid Model	52
Figure 5.1. Cone Injection for 3D Hollow Fuel Spray (Anonym 2003).....	55
Figure 5.2. Dome-Swirlers Model.....	60
Figure 5.3. Dome Swirled Flow Prediction	60
Figure 5.4. Comparison of Predicted Combustor Liner Airflow to Conventional Designs	64
Figure 6.1. Predictions at 5-inches Extension Mid-section: Rake 1 and Rake 2	70
Figure 6.2. Predicted Temperature Profiles with Different Grid Density.....	70
Figure 6.3. Effects of Turbulence Intensity to Combustion Simulation	72
Figure 6.4. Velocity Vectors of Combustion Zone.....	77
Figure 6.5. Comparisons of Combustor Flowfields: A. Zamuner et al (2002), B. Adami and Martelli (2000), C. Current Combustor.....	77
Figure 6.6. Kerosene and Diesel Combustion Temperature Distributions	79
Figure 6.7. Combustion Zone Temperature Distribution.....	81
Figure 6.8. Predicted Temperature Distributions with Different Combustion Models: Plane 1	83
Figure 6.9. Predicted Temperature Distributions with Different Combustion Models: Plane 2.....	84
Figure 6.10. Discrete Phase Fuel Injection Trajectory	88
Figure 6.11. Stochastic Tracking of Liquid Fuel Injection.....	89
Figure 6.12. Temperature Distributions in Combustor Predicted with RSM and $k-\epsilon$ Turbulence Models.....	91
Figure 6.13. Temperature Profiles at Test Rig Mid-Section Predicted with RSM and $k-\epsilon$ Models.....	91

Figure 6.14. Predictions Based on 1 st Order and 2 nd Order Discretizations	93
Figure 6.15. Convergence History of EDM Two-Step Diesel Combustion	94
Figure 6.16. Computing Time Reduction with Parallel Processing.....	96
Figure 6.17. Temperature of Combustion Flow at Test Rig Mid-Section	99
Figure 6.18. Liner Wall Temperature Predictions	99
Figure 6.19. <i>NO</i> Formation for Diesel Fuel (Adapted from Lefebvre 1999)	101
Figure A. 1. Combustor Liner Geometry.....	113
Figure A. 2. Layout of Liner Injection Holes	114
Figure A. 3. Geometry of Turbine Disk Shield	114
Figure A. 4. Geometry of Dome-Swirler Slots.....	115

List of Tables

Table 2.1. Classifications of Combustion Models.....	26
Table 2.2. Applications of Diffusion Combustion Models.....	29
Table 3.1. Engine Simulation Parameters at Take-Off Condition.....	40
Table 5.1. Liquid Phase Properties of Kerosene and Diesel Fuel.....	54
Table 5.2. Discrete Phase Model Initial Conditions	56
Table 5.3. Definition of Fuel-Air Mixture Properties.....	57
Table 5.4. Vapor Phase Properties of Kerosene and Diesel Fuel	58
Table 5.5. Grid Independent Study of the Dome-Swirl Model	61
Table 5.6. Dome-Swirl Airflow Distribution.....	61
Table 5.7. Boundary Conditions Specification	62
Table 5.8. Liner Airflow Split.....	63
Table 5.9. Boundary Conditions for CFD Simulations.....	65
Table 6.1. Grid Density Refinements with Grid Adaptions.....	69
Table 6.2. Maximum Temperature and Mass Weighted Average Outlet Temperature Predicted with Different Combustion Model.....	82
Table 6.3. Residual Convergence Criteria	92
Table 6.4. Convective Heat Transfer at Liner Wall.....	97
Table 6.5. <i>NO</i> Predictions at Combustor Outlet	100
Table A.1. Geometry Profile of Turbine Disk Shield.....	114
Table B.1. Lookup Table Species	116
Table C. 1. Combustor Annulus Air Properties.....	118
Table C. 2. Estimated Parameters for Convective Heat Transfer Calculations.....	118
Table C. 3. Estimated Convective Heat Transfer Coefficient for Liner Wall	118

Nomenclature

Symbols	Descriptions	Units
A	Modeling constant (Eqn. 2.4.1); Cross sectional area	(none); m^2
B	Modeling constant (Eqn. 2.4.2)	(none)
C_D	Drag coefficient	(none)
c_p	Specific heat	J/kgK
D	Diameter; Diffusivity	m ; m^2/s
D_{ij}	Binary diffusivity	m^2/s
f	Mixture fraction; Friction factor	(none); (none)
F	Force; Correction factor	N ; (none)
G	Gibbs free energy	J/mol
h	Enthalpy; Convective heat transfer coefficient	J/mol ; $\text{W/m}^2\text{K}$
H	Total enthalpy	J/mol
I	Turbulence intensity	%
$\bar{J}$	Diffusion flux	$\text{kg/m}^2\text{s}$
k	Turbulent kinetic energy; thermal conductivity	m^2/s^2 ; W/mK
l	Turbulence length scale	m
L	Physical length scale; Latent heat of evaporation	m ; J/kg
$\dot{m}$	Mass flow rate	kg/s
M	Molecular weight	kg/mol
N	Number of species	(none)
Nu	Nusselt number	(none)
P	Pressure	Pa
Pr	Prandtl number	(none)
r	Radius	m
R	Reaction rate	$\text{kg/m}^3\text{s}$
Re	Reynolds number	(none)
R_u	Universal gas constant	J/molK

s	Entropy	J/kgmolK
S_m	Mass source (Eqn. 2.2.1)	kg/m ³ s
T	Temperature	K
t	Wall thickness; Time	m; s
T_{ref}	Reference temperature	K
u	Velocity	m/s
x	Space coordinate	(none)
y	Space coordinate	(none)
Y	Mass fraction	(none)
z	Space coordinate	(none)
Z	Atom fraction	(none)

Greek Symbols

ρ	Density	kg/m ³
ϕ	Scalar quantity	-
τ	Viscous force tensor	N/m ²
θ	Injection angle	degree
μ	Dynamic viscosity	kg/ms
χ	Scalar dissipation rate	m ² /s
ε	Turbulence kinetic energy dissipation rate	m ² /s ³
ω	Turbulence kinetic energy specific dissipation rate	s ⁻¹
ν'	Stoichiometric coefficient for a reactant	(none)
ν''	Stoichiometric coefficient for a product	(none)
μ_t	Eddy viscosity	kg/ms

Subscripts

$fuel$	Fuel stream
i	Direction component; i^{th} atomic element; Inner diameter or radius
j	Direction component
k	k^{th} species
l	Liquid phase

o	Outer diameter or radius; Standard state condition
ox	Oxidant stream
P	Product
R	Reactant
r	r^{th} reaction
Superscripts	
$'$	Fluctuation quantity
o	Formation rate

Chapter 1

Introduction

The growing uses of gas turbine engines as power plants in industry and their dominant role in air transportation have led to a significant concern regarding gas turbine combustion emissions and the research for alternative combustion sources. For many years, scientists and engineers have made extensive efforts to design a gas turbine combustion system with high performance, high fuel efficiency, low emissions, and the ability to burn alternative fuels. These efforts include the study of combustion phenomena to further the understanding of the process of combustion, and the development of reliable and efficient simulation tools to supplement the conventional experimental design methodology.

Today, Computational Fluid Dynamics (CFD) combustion modeling has been incorporated greatly into the practical designs and developments of gas turbine combustion systems. To understand the increasing applications of CFD in gas turbine combustion, this thesis presents a CFD combustion simulation of a helicopter gas turbine engine combustion system to study the various issues regarding the usefulness and limitations of CFD simulation for a practical gas turbine combustor.

As an introduction, this chapter gives a brief overview of the major elements of modern gas turbine engines and their combustion systems, a brief foreword of CFD combustion simulations of gas turbine combustors, and presents the scope of the current research.

1.1 Gas Turbine Combustor

Detailed descriptions of a gas turbine (GT) engine and combustors are available in general gas turbine textbooks, like Saravanamuttoo et al (2001), Lefebvre (1999), and Mellor (1990). This section will provide a brief review.

The major components of a typical propulsion gas turbine engine are the engine inlet, compressor, combustion chamber (combustor), turbine, and nozzle as shown in Figure 1.1.

Figure 1.1. Gas Turbine Engine (Adapted from Anonym 1986)

Among these components, the combustor is an energy-conversion device where the fuel is mixed with the compressor air and combusted to release the thermal energy to power the engine. The modern gas turbine combustors could be categorized into a can, can-annular and annular combustor as shown in Figure 1.2. A gas turbine combustor can be described by conventional terminology as shown in Figure 1.3.

Depending on the flow configurations, a combustor can be further distinguished into straight flow or reverse flow combustors, where the straight flow combustor is widely used for larger gas turbine engines, while the reverse combustion flow configuration is generally used for smaller gas turbine engines such as those used in helicopters, because of their short length and small volume.

Figure 1.2. Gas Turbine Combustors (Adapted from Lefebvre 1983)

Figure 1.3. Gas Turbine Combustor Terminology (Adapted from Mellor 1990)

1.2 Computational Fluid Dynamic Combustion Simulation

In general, Computation Fluid Dynamics (CFD) could be viewed as a computer program that simulates the fluid flowfield of an engineering device for design purposes and research interest. The basic structure of a typical CFD model could be represented as in Figure 1.4.

Figure 1.4. General Structure of CFD modeling

From Figure 1.4, it can be seen that CFD modeling is a task requiring knowledge of various engineering practices. The geometry of the device is constructed in pre-processing with the software solid modeler or CAD software, and is subsequently “meshed” with computational grids for numerical simulation. These processes require engineering justifications for device geometry simplifications and grid generation methods to obtain an accurate CFD simulation while retaining the reasonable computation time. In solving the problem, the appropriate physical models, such as the turbulence models, combustion models, heat transfer models, etc., have to be selected carefully based on specified parameters with awareness of the varied sophistications and limitations of these models. Results of the simulations are compared against scientific or technical data to ensure their validity.

CFD simulations of a gas turbine combustor inherently deal with turbulent flow with combustion that can be classified into a diffusion (non-premixed), premixed, and partially premixed flame. Non-premixed combustion is where the fuel and the oxidant (air) are initially separated and combustion occurs when the fuel stream and the oxidant stream become mixed and ignited. For premixed combustion, the fuel and the oxidant are initially mixed at a molecular level, and the propagation of the flame front controls combustion. The partially premixed combustion system includes premixed flames with non-uniform fuel-oxidizer mixtures.

There are different approaches for combustion modeling for the different combustions flames. Both approaches are concentrated on the efforts to model the chemistry and turbulence interaction. For the modeling of diffusion combustion, additional effort is required to model the injection and atomization of the liquid fuel. This thesis is based on the CFD modeling of diffusion combustion, which is employed in most practical engineering devices, such as conventional gas turbine engine combustors.

1.3 Thesis Overview

This thesis is part of a program to establish a new gas turbine combustion research laboratory at Carleton University. In particular, a Rolls-Royce Allison 250 gas turbine engine is being installed for future applied research activities. This thesis is to establish a baseline CFD model of the engine combustor when burning diesel fuel.

The combustion simulations were done with a commercial CFD package, FLUENT™ 6.1. The predicted flow properties of the combustor flowfield are compared with published literature and empiricisms to assess the validity of the CFD simulations, and to investigate the appropriateness of turbulence combustion models that are commonly applied for practical gas turbine diffusion combustion system simulations.

In the following chapter, a literature review and the principal theory elements of CFD combustion simulation of a gas turbine with diffusion combustion are presented. The specifications of the Allison 250 gas turbine engine and the detailed description of its combustion system are given in Chapter 3. In Chapter 4, the construction of the solid model of the combustor for computational purposes, and the meshing of the combustor model are discussed. The details of the boundary conditions specification and modeling parameters are discussed in Chapter 5. The CFD combustion simulations and the results of the simulation, which include the models for turbulence and combustion modeling, the fuel injection model, and the predictions of liner wall temperature and NO_x emissions, are discussed in Chapter 6. The thesis concludes with discussions of the validity and credibility of the present simulation methodologies for the particular gas turbine combustion system and possible future improvements that could be made to refine the simulations.

Chapter 2

Theoretical and Literature Reviews

CFD combustion simulation of a practical gas turbine combustor is a highly complicated task that involves a broad range of knowledge and principles. The purpose of this chapter is to review CFD combustion simulation for gas turbine combustion systems with diffusion flame.

The review is concentrated on the modeling of turbulent flow, turbulent combustion, fuel injection and droplet dispersion, and NO_x emissions prediction in a gas turbine combustion system. It also discusses radiation heat transfer phenomena in a gas turbine combustor and the commonly applied numerical techniques for CFD combustion simulations.

The review is based largely on published literature such as the works of Jones and Whitelaw (1982), Peters (2000), and Veynante and Vervisch (2002). Theories that are listed for the ease of discussion are mainly adapted from Anonym (2003) unless otherwise specified. Examples of CFD simulations of practical gas turbine combustion with different turbulence combustion models are presented to study the features of these representative models based on the theoretical assumptions, computational efficiency and robustness, accuracy of predictions, and appropriateness for the type of combustor being modeled.

2.1 CFD Combustion Modeling

The basic definition of CFD is “a computer software that simulates any fluid flow by solving numerically the governing equations, which are based on the conservation principles of mass and momentum (Navier-Stoke equations), the conservation of energy, the equation of state, and the conservation of chemical species for reacting flow. These equations can be expressed as mathematical equations in the form of partial differential equations, and, CFD is, in part, the art of replacing the governing partial differential equations of fluid flow with numbers, and advancing these numbers in space and/or in time to obtain a final numerical description of the complete flowfield of interest.” (Wendt et al 1996)

The incorporation of CFD in the design of combustion systems took place as early as the 1950's (Chang and Zhou 1999), and with the application for gas turbine combustion beginning in the 1970's by Spalding (Spalding 1999). Prior to this, “the development of a gas turbine combustor in the earliest days was referred to as ‘black art’ by Lefebvre (1983), which was based on, if not entirely but intensively on trial-and-error parameter testing. The rule-based empirical design technique that rely on experimental correlations is important for the initial design phase, however, it is not very efficient and there is little innovation due to the excessive experimental costs that require proving a new design” (Lefebvre 1983).

As CFD simulation is relatively inexpensive and has less limitations than the experimental techniques, it has quickly become a powerful design tool for practical combustor design and a research tool for studying combustion phenomena. In the past decades, higher operating temperatures and pressures of an advanced gas turbine combustion chamber and stringent emission regulations, particularly NO_x emissions, have initiated the extensive applications of CFD in gas turbine combustion design.

Today, the CFD simulation of a gas turbine combustor is more feasible with the constant increase in computer power, and is more reliable with the development of advanced numerical and grid generation techniques and a better understanding of the parameters affecting turbulent combustion flow. CFD combustion simulation is widely employed in industry, as well as in research institutes and the academic sector for research and study purposes. CFD software that is implemented with turbulent combustion modeling is widely available commercially and includes CFX™, FLUENT™, and CFD-ACE.

The increasing usage of CFD combustion simulation has drawn great interest from scientists, researchers, and engineers to critically observe and evaluate its validity and ability or potential ability. Jones and Whitelaw (1982) reviewed and evaluated the calculation methods of the conservation equations in turbulent reacting flow; Bilger (2000) summarized the implementations of turbulent flame structure research on modeling; Libby and William (1980, 1994) co-edited academic releases that reviewed the development of turbulent combustion; and Veynante and Vervisch (2002) provided comprehensive generic reviews of the approaches and modeling strategies of turbulent combustion modeling. Practically, Eaton et al (1999) presented experimental validated applications of furnace combustion CFD simulation, Mongia (1993) summarized the applications of combustion models and methodology in the design and development of gas turbine combustion systems that were formulated, developed, and refined by himself and his coworkers over two decades. The following sections present a similar review, however, the subjects reviewed are concentrated on CFD modeling of diffusion combustion systems.

2.2 Governing Equations in Turbulent Reacting Flow

The motion of all fluid flow can be described by the Navier-Stokes equations, which are the instantaneous conservation of mass (continuity) and momentum that can be written in general form as:

Continuity ($i = 1, 2, 3$):

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = S_m \quad (2.2.1)$$

Momentum ($j = 1, 2, 3$):

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} + F \quad (2.2.2)$$

Where u_i is the velocity vector, ρ is the flow density, S_m is the mass source added to the continuous phase, i.e., fuel injection vaporization, P is the static pressure, F is the body force, and τ_{ij} is the viscous force tensor as defined based on Newtonian fluid.

For reacting flow, additional conservation equations are written for energy and chemical species of finite-rate transport in combustion flow. The species conservation equation is written as:

Species (N species with $k = 1 \dots N$):

$$\frac{\partial}{\partial t}(\rho Y_k) + \frac{\partial \rho u_i Y_k}{\partial x_i} = -\frac{\partial \bar{J}_i^k}{\partial x_i} + R_k \quad (2.2.3)$$

where Y_k is the mass fraction of species k , and R_k is the rate of formation through reaction of species k . The diffusion flux, $\bar{J}_i^k$ of species molecular k that arises due to concentration gradient is generally defined according to Fick's law (Veynante and Vervisch 2002, Turns 1996).

The assumptions of unity Lewis number and negligible pressure work for incompressible flow are generally made to simplify turbulence combustion modeling (Veynante and Vervisch 2002). With these assumptions, the energy equation in the form of total enthalpy, H , is written in a simplified form as:

Enthalpy:

$$\frac{\partial \rho H}{\partial t} + \frac{\partial \rho u_i H}{\partial x_i} = \frac{\partial P}{\partial t} + \frac{\partial}{\partial x_i} \left[\sum_{k=1}^N J_i^k + u_i \tau_{ij} \right] + u_i F \quad (2.2.4)$$

The total enthalpy H is defined as

$$H = \sum Y_k H_k \quad (2.2.5)$$

and

$$H_k = \int_{T_{ref,k}}^T c_{p,k} dT + h_k^o(T_{ref,k}) \quad (2.2.6)$$

h_k^o is the formation enthalpy of species k at the reference temperature $T_{ref,k}$, and $c_{p,k}$ is the heat capacity of the species.

2.3 Modeling Turbulence

In many engineering devices such as a gas turbine combustor, the solution for the turbulent flow is always a challenging task that remains “unresolved and yet to be fully understood” (Peters 2000). The results of intensive research activities of engineers, researchers, and scientists, have led to the various approaches of modeling turbulent flow. These approaches or models have been implemented in CFD simulations with substantial success with their quality in simulating turbulent flow for practical engineering applications. These various approaches are semi-empirical models based on the turbulence theory with empirical inputs, which include Reynolds Average Navier-Stokes (RANS), Large Eddy Simulation (LES), and Direct Numerical Simulation (DNS). The theory of these approaches and their applications in gas turbine turbulent combustion modeling are reviewed in this section.

2.3.1 Limitations of DNS in CFD Combustion Simulation

Turbulent flows can be described as a fluctuating velocity field that induces the fluctuations of the transport quantities in a flowfield such as momentum, energy, and species concentrations. Since these fluctuations could be small scale and have high frequency, the direct numerical simulation of the resulting “fluctuation governing equations” will require extremely fine computational grid cells and time steps to fully resolve these fluctuating quantities. With limited computer power and memory storage, the application of direct numerical simulation (DNS) is limited to simplified problems, where the number of time and length scales present in the turbulent flow are not great.

The application of DNS in turbulent reacting flow is restricted to simplified cases as a tool to study the phenomena of a turbulent reacting flowfield, or as the validating tools for other turbulence combustion models. Its application for practical engineering devices such as a gas turbine combustor is limited by the computer power even for the foreseen future (Veynante and Vervisch 2002).

2.3.2 RANS Turbulence Models

With the difficulties in practical application of DNS, scientists and engineers have come up with semi-empirical turbulence models to resolve the need for solutions of turbulent flow. The classical approach is the use of turbulence models based upon the Reynolds Averaged Navier-Stokes (RANS). These types of models are widely applied and generally accepted as a reasonable representation of turbulent flow for both non-reacting and reacting turbulent flowfields.

In the RANS turbulence simulation, turbulent flow is expressed into mean flow and fluctuation as:

$$\phi = \bar{\phi} + \phi' \quad (2.3.1)$$

where ϕ represents a scalar quantity, such as velocity components, pressure, energy, or species concentrations. Substituting these expressions into the instantaneous continuity and momentum equations, and taking an ensemble average (Reynolds averaging), the equations can be simplified by dropping the over-bar on the mean component, thus giving the ensemble-averaged Navier-Stokes equations as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \quad (2.3.2)$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial}{\partial x_j}(-\overline{\rho u_i u_j}) \quad (2.3.3)$$

The Reynolds Averaged Navier-Stokes (RANS) approach has bypassed the enormous computational expense of modeling the exact Navier-Stokes equations by representing the resulting equations with a mean flow velocity. However, there is an additional term on the RHS of Equation (2.3.3) representing the effects of turbulence (Reynolds stresses), which requires additional closure. Turbulence modeling is thus the introduction of the closure hypothesis relying on physical arguments and empirical inputs to solve the second order moments of turbulent flow (Peters 2000).

Depending on the number of additional closure equations, these models can be classified as zero-equation models, one-equation models, or two-equation models. For examples, Spalart-Allmaras' (1992) one-equation model, Launder and Spalding's (1972) k - ε two-equation models, and Wilcox's (1998) k - ω model. These models are also referred to as "eddy viscosity models", as they are all based on Boussinesq's hypothesis that the Reynolds stresses can be related to the mean velocity gradient as:

$$-\overline{\rho u_i u_j} = \mu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (2.3.4)$$

The disadvantage of the Boussinesq's hypothesis is that the eddy viscosity, μ_t , is assumed as an isotropic scalar quantity, which is not strictly true in turbulent flow (Anonym 2003). Among these eddy viscosity type turbulence models, the k - ε model (Launder and Spalding 1972) is widely used in turbulent combustion flow with its computational robustness, economy, and reasonable accuracy. The k - ε model defines the eddy viscosity as a function of turbulence kinetic energy (k) and its dissipation rate (ε), therefore, the CFD simulation of turbulent flow with the k - ε model requires solving additional transport equations of k and ε , as discussed in more detail in Jones and Whitelaw (1982).

Although often criticized for its lack of agreement with experimental data for some applications, the k - ε model is still the most commonly used turbulence model with its numerical stability and applications widely documented, particularly the implementations of more elaborate turbulence models are not justified in turbulent combustion simulations. Some examples of the applications of the k - ε turbulence model in a gas turbine combustion simulation include: Lau (1995) investigated the performances of different combustion models based on the k - ε model; Gulati et al (1995) investigated the effect of dilution air on the combustion flow with k - ε model; Crocker et al (1999) and McGuirk and Spencer (2000) used the k - ε and the modified k - ε model respectively to investigate the coupling effect of the combustion annulus and inlet flowfield.

Modifications of the original k - ε model based on the RNG mathematical theory (Yakhot and Orszag 1992) have been suggested for modeling of the flow with strong streamline curvature, vortices, and rotation. Nonetheless, the investigation of a 3D diffusion combustion flow by De Champlain et al (1994) showed that no significant improvement was found with the application of the RNG k - ε model over the standard k - ε model. They explained that the intense dilution jets and swirl recirculation flow corresponded with the isotropic assumption of these models, therefore, the application of the RNG k - ε model will not yield significant improvement. Xia et al (1998) have also revealed that the RNG k - ε model gives little improvement over the standard k - ε model by comparing numerical results against experimental data in their swirling flow study with a water-modeled combustor.

The k - ω turbulence model is incorporated with the modifications for low-Reynolds-number effects, compressibility, and shear flow spreading. The applications of this lately developed two-equation turbulence model in turbulent reacting flow is not as well established as the classical k - ε model. Adami and Martelli (2000) have incorporated the k - ω turbulence model in their non-premixed reacting flow solver, however, they have not investigated the advantage of implementing this turbulence model over the classical k - ε model.

2.3.3 Reynolds Stress Model

The Reynolds Stress Model (RSM) is a more elaborate turbulence model that solves the transport equations for the Reynolds Stress in Equation (2.3.3) to account for the anisotropic effect of turbulent flow with strong swirl. Therefore, it theoretically allows a more accurate prediction for complex flow, such as the one in a combustor.

In the investigations of Xia et al (1998), and Maidhof and Janicka (1993), their findings suggested that the RSM model has a superior performance over the $k-\varepsilon$ model in combustor flowfield prediction compared against experimental data. They showed that the RSM model succeeded in predicting the recirculation zone and corner swirling of flow toward the outlet of the combustor model, while the $k-\varepsilon$ model predicted the “solid-body-rotating-type” flow at the downstream. However, the superiority of the RSM model in a combustion flowfield was not reported in Xia et al (1998). In the combustion flow predictions of Maidhof and Janicka (1993), discrepancies were present in both the RSM and $k-\varepsilon$ model, with the superiority of the RSM model in combustion flow modeling certainly not realized. Other applications of RSM include Ma et al (1999), who predicted a turbulent diffusion flame based on the RSM with the implementation of two different combustion models.

Although the Reynolds Stress turbulence model is proven superior in the predictions of strongly swirled flow, such as the one in a combustor, there are no reports of substantial improvement to combustion flow calculation. The application is limited to the reliability of the closure assumptions employed for the Reynolds stresses tensor and additional computational times to solve the extra equations. As reported by Xia et al (1998), a CPU time that is 2.7 times greater than the $k-\varepsilon$ model per iteration, and an excessive under-relaxation factor must be applied to obtain a convergence solution, which also increases the total calculation times.

2.3.4 Large Eddy Simulation

Large eddy simulation (LES) is an alternative approach for turbulence modeling. LES is situated between the DNS and the RANS approach. The largest scale turbulence structures are explicitly computed while the effects of the smaller scale turbulence are modeled (subgrid-scale model).

Since the large scale mixing between fuel and oxidizer is fully resolved and simulated, LES provides an attractive feature that resolves the limitations of the RANS models in modeling large scale mixing of turbulent combustion flow, which controls many properties of the combustion chamber (Veynante and Vervisch 2002). At the small-unresolved scale, interactions between turbulence mixing and combustion still need to be modeled in the LES approach. As discussed in Peters (2000), the subgrid model for turbulence combustion closure can be easily adapted from some successful RANS combustion models, such as the extension of the flamelet model (which will be discussed later in the section) for LES modeling by Pitsch (2000).

The LES approach has less restrictive mesh resolution requirements than DNS, however, extremely fine meshes and long computational time are still necessary. As in the work of Jones (2002), 1.25 millions grid cells were required for the computation of a simple geometry combustor. Forkel and Janicka (2000) conducted a LES simulation of a coaxial flow hydrogen fuel combustor with simple cylindrical geometry with 24 cm in diameter and 38 cm in length that comprises of 500 000 grid cells in two weeks with a single workstation.

The applications of LES in combustion simulation is gaining popularity and has shown to improve the inaccuracy associated with RANS models, while its application to practical combustion systems is still in its early stages.

2.4 Turbulent Combustion Modeling

In combustion flow simulations, the accuracy of the flow properties depends on:

- The reacting species present in the flow and the reaction steps that are described by the chemical kinetic mechanisms;
- The calculations of the formation and destruction rates of each species involved in the turbulent combustion flowfield.

As the chemical source terms, R , that emerge in the species concentrations equations (Equation 2.2.3) are highly nonlinear functions of temperature and species concentrations, and strongly interact with the turbulence, the determination of the mean reaction rate is a major difficulty for turbulent combustor flow. According to Veynante and Vervisch (2002), the combustion models for a turbulent diffusion flame can be categorized into three major groups based on the following hypotheses:

- Infinitely fast chemistry, i.e., “mixed is burnt” models;
- Finite rate chemistry assuming that the local in-equilibrium between diffusion and reaction is similar to the one observed in laminar flames, i.e., flamelet assumption;
- The treatment of molecular and heat transport separated from chemical reaction with the probability density function transport methods.

The following sections review turbulent diffusion combustion modeling with a foreword of chemical kinetics, followed by the overviews of the modeling approaches based on these three hypotheses. Examples using practical applications with these approaches are discussed to reveal the strengths and weaknesses of these approaches for CFD diffusion combustion modeling in a practical gas turbine combustor.

2.4.1 Finite-Rate Chemical Kinetics

Ideally, the chemical mechanism of the combustion of a fuel should be described with detailed chemical kinetics by including the elementary reactions of all species involved. Unfortunately, detailed chemistry kinetics descriptions of practical hydrocarbon fuels require hundreds of chemical species and thousands of reactions steps, which prohibits the implementation of detailed kinetics of chemical combustion in a CFD simulation due to the limitations of CPU power and memory storage. Therefore, the chemical mechanisms of reduced kinetics, one-step global reaction and quasi-global reaction are commonly applied for CFD combustion modeling.

As discussed by Jones and Whitelaw (1982), the one-step reaction can lead to errors up to three orders of magnitude in the evaluation of the mean quantities. Thus, it is important to minimize the number of species while retaining the essential features of the chemical kinetics based on the information desired for the simulation. Correa (1995) developed a reduced scheme starting from a multi-step scheme for high intensity turbulent flow. Montgomery et al (2000, 2001) employed an automated mechanism reduction process to generate reduced kinetics for a JP-8 fuel that could be employed in LES and RANS simulation of gas turbine combustion. Results revealed that the generated reduced kinetics yielded good comparisons to the predictions from detailed kinetics depending on the specific properties of the flowfield and corresponding operating conditions.

Since the reduced kinetics of hydrocarbon fuels is complex and not commonly known, CFD simulations of gas turbine combustion generally employ a simpler fuel to represent complex hydrocarbon fuels, such as the use of $C_{12}H_{26}$ to represent diesel fuel in the CFD simulation of gas turbine combustion conducted by Liever et al (1998). As will be discussed in the following section, the use of global step reaction and reduced kinetics is common practice for CFD combustion simulations with complex hydrocarbon fuels.

2.4.2 Eddy-Break-Up and Eddy Dissipation Model

In general, the solutions of the mean formation rates are determined from the Arrhenius expressions, as discussed in Turns (1995) and Mellor (1990), based on the chemical mechanisms describing the chemical reaction. The introduction of the Eddy-Break-Up Model (Spalding 1971) and the extended Eddy Dissipation Model (Magnussen and Hjertager 1976) provides closure for the mean reaction source term in turbulent reacting flows based on the intuitive argument that turbulent reaction is controlled by turbulence mixing rather than the finite-rate chemical kinetics. Therefore, computation of the chemical reaction rate based on the Arrhenius expression could be safely neglected.

Turbulence mixing can be viewed as the cascade process of the fuel-containing eddies and the oxidant-containing eddies from the integral scale down to the molecular scale, where chemical reaction occurs. Assuming the chemical reaction time scale is infinitely fast compared to the turbulence time scale, turbulent reaction is thus controlled by the cascade process, i.e., turbulence mixing control. For most combustion cases of hydrocarbon fuel in diffusion flames, the kinetic rate is usually higher than the turbulence mixing rate and combustion can be assumed mixing controlled, and the Eddy-Break-Up (EBU) type combustion models can be applied.

In the Eddy Dissipation model (EDM), the reaction rate is determined from the minimal value of the expressions as a function on the mass fraction of the reactants (fuel and oxidant) or product for species k in reaction r written as:

$$R_{k,r} = \nu_{k,r}' M_k A \rho \frac{\varepsilon}{k} \min_R \left(\frac{Y_R}{\nu_{R,r}' M_R} \right) \quad (2.4.1)$$

$$R_{k,r} = \nu_{k,r}' M_k A B \rho \frac{\varepsilon}{k} \frac{\sum_P Y_P}{\sum_j^N \nu_{k,r}'' M_k} \quad (2.4.2)$$

Where Y_P and Y_R are the mass fraction of any product P and reactant R respectively, ν is the stoichiometric coefficient, M is the molecular weight of species, and A and B are empirical modeling constants with the default value of 4.0 and 0.5 respectively (Magnussen and Hjertager 1976). These equations show that the combustion proceeds whenever turbulence is present ($k/\varepsilon > 0$), where k is the turbulence kinetic energy and ε is its dissipation rate.

2.4.3 Mixture Fraction Conserved Scalar Approach

The mixture fraction, f , is a normalized quantity such that its value is unity in the fuel stream and zero in the oxidant stream, which is written in terms of the atomic mass fraction as:

$$f = \frac{Z_i - Z_{i,ox}}{Z_{i,fuel} - Z_{i,ox}} \quad (2.4.3)$$

Where Z_i is the elemental mass fraction of element i , the subscript *ox* denotes the value at the oxidizer stream inlet and the subscript *fuel* denotes the value at the fuel stream inlet.

Under the assumption of equal diffusivities for all elements, $D_i = D$, all mixture fractions are equal irrespective of the element from which they are formed (Bilger 1989). As the atomic element is conserved in a chemical reaction, the species conservation equations can be reduced to the transport equations for a mixture fraction conserved scalar, and the modeling of the reaction source terms in the species equations is not required.

To model the turbulent diffusion flame, the transport equations of mean mixture fraction, $\bar{f}$, and its variance, $\overline{f'^2}$ are solved. Thermochemical properties are uniquely related to the predicted mixture fraction at each point in the flowfield to compute the instantaneous values of individual species mole fractions, density, and temperature. The calculations of thermochemical scalars are preprocessed and tabulated in a lookup table assuming infinitely fast chemistry and chemical equilibrium, therefore, species mole fractions and the flow properties can be computed from f by minimizing the Gibbs free energy (Kuo 1986). This functional relationship can be generalized as:

$$\phi_i = \phi_i(f) \quad (2.4.4)$$

where ϕ represents the instantaneous species mass fraction, density, or temperature.

In the determination of the time-averaged values of flow properties, $\bar{\phi}_i$, interaction between chemistry and turbulence can be accounted for with a presumed shape Probability Density Function (PDF), $p(f)$, written as:

$$\bar{\phi}_i = \int \phi_i(f) p(f) df \quad (2.4.5)$$

Among the various PDF functions that have been proposed, which have been discussed in the review of Jones and Whitelaw (1982), the β -function PDF is most widely used and agreed upon based on experimentation. As in the CFD combustion codes of Tolpadi et al (1998), and Adami and Martelli (2000), the β -PDF has been assumed. The dependence of mean scalar values to the prediction of $\bar{f}$, and $\overline{f'^2}$ is illustrated in Figure 2.1.

Figure 2.1. Lookup Table Concept (Anonym 2003)

2.4.4 Laminar Flamelet Model

Although the infinitely fast chemistry combustion models give an acceptable prediction for turbulent combustion flow, they impose drawbacks and limitations in the simulation for combustion flow where finite rate chemistry and in-equilibrium effects, such as the locally fuel rich condition, rich or lean blowout, and ignition, are becoming more important. The laminar flamelet model is a direct improvement of the mixture fraction conserved scalar approach through the introduction of the scalar dissipation rate, χ , to include the finite rate effect for local in-equilibrium due to aerodynamic strain in turbulent combustion flow. The theories of the flamelet model are reviewed extensively by Peters (2000).

The instantaneous scalar dissipation rate can be thought of as the diffusivity in mixture fraction space, where diffusivity is multiplied by the square of the gradient of mixture fraction (Peters 2000), defined as:

$$\chi = 2D|\nabla f|^2 \quad (2.4.6)$$

By adding the scalar dissipation rate, the functional relation $\phi(f, \chi)$ must be determined and tabulated to create a flamelet library, and the $p(f, \chi)$ joint PDF must be presumed. The $\phi(f, \chi)$ is generally tabulated from the solution of a counter-flow diffusion flame, where the complex chemistry reaction rate is reduced and described by two parameters, f and χ . The mixture fraction and its dissipation rate are assumed to be uncorrelated in most flamelet models, and the joint PDF can be determined with a presumed shape as:

$$p(f, \chi) \approx p(f) \cdot p(\chi) \quad (2.4.7)$$

2.4.5 PDF Transport Model

Instead of prescribing the shape of PDF to provide closure for turbulence mixing in combustion simulation, it is possible to construct the PDF by solving the transport equation for composition PDF or velocity-joint composition PDF. These methods have more advantages than the prescribed PDF because the transport equation of composition PDF for the thermo-chemical variables, species, temperature, and the velocity field statistics can be written to capture the effects of detailed chemistry and the interactions with turbulence.

The multidimensional assumed-shape PDF can be used to model finite rate kinetics of detailed chemistry by assuming statistical independence of the reaction progress variables, such as that employed by Repp et al (2002) and Klose et al (2000). Nonetheless, this method is impractical, since the prescriptions of PDF become very complex and problem dependent as discussed by Tolpadi et al (1997, 1997a).

As the PDF transport equation requires more independent variables than the typical mean flow equations, a numerical treatment, the Monte Carlo simulation (Pope 1990) is required for the PDF transport method. Tolpadi et al (1997, 1997a) presented a representative application of composition PDF in a CFD simulation for a practical gas turbine combustor. The applications of these combustion models in combustor modeling will be compared with previously discussed combustion models in the following section.

2.4.6 Comparisons between Different Combustion Models

The previously introduced combustion models are widely applied for CFD combustion modeling for gas turbine combustors. According to the assumptions about chemistry and the degree of complexity and sophistication, these combustion models are summarized in Table 2.1.

Table 2.1. Classifications of Combustion Models

Combustion Model	Chemistry Assumptions	Turbulence Closure
Eddy-Break-Up/ Eddy Dissipation	<ul style="list-style-type: none">• Infinitely Fast Chemistry• Neglected Chemical Reaction• Improvements with Finite Rate Chemistry and Extinction Model	Turbulence Mixing Time Scale: k/ϵ
Conserved Scalar Mixture Fraction Model with Presumed PDF	<ul style="list-style-type: none">• Infinitely Fast Chemistry• Equilibrium Chemistry Reaction	Presumed Shape PDF
Laminar Flamelet Model based on Mixture Fraction	<ul style="list-style-type: none">• Finite Rate Chemistry• Chemistry In-equilibrium	Presumed Shape PDF
PDF Transport Model	<ul style="list-style-type: none">• Finite Rate Chemistry• Account for Complex Chemistry and Turbulence Interaction Implicitly	Computed Composition Joint PDF with Monte Carlo Method

The various practical applications of these combustion models in the gas turbine combustor simulation have been reported in the literature with detail. The abilities and limitations of these models are widely understood based on theoretical studies as well as experimental validations for both prototypes and practical combustors.

As the Eddy-Break-Up type models replace the chemical time scale by the turbulence time scale based on a single global step chemical mechanism, these models are always criticized for the lack of physical representation and classified as out of date. It is also known that the empirical modeling constants in these models have to be tuned over a wide range to obtain reasonable results.

A study of modeling of a natural gas diffusion flame conducted by Ma et al (1999) and Islam and Hossain (1996), showed that the value of modeling constant, A , has to be changed from the value of 4.0 to 1.5 and 1.25 respectively to yield a reasonable prediction of the flowfield temperature to match the experimental data. An interesting work conducted by Brizuela and Bilger (1996) showed that a fuel-independent value of A can be derived as a function of the mixture fraction and its variance of the flow based on the assumption of fast chemistry.

To account for the shortcomings of these models, various modifications have been made to these models to improve the quality of predictions including the implementations of the multi-step chemical mechanism for hydrocarbon fuels combustions, and the inclusion of finite-rate kinetics in the calculation of mean reaction rate. There are various successful applications of these combustion models in gas turbine combustion modeling.

Gran et al (1994) modeled the influences the local extinction characteristic in combustion flow by extinction time scale in Eddy Dissipation combustion model. Tolpadi et al (1998) successfully implemented this concept in the axisymmetric diffusion flame modeling and show that the EDM with extinction time scale more closely agrees with experimental data relative to the EBU model for both flowfield properties and emission predictions. Another improvement includes the implementations of two-step or four-step global reaction mechanisms in this model, such as the modeling of methane combustion by Brink et al (2000).

From practical experiences using these models, as discussed in the literature, it showed that even reasonable predictions of the temperature flowfields can be obtained with the models based on infinitely fast reaction and equilibrium chemistry assumptions, the predictions of NO_x and CO emissions can be off by a magnitude since the chemical reactions are significant for the determination of emissions. However, reasonable predictions of the NO_x emission can be achieved with the post-processing method from the prior determined combustion flowfield as will be discussed later in this chapter.

Tolpadi et al (1998) showed that the conserved scalar with assumed shape PDF model yielded a superior performance in the prediction of temperature profiles and NO_x emissions compared to the two-step based Eddy-Break-Up and Eddy Dissipation models. Lau (1995), with the use of both the Eddy Dissipation implemented with four-step global mechanism and the transport PDF Monte Carlo model, showed that the later model yielded “outstanding results” compared to experimental data, with the EDM model giving a reasonable prediction of the overall combustion performance but with errors in orders of magnitude in emissions prediction.

As the models in the “infinitely fast chemistry” categories can not rigorously account for the turbulence chemistry interaction, these models are not readily extended to the modeling of slow solution reactions such as CO , soot formation, ignition, and extinction. However, the time dependent flamelet model is employed to study the unsteadiness in combustion such as extinction and re-ignition that was done by Pitsch et al (2003). The transport PDF method is proposed to give an accurate estimation of the emissions of CO and unburned hydrocarbon (UHC) by calculating chemical reaction with turbulence mixing simultaneously as discussed in Tolpadi et al (1997, 1997a). Nonetheless, the applications of these models are limited due to their complicated formulations and high computing requirements, and the prior knowledge of detailed chemistry.

Based on the above reviews, it can be concluded that:

Table 2.2. Applications of Diffusion Combustion Models

Combustion Simulations (Modeling Requirements)	Combustion Models
General Combustion Flowfield Estimation (Turbulent Reaction Interaction)	<ul style="list-style-type: none">• EBU/EDM• Prescribed PDF Approach• Flamelet Model• Transport PDF model
<i>CO</i> or <i>UHC</i> Emission Prediction (Detailed Chemical Kinetics and Instantaneous Turbulent Reaction)	<ul style="list-style-type: none">• Flamelet Model• PDF Transport Model• EDM With Kinetic Time Scale Enhancement
Extinction or Ignition Simulation (Detailed Chemical Kinetics and Instantaneous Turbulent Reaction)	<ul style="list-style-type: none">• Unsteady Flamelet Model• PDF Transport Model

2.5 Discrete Phase Model

The performance of diffusion gas turbine combustors is strongly influenced by the problems with the fuel injection, including the aerodynamics within the atomizer passage, formation of the liquid droplet via fuel filming, ligament formation and breakup, droplet dispersion, heat and mass transport, and fuel-air mixing.

For diffusion combustion simulation, the primary atomization of a liquid droplet is usually not included in the simulation, however, the injection of the droplet is treated as a fully atomized liquid fuel with spherical droplets, such as that employed in Tolpadi et al (2000), and Čížek and Jícha (2000). The modeling of fuel injection is done to predict droplets trajectory in a Lagrangian reference frame coupled with heat and mass transfer interaction with a continuous phase. For a more elaborate model, the droplet collisions and coalescence as well as the aerodynamic breakup can be employed such as that employed by Su and Zhou (1999). The Eulerian fuel injection model is also employed for combustion simulation, as Zarzalis et al (2002) and Klose et al (2000) demonstrated. Nonetheless, due to the limits of the scope of this review, only the more common Lagrangian approach will be discussed.

The trajectory motion of the fully atomized droplets is dependent on the particles inertia and aerodynamic drag force based on the particle solid-sphere law. Several expressions for drag coefficient, C_D , are available for the spherical drag law in literature, such as the expression of Wallis employed in Tolpadi (1995) and Zamuner et al (2002). In the model of Čížek and Jícha (2000), the hydrostatic lift that is calculated from the ambient pressure gradient is also accounted for in the trajectory motion of the droplet. Yet, many of the discrete phase models only account for aerodynamic drag as it is dominant in turbulent flow. For droplet size distribution, the Rosin-Rammler droplet distribution function is commonly employed in combustion simulation as discussed in Lefebvre (1999) and Mellor (1990). However, as discussed in Babinsky and Sojka (2002), the popularity of this function is primarily due to its simplicity rather than its validity in describing droplet size distributions in combustion field.

Heat and mass transfer with the continuous phase are governed by sequential heating and evaporation of the droplet assuming infinite conductivity of the droplet, i.e., constant droplet temperature. For a more advanced method, Tolpadi et al (1998) modeled droplets heating and evaporating simultaneously, however, infinite conductivity was still applied. The infinite conductivity of a droplet is justified with the droplet internal mixing at a high droplet Reynolds number as discussed in Zamuner et al (2002).

Droplet heating is generally governed by convection heat transfer, with the inclusion of radiation heat transfer rarely reported. The rate of vaporization is governed by gradient diffusion, with the flux of droplet vapor into the gas phase related to the gradient of the vapor concentration between the droplet surface and continuous phase. Since droplet surface vapor concentrations of complex fuels, such as kerosene and diesel, are difficult to determine, some models employ empirical correlation, such as the correlation by Spalding employed in Tolpadi (1995). The mass rate of droplets evaporation is contributed in the continuous phase conservation equation as a source term.

The effects of the turbulence dispersion could be included in the trajectory of the droplet via the stochastic eddy lifetime approach, such as that employed in Tolpadi (1995), Zamuner et al (2002), and Su and Zhou (1999). The interaction between the described discrete liquid phase and continuous phase is accomplished by solving the discrete and continuous phase equations alternately until the solutions in both phases have converged, as illustrated in Figure 2.2.

Figure 2.2. Coupling between Discrete Phase and Continuous Phase (Anonym 2003)

2.6 NO_x Predictions

The emissions from the combustion of hydrocarbon fuel include NO_x emissions, CO , and unburned hydrocarbon (UHC). NO_x , oxide of nitrogen, is an atmospheric pollutant that contributes to the formation of acid rain and photochemical smog, and the depletion of the ozone. With the increasing stringent regulations on the emission of NO_x , research for low emission gas turbine combustors has become one of the driving force of CFD combustion simulation (Eaton et al 1999).

As discussed in the previous section, the prediction of NO_x formation in gas turbine combustion has obtained a convincing level of accuracy with the various combustion models. Therefore, this section reviews its prediction methods.

Typically, NO_x emission primarily consists of nitric oxide (NO) with the significantly lower contribution from nitrogen dioxide (NO_2). Guo et al (2002) conducted a numerical investigation of the production of NO_2 , nevertheless, the formation is usually excluded in gas turbine combustor simulation.

The concentration of NO is generally much lower than the concentration of other species in the combustion flowfield. Its formation has negligible influence on the combustion reaction and the thermodynamic state of the flow. Therefore, the modeling of NO formation is commonly post-processed from the converged combustion flow calculation. With the flamelet combustion model, the instantaneous formation rate of NO can be obtained from the flamelet library and the corresponding mean formation rate can be obtained by the averaging process with prescribed PDF, such as the approach of Volkov et al (2001). However, this method disagrees with the post-flame formation mechanism of NO and the residence time scale for NO formation is irrelevant, as discussed by Held and Mongia (1998).

The formation of NO in diffusion combustion is governed mainly by the thermal or Zeldovich mechanism and the prompt or Fenimore mechanisms, with less significant contribution of fuel NO and NO re-burning. Thermal NO is formed by the oxidation of atmospheric nitrogen present in the air. Its formation rate is calculated by the extended Zeldovich mechanism based on the assumptions of the steady-state of N concentration and equilibrium or partial equilibrium between O and O_2 . Prompt NO_x is formed by the high-speed reaction of combustion. The actual formation involves series reaction of CH and CH_2 in the fuel (Turns 1995, Anonym 2003).

Thermal NO formation is typically concerned in the high temperature region of around 1900 K, where it contributes 60 % of its total NO . Prompt NO formation is important at lower temperatures around 1500 K where it contributes 65 % of its total NO (Lefebvre 1999). It was also shown that the formations of thermal and prompt NO are coupled (Ju and Niioka 1997), therefore, to predict accurately the rate of NO emission both mechanisms have to be considered.

In general, the predictions of NO emissions with the post-processing method in conjunction with the infinitely fast and equilibrium chemistry combustion models, and the turbulence mixing prescribed with the assumed shape PDF function make reasonable predictions of NO_x emissions (Tolpadi et al 1997).

2.7 Radiation Heat Transfer

Although the effect of radiation is important in the modeling of gas turbine combustion, the simulation of radiation heat transfer is generally neglected in CFD combustion simulation, such as Tolpadi (1995) and Liever et al (1998). The publications and literature on the theory and modeling of radiation heat transfer are plenty but the reports of practical application in CFD gas turbine combustion modeling is limited.

There are two difficulties associated in solving the radiative-transfer equation (RTE); knowledge of the spectral radiative properties involved in the high temperature gas and the efficient methods for solving the RTE. The common method for defining the radiative properties is the weighted-sum-of-gray-gas model (WSGGM). The discrete ordinates radiation model (DOM) and the discrete transfer radiation model (DTRM) are commonly applied for the calculation of radiation transfer (Viskanta 1998, Oran and Boris 2001).

2.8 Numerical Schemes

Advances in numerical techniques have benefited the application of CFD simulations for practical gas turbine combustors. This section reviews some of the commonly used numerical schemes, as described in Oran and Boris (2001), and Anonym (2003), for CFD combustion simulation.

CFD simulation of gas turbine combustors typically requires a 3-dimensional (3D) solid model to describe the complex geometry involved. Multi-block grids and the unstructured grids are of great interests in gas turbine combustor simulations with the high geometry flexibility and robustness in the meshing of the computational domain. As shown by Crocker et al (1999), using eleven multi-blocks allows the use of 80 000 grids to describe the combustor model from compressor diffuser exit to turbine inlet, whereas over a million grid sizes will be required if a single block grid is used.

Finite volume based techniques are employed to discretize the governing equations for individual computational grids, where it can be a staggered and unstaggered type grid. In a staggered grid, different variables (solutions of governing equations) are defined at different points on the grid such as the center, corner, or surface. In an unstaggered grid, all variables are defined at the same location.

The discretized systems of equations are linearized explicitly or implicitly based on the coupled or segregated solution methods to obtain a converged solution. The multigrid method, such as AMG (algebraic multigrid), is commonly applied to speed up the convergence. The SIMPLE (Patankar 1980), "Semi-Implicit Method for The Pressure Linked Equation", algorithm is employed for pressure-velocity correlation for a segregated solver to enforce mass conservation. Some recent publications also report the use of a SIMPLE-Consistent (SIMPLEC) algorithm (Vandoormaal and Raithby 1984) for faster convergence, such as Xia et al (1998).

The discretization schemes commonly used are the first order and second order upwind schemes, the QUICK scheme “Quadratic Up-Wind Interpolation for Convective Kinematics”, center different scheme, and even higher schemes such as the fourth order upwind employed by Ju and Niioka (1997). In general, higher order discretization schemes are more accurate, however they tend to result in longer computing time and are more prone to convergence problems.

2.9 Basis for Current Combustion Simulation

Based on the review of CFD simulations for gas turbine diffusion combustion, the methodology that will be employed for the current gas turbine combustion simulation is as follows:

- The application of a two equation turbulence model, specifically the $k-\varepsilon$ model, will be used for the gas turbine combustion simulation since other RANS turbulence models have not proven more accurate. LES provides attractive features, however, its application for a practical gas turbine system is only possible with massive increase of current computer speed and more mature development of sub-scale combustion models.
- The implementation of detailed chemistry mechanisms for practical hydrocarbon fuel combustion is prohibitive. Simulation of hydrocarbon combustion will be based on global reaction schemes, reduced kinetics, and the use of a simpler fuel.
- Combustion models with various levels of sophistication are available for diffusion combustion, which have achieved representative and qualitative simulation for turbulent combustion flow. It has been shown that for accurate emission prediction, the effect of chemical kinetics must be included in conjunction with turbulence closure. However, if extinction, ignition or other in-equilibrium chemical effects are not of interest, the combustion models based on infinitely fast reaction and equilibrium is economic and appropriate for practical combustion systems burning complex hydrocarbon fuels.
- Although the effect of radiation heat transfer is argued to be important for flowfield and emission prediction, its implementation in gas turbine combustion simulation is not widely employed due to the difficulties in obtaining details in the modeling parameters.

- For the prediction of NO_x emissions, knowing the importance of their formation mechanisms in a gas turbine combustor, both thermal NO and prompt NO are considered.
- Advances in numerical techniques have benefited the numerical modeling of gas turbine combustors in many ways. Flexibility of unstructured grids is an asset for complex geometry modeling, and the use of parallel processing has allowed the feasibility of CFD as a practical design tool.

The issues regarding the determinations of boundary conditions for combustor models for CFD simulation are not mentioned in the review. This will be discussed in a later chapter where related issues are addressed.

Chapter 3

Roll-Royce Allison 250 GT Engine

This thesis is based on the CFD modeling of a Rolls-Royce Allison gas turbine engine combustion system, which is being installed for combustion research activities. Easy accessibility of the engine combustion system makes it suitable for a gas turbine combustion test bed. As for the current project, the combustion system was disassembled from the engine to study the combustion flow system and to obtain the details dimensions to construct a representative computational combustor model for CFD simulation.

This chapter gives a brief introduction of the gas turbine engine and its combustion system, with information mainly obtained from Anonym (1999) unless otherwise specified.

3.1 Allison 250 Engine Specifications

The Allison 250 Gas Turbine Engine, also known by its military designation as T63, is one of the most successful helicopter turbo-shaft engines powering the Bell JetRanger, SeaRanger, and Agusta 206A. The specific model used in the current research is the Roll-Royce Allison 250 C20B gas turbine engine. The engine has a power output of 420 shp (313 kW) with a maximum shaft speed of 6016 rpm and a specific fuel consumption of 0.650 lb/shphr (395.38 mg/Whr).

The performance of the engine during sea level take-off operating conditions, which is obtained from Hendrick (1999), is summarized in Table 3.1. As will be discussed in Chapter 5, these operating parameters and engine performance information were adapted as the boundary conditions for the CFD combustion simulations in the current study.

Table 3.1. Engine Simulation Parameters at Take-Off Condition

Airflow rate	3.82 lb/s	1.733 kg/s
Fuel flow rate	0.0766 lb/s	0.035 kg/s
Power (take-off)	450 SHP	335 kW
Compressor exit temperature	1039 °R	577 K
Compressor exit pressure	116 psia	800 kPa
Combustor exit temperature	2430 °R	1350 K
Combustor exit pressure	113 psia	776 kPa

3.2 Engine Configuration and Combustion System

The Allison 250 is a twin spools engine with a single-can combustor located at the aft end of the engine for easy accessibility for liner, fuel nozzle and igniter maintenance or replacement during battlefield operations. This modular design of a combustion system not only makes the engine distinctive from other gas turbine engines in a similar category (where reversed flow combustion systems are mainly used), but it also makes it particularly suitable to be adapted as a combustor test bed.

As shown in Figure 3.1, the engine has an unique “back-to-front” combustion flow design. Air enters the engine through the compressor inlet and is compressed by six axial compressor stages and one centrifugal compressor stage. The compressor air is discharged into two ducts on both sides of the engine, which deliver the air into the single-can combustion section.

The combustion system consists of the outer casing and the combustion liner with the outlet facing the front of the engine. Air enters the combustor liner through holes in the liner dome and skin, mixed with fuel sprayed from the fuel nozzle mounted at the aft end of the engine, and combusted. Combustion air moves forward, expands through the two stage power turbine that is mounted in the mid-section of the engine, and exhausts through the twin ducts exhaust collector.

Figure 3.1. Allison 250 Engine Airflow (Adapted from Anonym 1999)

3.3 Combustor Liner Geometry

The single-can combustion liner of the Allison 250 engine is 23 cm in length and 15.45 cm in diameter at the outlet. The liner can be described by three zones, the dome-swirler zone, primary zone, and dilution zone, as shown in Figure 3.2

The dome-swirler zone consists of the mounting ports for the fuel injection nozzle and igniter, and the dome-swirler wall orifices. The primary zone starts with a wigglestrip cooling slot and 12 primary injection holes. A similar cooling slot is used on the dilution zone, followed by 14 dilution holes and 2 dilution holes. The details of the combustor liner geometry are demonstrated in Appendix A.

There are two symmetry plans that can be used to describe the combustor with half geometry to capture the layouts of these injection holes and the swirling flow inside the combustor. Nonetheless, it was decided to employ a full geometry to simulate the current combustor. The following chapter describes the construction of the 3D solid model of the combustor.

Figure 3.2. Allison 250 Gas Turbine Engine Combustion Liner

Chapter 4

Combustor Solid Model and Grid Generation

A 3D solid model has been built for the CFD combustion simulations of the Allison 250 combustor to capture the swirling flowfield and the multi-injection flows on the liner. The 3D model has been built with simplifications of the liner geometry, while retaining the important features on the liner and the combustion flowfield. The unstructured grid generation method has been used for the meshing of the model, as it is more robust and flexible, and can lend itself to the advance grid adaptive method for grid cell refinement. Combustor models with grid density of 296 000, 550 700, and 567 600 have been modeled to ensure that a grid independent solution is obtained.

4.1 Simplified Solid Model

To avoid using extremely high grid density to define the entire computational domain and retaining the presences of the swirling flows, circular dilution jets, and liner cooling scheme, the combustor model was built with the following simplifications:

- The model was built to simulate the internal flowfield of the combustion liner;
- Liner thickness was not included in the model;
- Complex dome-swirler and cooling slots flow path were simplified.

The outlined shape that describes the liner internal fluid domain was first constructed with CAD software, and imported into the FLUENT™ preprocessor Gambit™ software package (a geometry modeler and meshing tool) to set up the detailed geometries and boundary conditions, i.e., walls, dome swirled inlet, injection holes, cooling slots, and outlet.

At the dome-swirler, swirling air is injected into the combustion liner in different direction through the liner orifices and the louver flat plates, as shown in Figure 4.1 and Figure 4.2. For the first 3D full combustor model that was built for combustion modeling, the dome swirled flow injections were modeled with circular holes on the wall by specifying the tangential injection direction, as shown with the arrows in Figure 4.3. Instead of modeling the diffuser-like flow path of the wigglesstrip cooling slots, circumferential slots were used as the inlet boundaries of the cooling film injections. These cooling slots were divided into sections and specified as inlet boundaries and wall boundaries to model the injection pattern of the cooling films. All injections holes on the model were retained in a circular shape defined with 2D triangular grid.

Figure 4.1. Dome-Swirler Holes Distribution and Swirled Flow Direction

Figure 4.2. Dome-Swirler Louver Plates

Figure 4.3. Preliminary Combustor Solid Model

Figure 4.4. Simplified 3D Combustion Solid Model

Figure 4.5. Turbine Disk Shield at Combustor Outlet

The solid model was later refined to better simulate the inlet and outlet boundaries of the combustor. A 5 inch (12.7 cm) extension was also added to simulate a combustion test rig to allow investigations of the evolution of the combustion flow and the mixing of the diffusion flame at the combustion downstream, as shown in Figure 4.4.

For the later solid model, the dome wall orifices were replaced by rectangular “cut-out” to simulate the injections of the swirled flow that generated by the louver plates. The cooling slots were simplified to continuous circumferential slots, as this seems to yield better descriptions for the inlet boundaries of the cooling films from the wigglesstrip slots. A fuel nozzle port was added to the solid model for more accurate specification of the position of the fuel injection. The last refinement to the model was the addition of a turbine disk protecting shield at the outlet, as shown in Figure 4.5. This modification was crucial to simulate the realistic outflow boundary condition of the combustor.

4.2 Unstructured Grid Generation

The FLUENT™ preprocessor Gambit™ package was used for the grid generation of the combustor model. The meshing of the solid model with 5 inch extension is illustrated as an overview of the grid generation technique that is employed in the current study.

Unstructured grids were used for meshing the solid model because this technique is easier to be applied in defining the geometry of the combustor and allows the use of grid adaption for grid density refinement. The method avoids the difficulties in defining a complex geometry with structured grids, such as circular orifices and curvatures of the combustor.

The meshing of the combustor solid model started with “line mesh” by sectioning the edges of the surfaces to ensure significant features of the geometry were defined (Figure 4.6 A). The surfaces of the solid model were then meshed with 2D triangular grids (Figure 4.6 B). The aspect ratio of these 2D triangular grids were maintained in a reasonable range to ensure uniform 3D pyramid cells can be generated for the entire volume. The final mesh of the combustor solid model is presented in Figure 4.7. This demonstrated that the higher mesh density has been generated at the region of the dome-swirler and near the liner injections, where strong interaction and mixing of the flow occurred.

After the set up of the computational domain for the combustor solid model, it is required to specify the boundary conditions and interior fluid properties of the computational volumes for combustion simulations. This is addressed in the following chapter.

Figure 4.6. Meshing of Combustor Solid Model: A. Line Mesh, B. Face Mesh

Figure 4.7. Final Mesh of the Combustor Solid Model

Chapter 5

Boundary Conditions Specification

For spray combustion modeling, it is required to specify the boundary conditions for the continuous phase (the gaseous phase) and the discrete phase (the liquid droplets). In this chapter, the specifications of the boundary conditions and fluid properties of the two fluid phases in the computational domain as described previously are detailed.

A Discrete Phase Model (DPM) with 3D cone injection has been employed for the fuel injection of the two working fuels, kerosene and diesel, that were used to simulate the combustion performance of the gas turbine engine. The properties of kerosene were kept as in the FLUENT™ database, while the properties of the diesel fuel were specified with the information obtained from the literature.

For the modeling of the continuous phase, both constant value fluid properties and detailed value, as function of temperature, have been used in defining the interior fluid properties of the computational domain. Without the experimental data for the combustor airflow distribution, the boundary conditions for the combustion simulation were estimated based on the engine performing information given in the literature.

The following will first cover the boundary conditions for the DPM. The definition of the combustor interior flow properties and the estimation of the boundary conditions for the continuous phase then are discussed.

5.1 Discrete Phase Model Boundary Condition

The standard atomizer for the Allison 250 gas turbine combustor is a dual-orifice pressure-swirl atomizer with the primary orifice used for fuel atomization during ignition, and the secondary orifice supplying the bulk of the fuel for higher power operation of the engine. The specification of the fuel injection was adapted from the experimental work of Naegelli et al (1991), who employed the same combustor for their fuel atomization study.

5.1.1 Liquid Fuel Properties

The default properties of kerosene fuel in the FLUENT™ database (Anonym 2003) were used to simulate the combustion of kerosene fuel. These properties were then modified based on the diesel fuel properties obtained from Odgers and Kretschmer (1986) to simulate the diesel fuel combustion. The liquid phase properties of these fuels are summarized in Table 5.1.

Table 5.1. Liquid Phase Properties of Kerosene and Diesel Fuel

	Kerosene	Diesel
Density ρ (kg/m ³)	780	840
Specific Heat c_p (J/kgK)	2090	1930
Thermal Conductivity k (W/mK)	0.149	0.134
Latent Heat L (J/kg)	226 000	228 000
Vaporization Temperature T_{vap} (K)	341	341
Average Boiling Temperature T_B (K)	477	538
Binary Diffusivity D (m ² /s)	3.79×10^{-6}	3.79×10^{-6}
Average Saturation Vapor Pressure $P_{saturated}$ (Pa)	1329	1400

These properties are significant in the simulation of the discrete phase model. As they control the heating and evaporation rate of the liquid droplets, they also control the contributions of the mass source and energy source to the continuous phase. Nevertheless, the use of constant values for these properties will be sufficient since a constant liquid droplet temperature has been assumed for the discrete phase model that has been employed in the current study.

5.1.2 Discrete Phase Injection Initial Point Properties

The modeling of the pressure-swirl atomizer in the current study was simplified to a 3D hollow cone fuel injection model specified with the injection position and axis (x , y , z), nozzle inner radius (r), and angle of injection (θ) as shown in Figure 5.1. The fuel injection was assumed to be fully atomized into spherical droplets without modeling the formation of stream ligament and droplet break-up.

Figure 5.1. Cone Injection for 3D Hollow Fuel Spray (Anonym 2003)

The origin of fuel injection was positioned at the injection port that was shown previously in Figure 4.4, with an orifice radius of 1 mm, and an injection angle of 45° . The initial point properties of the injection of the fuel stream were specified with inlet velocity, droplet temperature and diameter, and fuel flow rate.

The initial velocity of the fuel droplet was estimated with the equation suggested by Mellor (1990) as:

$$u = \sqrt{\frac{2\Delta P}{\rho}} \quad (5.1.1)$$

where ΔP is the nozzle differential pressure with a value of 862 kPa (Naegeli et al 1991), and ρ is the density of the fuel at the fuel injection temperature of 300 K (Naegeli et al 1991).

The initial conditions of the cone injection of kerosene and diesel fuel with the fuel flow rate of 0.035 kg/s are specified with the estimated inlet velocity of 47 m/s and 45 m/s respectively. The droplet size distributions of the spray are not modeled in the study, the constant droplet diameter of 50 μm were employed, which is the mean diameter measured by Naegeli et al (1991). The initial boundary conditions of the discrete phase model are summarized in Table 5.2.

Table 5.2. Discrete Phase Model Initial Conditions

	Kerosene	Diesel
Temperature, T (K)	300	300
Density, ρ (kg/m ³)	780	840
Fuel flow rate (kg/s)	0.035	0.035
Velocity, u (m/s)	47	45
Radius, r (m)	0.0005	0.0005
Droplet Diameter, (μm)	50	50
Injection angle, θ (degree)	45	45

5.2 Continuous Flow Boundary Conditions

5.2.1 Combustor Interior Fluid Properties

The air and fuel mixture properties inside the computational domain for combustion simulations were defined according to the mixing law given in Anonym (2003) as summarized in Table 5.3.

Table 5.3. Definition of Fuel-Air Mixture Properties

	Kerosene-Air/Diesel-Air Mixture Properties
Density ρ (kg/m ³)	Volume weight mixing law, $\rho = \frac{1}{\sum_k Y_k / \rho_k}$
Specific Heat c_p (kJ/kgK)	Mixing law, $c_p = \sum_k Y_k c_{p,k}$
Thermal Conductivity k (W/mK)	Mass weight mixing law, $k = \sum_k Y_k k_k$
Viscosity μ (kg/ms)	Mass weight mixing law, $\mu = \sum_k Y_k \mu_k$

The specifications of the properties of the air, which include the density, thermal conductivity, specific heat capacity, and viscosity of O_2 , N_2 , and CO_2 , were based on the constant values as given in the FLUENT™ database and further defined with detailed values based on the piecewise-linear functions of temperature obtained from Çengel (2003). The two different methods for the definition of the air properties were used to investigate the impact of using detailed fluid properties on the accuracy of combustion simulations.

The properties of the vapor kerosene fuel, $C_{12}H_{23}$, were taken from the FLUENT™ material database, and the properties of the diesel fuel, $C_{10.8}H_{18.7}$, were adapted from Turns (1996). The vapor phase properties of these fuels are summarized in Table 5.4.

Table 5.4. Vapor Phase Properties of Kerosene and Diesel Fuel

	Kerosene	Diesel
Density ρ (kg/m ³)	7.1	7.1
Specific Heat c_p (kJ/kgK)	2571	Piecewise- Linear Function
Thermal Conductivity k (W/mK)	0.0178	0.0178
Viscosity μ (kg/ms)	7.0×10^{-6}	7.0×10^{-6}
Molecular Weight M (kg/kmol)	167.31	148.6
Standard State Enthalpy h_o (J/kgmol)	-250 000 000	-1 218 000
Standard State Entropy S_o (J/kgmolK)	0	0
Reference Temperature T_{ref} (K)	298.15	298.15

The specific heat, c_p , of vapor diesel was specified by a piecewise linear function with the values obtained from the curve fit data given in Turns (1996) as:

$$c_p (J/kgK) = \frac{4184(-9.1063 + 246.97\theta - 143.74\theta^2 + 32.329\theta^3 + 0.0518\theta^{-2})}{148.6}$$

where $\theta = T/1000$, T is the temperature with the units in Kelvin (K). Since there is no reliable source for the other vapor properties of the diesel fuel, the properties of kerosene fuel as given in the FLUENT™ database were employed.

It was realized that the thermal properties of vapor fuel are a function of the combustion temperature, the use of constant properties of vapor fuel will have minor effect on the accuracy of the flowfield predictions. However, the detailed definition of the properties of the air is more significant since the overall air fuel ratio of the current combustion flow is rather high with a value about 50.

5.2.2 Estimations of Continuous Flow Boundary Conditions

The boundary conditions at the various liner inlets, such as turbulence characteristics, injection angle, pressure distribution around the liner, etc., are usually assumed or estimated using 1D flow analysis without detailed experimental measurements, such as the one-dimensional external flow code used by AlliedSignal (Liever et al 1998). The difference between the current combustor airflow configuration and conventional coaxial liner external and internal flow configuration has precluded the use of empirical 1D analysis, therefore the boundary conditions of the combustor liner for the CFD combustion simulation are estimated based on the known engine operating parameters from Hendrick (1999).

The estimations of the airflow distribution of the combustion zone is based on the assumption that the pressure is uniformly distributed around the combustor liner with the compressor discharged stagnation pressure. The assumption is obtained from the design criteria for a compressor diffuser where “the discharged air pressure is fully recovered and the pressure is uniformly distributed around the combustor liner” as discussed in Lefebvre (1999).

5.2.2.1 Dome Swirled Flow Prediction

At the dome-swirler, air enters the liner through the 3-holed and 6-holed dome orifices and redirects by the flat-pressed louver plates, which introduce the opposite direction swirled flows into the primary zone, as shown previously in Figure 4.1 and Figure 4.2. To model the 3 mm gaps between the dome wall and louver plates requires extremely fine grid to describe the geometry, which would result in an unreasonable high grid density for the entire combustor model. Therefore, a rectangular computational volume with the detailed section of the dome-swirler that consists of a row of six orifices with two louver plates was modeled separately from the whole combustor to predict the distribution of airflow from the dome, as shown in Figure 5.2.

Figure 5.2. Dome-Swirl Model

Figure 5.3. Dome Swirled Flow Prediction

The average mass flow rates from the five injection planes of the model, as shown in Figure 5.3, were predicted to provide an estimation for the dome swirled flow injection boundary condition for the full CFD combustor simulations. The estimation was accomplished with the $k-\varepsilon$ turbulence model with the assigned pressure inlet, pressure outlet, and wall boundary conditions as shown in Figure 5.2.

The volume of the computational model and the grid density were increased to ensure wall effect independence, to allow the grid density independent results to be obtained. Both first order and second order discretization schemes were employed in the simulations, as shown in Table 5.5.

Table 5.5. Grid Independent Study of the Dome-Swirler Model

Case	Volume ($x \times y \times z$) (cm ³)	Grid Cells	Discretization Scheme
1	13 × 10 × 10	521 498	1 st order
2			2 nd order
3	13 × 10 × 10	852 505	1 st order
4			2 nd order
5	20 × 13 × 15	668 249	1 st order
6			2 nd order

It is shown that the models with larger volumes yield no significant difference in the results, thus the airflow rates predicted from case 4 with a volume of 13 × 10 × 10 and 852 505 grid cells, given in Table 5.6, are employed as the swirled flow rate in the combustion simulation.

Table 5.6. Dome-Swirler Airflow Distribution

	Dome Swirled Flow Rate (kg/s)
Plane 1	0.00150
Plane 2	0.00475
Plane 3	0.00164
Plane 4	0.00475
Plane 5	0.00150

5.2.2.2 Liner Flow Distribution

Based on the assumption of the uniformly distributed total pressure around the combustor liner, the inlet boundaries of the combustor model were specified with compressor discharged stagnation pressure of 699 kPa and temperature of 577 K with flow direction normal to the inlet. The specification of the combustor outlet boundary condition requires the static pressure at the combustor outlet. Since only the stagnation pressure of 675 kPa at the combustor outlet can be obtained from the available information, the static pressure was estimated with a trial-and-error method based on a non-reacting flow simulation using the $k-\varepsilon$ model, “cold-flow” simulation. To meet the combustor total outlet gauge pressure of 675 kPa, the static pressure of 641 kPa was obtained from the iterative solution of the “cold-flow” simulation.

The specification of the boundary conditions for the CFD combustion simulations are summarized in Table 5.7.

Table 5.7. Boundary Conditions Specification

Boundary Conditions	Definition	Specified Values
Dome swirled flow injection	Mass flow inlet	As predicted previously
Cooling slots	Total Pressure Inlet	699 kPa, 577 K
Primary zone dilution holes	Total Pressure Inlet	699 kPa, 577 K
Dilution zone dilution holes	Total Pressure Inlet	699 kPa, 577 K
Outflow	Static Pressure	641 kPa

The flow split around the combustion zone was further estimated using the Eddy Dissipation combustion model. The mass flow rates around the combustion zone predicted with these two methods are similar, as summarized in Table 5.8. It should be noted that the mass flow rate at the dome-swirler zone was predicted uncoupled from the whole geometry as discussed in the previous section.

Table 5.8. Liner Airflow Split

	Airflow rate (kg/s) Cold Flow Model	Airflow rate (kg/s) Combustion Model
Dome-Swirler Zone	0.131	0.131
Primary Zone Cooling Slot	0.196	0.186
Primary Zone Injection Holes	0.381	0.361
Dilution Zone Cooling Slot	0.268	0.256
Dilution Zone Injection Holes	0.610	0.577
Total Mass Flow Rate	1.587	1.512

The predicted mass flow distributions are further justified in comparison to conventional design parameters from literature (Mellor 1990), as shown in Figure 5.4. For a total engine mass flow rate of 1.733 kg/s, the cold flow model predicted 92 % of the airflow through the combustor, while the Eddy Dissipation Model predicted 87 %.

The predicted liner airflow distributions and the predicted swirled flow distributions are employed as the boundary conditions for the CFD combustion simulation in the current study. These estimations are sufficient to provide reasonable boundary conditions for the current CFD combustion simulation, until more reliable resources about the airflow split of the current are available or the fully-couple liner annulus and liner internal flowfield simulation are performed.

Figure 5.4. Comparison of Predicted Combustor Liner Airflow to Conventional Designs

5.3 Summary of Continuous Phase Boundary Conditions

The current CFD combustion simulation is to model the performance of the Allison 250 gas turbine engine combustion system under the engine take-off operating condition as adapted from Hendrick (1999) with kerosene and diesel fuel. These two working fuels were employed to simulate the operation of the combustor, considering the engine will be operating with diesel fuel after the set up of the combustor test bed.

Airflow distributions around the combustor liner were predicted based on the engine performance parameters, and the results of the simulations as discussed in section 5.2.2 were applied as the boundary conditions for the CFD simulation. This is summarized in Table 5.9.

Table 5.9. Boundary Conditions for CFD Simulations

Mass Flow Inlet Boundary Conditions	Airflow Rate (kg/s)	Number of Injections
Swirler Plan 1 and 5	0.00150	24
Swirler Plan 2 and 4	0.00475	18
Swirler Plan 3	0.00164	6
Primary Zone Cooling Slot	0.187	1
Primary Injection Holes 1	0.0339	6
Primary Injection Holes 2	0.0263	6
Dilution Zone Cooling Slot	0.256	1
Dilution Injection Holes 1	0.189	2
Dilution Injection Holes 2	0.0143	14
Pressure Outlet		
Outlet Static Gauge Pressure	641 000 (Pa)	

As the simulation was uncoupled from the full combustor, the effects of the liner walls and the neighboring flow were not accounted for in the predicted flow rate. Even so, the predictions provide a reasonable dome airflow injection distribution in different directions that generate the swirling flow in the primary combustion zone.

Fully coupled internal and external combustor liner models with detailed geometries of the dome orifices and guide plates could be used to obtain a more accurate estimation of the swirled flow distribution, such as that suggested by Karki et al (1992), McGuirk and Spencer (2000), and Crocker et al (1999).

However, there are associated difficulties that have to be resolved in order for fully coupled internal and external combustion flow to be modeled. They include:

- The complicated geometry of the liner annulus, which consists of various contraction and diffusion cross sectional areas, makes it difficult to obtain the dimensions and to model with the CFD;
- The diffuser discharged airflow parameters are unknown, and the estimates for the airflow distribution initiating from the compressor discharge involves additional assumptions, where the accuracy of improvement is not guaranteed;
- Current computer resources limit the simulation of the extremely fine grid density that is required to describe the fully coupled complex geometry. This difficulty should be partly resolved with recently available workstations with better performance than those used for this analysis (discuss in the later chapter).

Chapter 6

CFD Combustion Simulations and Discussions

In this chapter, the detailed CFD simulations of Allison 250 gas turbine engine combustion flowfield with the commercial CFD solver, FLUENT 6™, are discussed. The combustor solid model that was meshed with the computational grid cells and specified with the predicted boundary conditions as discussed previously was employed for the CFD simulations.

The discussions in this chapter are arranged as:

- Grid independent study;
- Specification of turbulence characteristics with the $k-\varepsilon$ model;
- Predictions of temperature distribution with the infinitely fast chemistry combustion models, i.e., the Eddy Dissipation Model and the mixture fraction conserved scalar approach with presumed PDF;
- Discrete phase model trajectory and the interaction with the combustion flowfield;
- Differences in flowfield prediction between the $k-\varepsilon$ and RSM turbulence models;
- Numerical schemes and convergence difficulties;

- Computational efficiency with parallel processing;
- Liner wall temperature estimations;
- NO_x emission predictions.

The results of the simulations are examined to study the details of the flowfield inside the combustor and validate the assumptions made in the simulations by comparing the results against the literature. The limitations and advantages of the different turbulence combustion models are evaluated. Furthermore, important combustor design information, which includes the liner wall temperature and NO_x emissions, is obtained from the simulations.

6.1 Grid Independent Study

Two grid adaption methods in the FLUENT 6.1™ solver were used to refine the grid density of the combustor model, the volume adaption and the boundary adaption. The grid density of the entire computational volume was increased with the volume adaption to ensure no significant difference in combustion flowfield predictions was obtained with global refinement of the grid density. Subsequently, the grid density at the inlet boundaries of the computational domain was increased with the boundary grid adaption to ensure the grid density in this region was fine enough to capture the important flowfield interactions between liner injection flows and combustion main flow. The grid cells of the combustor model with grid adaption refinement are summarized in Table 6.1.

Table 6.1. Grid Density Refinements with Grid Adaptions

Cell Information	Prior Adaption	Volume Adaption	Volume and Boundary Adaption
Nodes	60 281	157 432	163 186
Faces	613 141	1 218 759	1 257 791
Cells	296 016	550 732	567 602
Mesh Name	cell000	cell001	cell002

The flowfield predictions were conducted with the $k-\varepsilon$ turbulence model and the Eddy Dissipation combustion model with first order discretization. Figure 6.2 shows the temperature profiles obtained at the mid-section of the 5-inch extension as demonstrated in Figure 6.1. Note that the symbols that appear in the figures indicate the data obtained from numerical simulations, and this is applied to the others figures that are presented in this thesis. The results of the simulations show that the error associated with numerical diffusion is minimized with the lowest grid density as the results of the predictions are essentially the same. Therefore, it can be concluded that the grid density independent solution is obtained with the grid cells employed.

Figure 6.1. Predictions at 5-inches Extension Mid-section: Rake 1 and Rake 2

Figure 6.2. Predicted Temperature Profiles with Different Grid Density

6.2 Turbulence Specification

The k - ε turbulence model with standard wall function improvement (Launder and Spalding 1972) was applied for turbulence modeling in the current study. As demonstrated in the literature review, the model is widely used for CFD combustion simulation because the model is computationally economic, numerically stable, and has acceptable accuracy for many classes of turbulent flow. To justify the conclusion drawn from Chapter 2, stating that the potential accuracy of applying other RANS models for combustion flow simulation is not realized in spite of the penalty in computing time, a trial simulation with the RSM turbulence model has been performed to investigate the impact of using this turbulence model compared to the k - ε RANS model in the later section.

Characteristics of turbulence boundary conditions are described with turbulence intensity, I , and turbulence length scale, l . The turbulence intensity is defined as the ratio of the velocity fluctuation to the mean velocity as:

$$I = \frac{u'}{u_{avg}} \quad (6.2.1)$$

Even though turbulence intensity of 10 % is typically used to simulate the fully developed turbulence flow in combustion simulation, the turbulence intensity as high as 15 %-18 % at the combustor outlet was reported by Barringer et al (2002). To study the effects of turbulence intensity on the CFD combustion flowfield predictions, turbulence intensity of 5 %, 10 %, 15 %, and 18 % have been specified at the inlet and outlet boundary conditions. The investigations were done using the EDM combustion model with the diesel fuel and constant fluid properties.

Figure 6.3. Effects of Turbulence Intensity to Combustion Simulation

As shown in Figure 6.3, the predicted temperature profiles, at the mid section of the 5-inches extension as in Figure 6.1, become uniform with higher turbulence intensity, whereas an undesired pattern factor is predicted with a turbulence intensity of 5 % (15). This reveals the requirements for the high turbulence injection flow in combustor design.

This study also demonstrated that the prediction of mixing of the flowfield is influenced by the specifications of turbulence intensity with the $k-\epsilon$ combustion model. This is contrary to the study of Ma et al (1999) who found that the predicted flowfields were essentially similar with turbulence intensity between 5 to 10 %. As the combustor model employed in their study consisted of 2D coaxial flow with much simpler geometry compared to the complicated mixing scheme of the current combustor, the effect of turbulence intensity is less significant.

The differences in temperature profiles with the higher in turbulence intensity is rather insignificant, therefore, the turbulence intensity of 10 % is justified to describe the fully developed turbulent flow in the combustor.

The turbulence length scale is a physical quantity related to the size of the energy-containing large eddy in turbulent flows. For a fully developed internal flow, the turbulence length scale is defined by its relation to the approximation of the physical length as (Anonym 2003):

$$l = 0.07L \quad (6.2.2)$$

The hydraulic diameter for the liner annulus has been used as the physical length scale, which is defined as:

$$L = 2(r_o - r_i) \quad (6.2.3)$$

where r_o is radius of the combustor casing and r_i is the liner external radius, measured at the combustor outlet as 17 cm and 15.45 cm respectively. As it is generally accepted that the turbulence length scale is closely related to the physical length scale, as discussed in Barringer et al (2002), this relationship was employed for all the CFD combustion simulations.

6.3 Combustion Flow Modeling

The EDM and the mixture fraction conserved scalar approach with presumed shape PDF were employed in the combustion modeling. The combustion with kerosene fuel was simulated with the EDM, while, the combustion of the diesel fuel was simulated with both combustion models.

6.3.1 Eddy Dissipation Combustion Model

The Eddy Dissipation Model that is based on the assumption of infinitely fast chemistry was employed frequently in the current study, as the model is robust and numerically stable. The model has been used extensively in the preliminary study of the combustion simulations, such as the grid independent study, and the investigation between kerosene and diesel fuel combustion.

Knowing the shortcomings of this model, as discussed in the literature review, various modifications have been made to the model to investigate the improvement in the prediction quality including the tuning of the modeling parameter, A , and the implementations of kinetics rate and two step global reaction.

The value of A was lowered from the value of 4 to 1.5 as suggested in the work of Ma et al (1999). Kinetics rate was implemented based on the Arrhenius modeling parameters for kerosene fuel as given in Anonym (2003). For the single-step and two-step global reaction of diesel fuel, the reactions are written as:

and

6.3.2 Conserved Scalar Approach with Prescribed PDF Combustion Model

The PDF model is frequently incorporated for the CFD diffusion combustion simulation of a practical gas turbine combustion system. This model is also based on infinitely fast chemistry assumptions as in the EDM model, however, the effect of chemistry is included with the assumption of equilibrium chemistry system.

As mentioned previously, only the combustion of the diesel fuel with the PDF model was conducted in the research. The lookup table for diesel fuel combustion was prepared with the FLUENT 6™ package preprocessor, *PrePDF*. Two different methods were used for the definitions of the diesel fuel, the ultimate analysis fuel components and the empirically defined fuel based on the atomic fraction of the fuel.

The ultimate analysis of the diesel is obtained from Odgers and Kretschmer (1986), given that the diesel fuel contains 86 % carbon and 14 % hydrogen in mass fraction. The empirically definition of diesel fuel is based on the chemistry composition of $C_{10.8}H_{18.7}$ given in Turns (1996). In preparing the lookup table, 12 species were included for the ultimate analysis of diesel fuel, and 13 species were included for the empirically defined diesel fuel, as further detailed in Appendix B.

For turbulence closure, the β -function PDF was employed, with the shape of the PDF defined as a function of $\bar{f}$, and $\overline{f'^2}$. This function was commonly employed for its good agreement with experimental data as discussed in the literature review.

6.3.3 Velocity Flowfield

The simulations of the flowfields inside the combustor based on the $k-\varepsilon$ turbulence model with the different combustion models are essentially the same. Figure 6.4 shows the velocity flowfield of a symmetry plane of the combustion zone predicted with the $k-\varepsilon$ model and PDF model with empirically defined diesel fuel.

High axial recirculation flow is found in the primary zone and diminished in the dilution zone. It is clearly seen that the injections in the primary combustion zone generated substantial mixing with the flow upstream, whereas the injections in the dilution zone flow toward the exit of the combustor without generating high axial recirculation. The velocity of the flow at combustor outlet is increased with the converging nozzle formed between the turbine disk protecting shield and the liner wall to provide high energy through the turbine expansion.

The velocity flowfield inside the combustor was compared with the results from the literature to verify the validity of the simulations. Figure 6.5 shows the flowfields inside three can combustors, Figure 6.5 A and B are adapted from the works of Zamuner et al (2002), and Adami and Martelli (2000), and Figure 6.5 C shows the flow pattern inside the current combustor. The combustor in Figure 6.5 A has an injection at the mid section, and the other two combustors have injections at both the primary zone and the dilution zone. The formations of axial recirculation flow are observed in both combustors. The circulation zone in the first combustor is created by the injection flow in the mid section, whereas, the circulation zones in the other two combustors are created by the injections at the primary zone while the injections in the dilution zone of these combustors have not created strong recirculation. The comparison of these flow patterns have revealed the similarities of flowfield inside a combustor, therefore, have suggested the validity of the current simulations.

Figure 6.4. Velocity Vectors of Combustion Zone

Figure 6.5. Comparisons of Combustor Flowfields: A. Zamuner et al (2002), B. Adami and Martelli (2000), C. Current Combustor

6.3.4 Kerosene and Diesel Combustion

Instead of using simple fuel with the simpler and more accessible chemistry reaction data, the kerosene and diesel fuels were employed in the current study to simulate the operating conditions of the Allison 250 combustor considering diesel fuel will be used after the set up of the experiment setup.

Combustions of the kerosene fuel and diesel fuel have been simulated with the Eddy Dissipation combustion model and the $k-\varepsilon$ turbulence model. The constant fluid properties have been used in the investigation, except that the heat capacity, c_p , of the vapor of the diesel fuel is defined as a polynomial function of temperature. This method has also been used to investigate the effects of turbulence intensities in previous section.

The differences of the temperature distributions in the combustor based on the kerosene and diesel fuel are relatively insignificant. As shown in Figure 6.6, the combustion zones with both fuels are similar except that the burning zone with diesel fuel combustion is more confined and the temperature has been diluted more by the cold flow from the dilution jets.

The rates of combustion reaction based on these fuel were expected to be similar in the primary zone because similar reaction parameters and fuel properties were used. Nonetheless, the more accurate definition of the c_p value for diesel fuel resulted in the more realistic temperature distributions inside the combustor.

The investigation showed that the accuracy of the flowfield prediction is based on the accuracy of the specifications of the fuel properties especially in the reaction zone. Also showed in Figure 6.6 is that the over predicted maximum temperature of 3100 K. As will be showed in the following section, the predicted maximum temperature is more realistic compared to the adiabatic temperature of the fuel with the detailed definition of the fluid properties.

Figure 6.6. Kerosene and Diesel Combustion Temperature Distributions

6.3.5 Temperature Distribution in Combustor

The temperature distribution inside the Allison 250 combustor with detailed specifications of fluid properties is showed in Figure 6.7. The prediction was based on the $k-\epsilon$ turbulence model and the PDF combustion model with empirically defined diesel fuel. The effect of liner wall heat transfer and the dispersion of the discrete phase were not accounted for in this simulation, these are discussed in later sections.

Several interesting phenomena about the combustion reaction and mixing of the flow inside the combustor were observed:

- the injection jets and the wall cooling films are clearly visible;
- the combustion zone is confined to the core of the flowfield;
- the combustion zone with the maximum temperature occurs slightly downstream of the primary zone indicating full combustion of fuel;
- the liner jets in the dilution zone mix with the upstream combustion flow and separate the hot stream into two;
- incomplete swirl mixing in the dilution zone resulted in the uneven temperature distribution at the combustor outlet.

The following section shows the temperature distributions in the combustor predicted with the other combustion models.

Figure 6.7. Combustion Zone Temperature Distribution

6.3.6 Temperature Distributions Predicted with Different Combustion Models

The temperature flowfields inside the combustor (Plane 1 and Plane 2 in Figure 6.7) predicted with the different combustion models are illustrated in Figure 6.8 and Figure 6.9. The four flowfields on the top are based on the EDM combustion models and the bottom two flowfields were predicted using the prescribed PDF approach with the ultimate analysis and empirically defined diesel fuel respectively. The maximum temperatures and the average combustor outlet temperatures corresponding to these models are summarized in Table 6.2.

The temperature distributions inside the combustor predicted with these combustion models show noticeable differences in the size of the burning zones and the maximum combustion temperatures. The differences of these predictions are closely related to the assumptions involved in these combustion models. By comparing the results of these models to the observations from the literature, the validities of these simulations can be evaluated.

Table 6.2. Maximum Temperature and Mass Weighted Average Outlet Temperature Predicted with Different Combustion Models

Combustion Models	Maximum Temperature (K)	Mass Weight Average Combustor Outlet Temperature (K)
EDM	2552	1419
EDM (with $A = 1.5$)	2430	1416
EDM (chemical kinetic)	2600	1424
EDM (Two Steps Reaction)	2169	1032
PDF (Empirical Defined Fuel)	2255	1446
PDF (Ultimate Fuel Analysis)	2268	1420

**Figure 6.8. Predicted Temperature Distributions with Different Combustion Models:
Plane 1**

**Figure 6.9. Predicted Temperature Distributions with Different Combustion Models:
Plane 2**

As can be seen from the results of the simulations, the EDM model has over predicted the size of the reaction zone with the combustion zone occurring very close to the spray. The predicted maximum temperature is higher than the adiabatic flame temperature of 2478 K, which was estimated with the software available from Gordon and McBride (1976), based on $C_{12}H_{26(l)}$ at the inlet temperature of 577 K and the equivalence ratio of 1.05. These observations agree with the numerical findings of Zarzalis et al (2002), who found that the high fuel consumption rate of the EDM model leads to an attached reaction zone. As the turbulence mixing rate is high in the primary zone with the strongly swirled flow, there was a predicted high reaction rate and high temperature in this region.

For the PDF model, the complete reaction of the fuel occurred downstream of the primary zone. Since the reaction of the PDF model is based on chemistry equilibrium, and the effects of dissociation are included in the equilibrium calculations, the maximum temperature is lower compared to the predictions of the EDM models. The spreading of the combustion to the dilution zone could be the result of the deficits in the estimated airflow distributions, nonetheless, the predicted combustion flowfield based on the PDF combustion model resulted in a realistic combustion flowfield inside the gas turbine combustor.

Changing the reaction constant A to the lower value of 1.5 actually improved the simulation with the predicted maximum temperature more closely (within 2 %) corresponding to the adiabatic temperature, and the maximum temperature zone that is more confined. The predictions with the inclusion of the Arrhenius finite rate and the two-step reaction in the EDM are unreasonable. The former has over predicted the maximum flame temperature; it is even higher than the one predicted from the EDM model, and the predicted reaction zone has attached closer to the fuel injection. The later, on the other hand, estimated lower maximum flame temperature and the combustor outlet temperature were under predicted by 20 %.

The discrepancies of these predictions are mainly due to the uncertainties in the reaction constants applied for Arrhenius calculation and the use of the two-step global reaction that has not been verified for a complex hydrocarbon fuel. The global reaction step employed in the Eddy-Break-Up type models as discussed in Chapter 2 is mostly based on simple fuel, such as methane. The employed global reaction steps are usually validated to give a reasonable representation of the chemistry reaction of the particular fuel.

If compared carefully, the pattern of the temperature distribution predicted by the EDM and the modified EDM model with A equal to 1.5 to the pattern predicted by the PDF with empirically defined fuel, it can be observed that the combustion in the primary zone is similar except that the temperature is lower. This is based on the assumption of infinitely fast chemistry, i.e. “mixed and burned”, however, the later also accounted for chemistry equilibrium and the effect dissociation, which lowered the maximum temperature. Since the diesel fuel was defined ultimately with the carbon to hydrogen mass fraction of six in the other PDF approach, it is less accurate than the empirically defined diesel fuel to represent the complex composition of the fuel.

Both models, except the EDM model with the two-step global reaction, estimated the outlet temperature reasonably well (within 5 %) compared to the given combustor exit temperature of 1350 K (Hendrick 1999). Based on this observation, the conclusion drawn from the literature review stating that the infinitely fast chemistry models are capable to predict the combustion outlet temperature reasonable well is confirmed.

Nonetheless, it is difficult to quantify the validity of these models experimentally based on test rig measurement at the combustor outlet since both models predicted the outlet temperatures in a close range. Both the intrusive and laser-based experimental techniques are limited by various practical difficulties in accessing the flowfield inside the combustor primary zone during the operation of the engine. Therefore, comparing the predicted maximum temperatures to the adiabatic temperature of the fuel with similar carbon level concluded that the current CFD combustion simulations provided representative predictions of the temperature distributions inside the combustor.

6.4 Fuel Injection Trajectory and Interaction with Continuous Phase

The interaction between the liquid fuel injection and the continuous phase was accounted for by trajectory tracking of the discrete droplets using spherical drag law in a Lagrangian frame of reference. The injection was specified with 100 discrete points, and a discrete phase calculation was performed for every 20 continuous iterations. Sequential droplet heating, evaporating and boiling is employed to determine mass source to the continuous flow domains assuming infinite conductivity of droplet temperature.

The predicted trajectories of the discrete fuel injection are shown in Figure 6.10, Figure 6.10 A shows the calculated trajectories with the EDM combustion model and Figure 6.10 B shows the calculated trajectories with the PDF combustion model. Full evaporation of the liquid droplets is indicated by the end of the trajectories. In Figure 6.10 A, full evaporation of the droplets happened in the primary zone, and Figure 6.10 B shows that the droplets traveled further downstream to the dilution zone before fully evaporating. These observations are consistent with the distributions of temperature flowfields inside the combustor, where the combustion zone based on the EDM model is confined in the primary zone with the higher combustion rate predicted by the EDM model, while the combustion is spread out into the dilution zone based on the PDF model.

The trajectories in the dome zone are well defined into the specified cone shape injection, and sprayed into the swirling flow downstream of the combustor. It can be seen that the cone spray in Figure 6.10 A is drawn toward the liner wall by the swirling flow, while the cone spray in Figure 6.10 B is unaltered. The spray is hardly influenced by the gas flow near the atomizer region since the momentum of the spray is high with the large fuel droplet and high injection velocity. The smaller droplets in the EDM combustion flowfield (because of the higher evaporation rate) explains why the injection is drawn by the swirling flow outward to the liner. These numerical observations agree with the numerical study of two-phase flow conducted by Zamuner et al (2002).

The greater influence from the continuous flow to the trajectory with smaller droplets (lower momentum) can be clearly seen in Figure 6.10 A, where the discrete phase trajectories were distorted and entrained into the core region by the primary zone injection. The common observation that the discrete streams with smaller momentum tend to flow into core region of the combustor can also be seen in Figure 6.10 B, where most of the trajectories are entrained by the swirled flow into the core region of the combustion zone with some trajectories flowing along the outer region near the liner wall.

Figure 6.10. Discrete Phase Fuel Injection Trajectory

The stochastic tracking of the droplets was investigated with 10 representative stochastic tries for every discrete injection. With the specified 100 discrete injections, the injection of the fuel is thus represented with a total of 1000 trajectories. Figure 6.11 shows the stochastic tracking with 10 number of tries from a single discrete point of the injection with the PDF combustion model. The effect of the “random walk” can be clearly seen with the 10 additional trajectories from the discrete point. It can also be seen that most of the trajectories are flowing into the core zone of the combustor, which confirms the observations previously discussed.

Despite the fact that the injection is represented with 900 additional trajectories, there is no noticeable change to the overall temperature distributions inside the combustion zone. The distributions of the discrete phase mass source and momentum source are improved slightly with the stochastic injection model. However, the difference is only noticeable in the primary zone and the effects to the entire combustion zone is rather insignificant. This suggested that 100 discrete injections is sufficient to represent the mixing between the continuous phase and discrete phase.

Figure 6.11. Stochastic Tracking of Liquid Fuel Injection

6.5 RSM and k - ϵ Turbulence Models

The combustion simulation of the current combustor was further investigated with Reynolds Stress turbulence model based on the PDF combustion model. The results of the investigations were compared with the prediction of the k - ϵ model to study the difference between these two RANS turbulence models. Contrary to the common findings as discussed in the literature review, the predicted velocity flowfields are very similar, however, the predicted temperature flowfields at the combustor outlet are different.

As shown in Figure 6.12, the upstream temperature distributions predicted by the two turbulence models are similar. Since the swirling flow is strong in the combustor upstream region, the isotropic assumption of the k - ϵ model is valid. The difference between the predictions is noticed at the downstream location near the combustor outlet. The flowfield predicted by the RSM model shows the continuous mixing between the cold dilution streams and the main combustion stream toward the outlet of the combustor at the core of the combustor. However, the k - ϵ model has not captured this mixing phenomena, the mixing of the flows was under predicted. These findings agree with the investigations of non-reacting flow conducted by Xia et al (1998), and Maidhof and Janicka (1993) as discussed in Chapter 2, where the k - ϵ model tends to under predict the strength of swirl flow.

From the temperature profiles at the mid section of the test rig (Figure 6.13), the temperature predicted with the RSM model is about 80 K lower in the core region. Theoretically, the RSM turbulence model takes into account the anisotropic effect of turbulent flow by modeling the Reynolds Stress directly will give better predictions of flowfield with high swirl. This numerical observation, unlike the investigations inside the combustion zone, can be validated with experimental measurements by installing a combustion test rig at the outlet of the combustor.

Figure 6.12. Temperature Distributions in Combustor Predicted with RSM and $k-\epsilon$ Turbulence Models

Figure 6.13. Temperature Profiles at Test Rig Mid-Section Predicted with RSM and $k-\epsilon$ Models

6.6 Numerical Schemes and Convergence Difficulties

The finite volume discretization scheme using a non-staggered grid with the variables defined at grid center was employed in the current study. The segregated method was employed for solving the system of governing equations, and the SIMPLE algorithm was employed for pressure-velocity correlation.

Solution convergences were monitored using the residuals of the governing equations. For single precision accuracy, the residual criteria for the converged solution are specified as shown in Table 6.3.

Table 6.3. Residual Convergence Criteria

Governing Equations	Convergence Criterion
Continuity	1×10^{-3}
Velocity Components	1×10^{-3}
Combustion Species	1×10^{-3}
Turbulence	1×10^{-3}
Energy	1×10^{-6}
<i>NO</i> Emission	1×10^{-6}

Both first order and second order upwind discretizations were investigated with the k - ε turbulence model and EDM combustion model. These simulations were based on diesel combustion with constant fluid properties that was used to investigate the differences between diesel and kerosene fuel combustion as discussed in section 6.3. As shown in Figure 6.14, the temperature profiles at the mid-section of the extension that were calculated based on the first order and second order upwind schemes yield a maximum difference in temperature of around 50 K. The overall trend of the profiles seem to agree with each other.

Figure 6.14. Predictions Based on 1st Order and 2nd Order Discretizations

Convergence difficulties were encountered for both first order and second order upwind discretizations. The under-relaxation factors were applied to control the change of solutions during the monitoring of the convergence history. In general, low values of the under-relaxation factors could be used to obtain stable convergences, however, this would result in longer iteration times.

As a compromise between high calculation times and convergence difficulties, under-relaxation values were refined during iteration. As illustrated in Figure 6.15, conservative values of under-relaxation factors were used at the beginning of the iteration, and the under-relaxation factors were changed to lower values as convergence difficulty is encountered, i.e., either there is fluctuation in the residual value or no further decrease in the residual values can be obtained.

Figure 6.15. Convergence History of EDM Two-Step Diesel Combustion

The convergence difficulties occurred while solving the energy equation, DPM interaction, the k and ϵ equations, and the CO_2 species for the two-step reaction EDM model. Under-relaxation factors of approximately 0.3 and 0.5 are sufficient to achieve convergence for DPM interaction and the k and ϵ equation respectively. For the energy equation and CO_2 species, an under-relaxation factor of 0.5 is sufficient to achieve residual values of 1×10^{-5} and 1×10^{-2} . However, a lower value is required to satisfy the specified residual values of 1×10^{-6} and 1×10^{-3} . In some cases, the solution is assumed to converge if the residual value is within one order of magnitude of the specified criteria and further decrease in the value of residual cannot be achieved within 50 to 100 extra iterations.

6.7 Computational Efficiency with Parallel Processing

Most of the CFD simulations were done using Pentium III dual processor systems until recently when two dual XEON™ processor SuperWorkstation become available.

These new computers provided the opportunity to study the computational efficiency of the CFD combustion simulations using parallel processing. The simulations were based on the combustor model with 567 600 grid cells and first order discretization. Each workstation was set up to allow for four virtual parallel processes with two processors.

Figure 6.16 shows the approximate reduction in computing time for the simulation with the $k-\varepsilon$ turbulence model and PDF combustion model. The total reduction of 70 % in computing time (average 2.5 minutes per 10 iterations) can be achieved with the parallel processing with two systems. Approximately 400 iterations are required to obtain a converged solution, therefore, a complete simulation can be preformed within two hours.

The computing times required for the $k-\varepsilon$ model with the EDM combustion model are approximately 10 % faster than the PDF combustion method. For the simulation with the RSM turbulence model and PDF combustion model, convergence can be achieved within 750 iterations with the 24 % additional computing time, therefore, the converged solution can be obtained within approximately four hours of simulation time.

Figure 6.16. Computing Time Reduction with Parallel Processing

6.8 Liner Wall Temperature Estimation with Convective Heat Transfer

The CFD simulations discussed previously assumed a combustor liner wall boundary condition that was adiabatic. The effect of including convection heat transfer of the combustor liner was investigated based on the PDF combustion model with the empirically defined diesel fuel. The following wall boundary conditions (Table 6.4) were specified in the combustor model for the heat transfer calculation of the liner wall.

Table 6.4. Convective Heat Transfer at Liner Wall

Free Stream Temperature $T_{free\ stream}$ (K)	577
Wall Thickness t (m)	0.002
Hastelloy Density ρ (kg/m ³)	9000
Hastelloy Specific Heat c_p (J/kgK)	460
Hastelloy Conductivity k (W/mK)	18.7
Heat Transfer Coefficient h (W/m ² K)	530

The compressor exit temperature (Hendrick 1999) was used for the liner external free stream temperature. The thickness of the combustor liner was measured to be approximately 2 mm, and the properties of Hastelloy X was obtained from Anonym (2003a). The method suggested by Çengel (2003) for the tube annulus was applied to estimate the convective heat transfer coefficient, h , of the combustor liner wall. The details of the determination of the heat transfer coefficient can be found in Appendix C.

The result of the simulation shows that the convective heat transfer on the liner wall has rather insignificant influences on the combustion flowfield. As shown in Figure 6.17, the temperature profiles at the test rig mid-section in the core region of the combustion flow are essentially the same with a maximum difference of 20 K near the wall. The average temperature at the combustor outlet is 1328 K compared to 1446 K when using the adiabatic wall condition.

The liner wall temperature distributions beginning from the primary zone to the combustor outlet that were predicted with and without the effects of convective heat transfer are showed in Figure 6.18. These temperatures are measured along the sides of the combustor without the dilution jets where the temperature of the flowfield is higher (Plane 1). The effects of the cooling films can be clearly seen from the predicted temperature distributions. The temperature of the wall is substantially lower in the beginning section of the primary zone and dilution zone with the cooling films injection, and begins to increase downstream. The wall temperature is about 250 K lower in the dilution zone section and 500 K lower in the rig section with the effects of the convective heat transfer.

This prediction is important in combustor design to ensure there is no apparent of local hot spots on the liner wall, which will shorten the service life of the combustor liner. For the present project, the predicted liner wall temperature provides useful information for the design of an experimental test rig that is planned to be installed on the engine. The predicted maximum temperature of the liner wall is within the acceptable operating range of 1100 K (Lefebvre 1999) for combustor liner material. This ensures that additional cooling is not necessary for the test rig. The simulations clearly show the importance of including convective heat transfer when predicting liner wall temperature.

Figure 6.17. Temperature of Combustion Flow at Test Rig Mid-Section

Figure 6.18. Liner Wall Temperature Predictions

6.9 NO_x Emission Estimation

The NO_x emission prediction is post-processed with the predicted combustion flowfield, therefore, the accuracy is dependant on the solutions of the combustion flowfield obtained from the combustion flow simulations. Since the effects of the chemistry and dissociation were included in the PDF combustion model, the NO_x emission prediction was based on the solution of the combustion flow simulation based on the PDF model with empirically defined diesel fuel.

Both of the thermal and prompt NO formation mechanisms were included in the estimation of NO_x emission. The dependence of the formation rate of the thermal NO on the equilibrium or partial equilibrium concentrations of O atom and OH radical, as discussed in Correa 1992 and Anonym 2003, were both investigated. For the prompt NO calculation that was based on the method of De Soete (Anonym 2003), CH_4 was defined as fuel species with the overall equivalence ratio of 0.33.

The predicted NO quantities at the combustor exit are summarized in Table 6.5. The conversion of the expression in parts per million by volume (ppmv) referenced to 15 % oxygen on dry basic can be found in Appendix D.

Table 6.5. NO Predictions at Combustor Outlet

	Mass Fraction	ppmv (dry)	Ppmv (corrected to 15 % O_2)
Thermal NO	1.25×10^{-4}	126	35.9
Thermal and Prompt NO	1.25×10^{-4}	126	35.9
Thermal and Prompt NO (partial equilibrium O and OH)	1.56×10^{-4}	157	44.7
Thermal and Prompt NO (partial equilibrium O)	1.56×10^{-4}	157	44.7

It can be seen that the total NO emission contributed from the prompt mechanism is rather insignificant, suggesting that the thermal mechanism is dominant in the formation of NO . As discussed by Correa (1992), such phenomena is the result of the presence of stoichiometric interfaces and high temperature in the non-premixed combustion. The inclusion of the partial equilibrium effects of O atom is more significant than the OH radical for thermal NO mechanism.

The predicted NO emission in the current study is in a reasonable range compared to the NO emission of diesel fuel with similar operating conditions as given in Lefebvre (1999), as shown in Figure 6.19. With the overall equivalent ratio of about 0.33, the measurement of the NO_x is in the range of 50 ppmv.

Figure 6.19. NO Formation for Diesel Fuel (Adapted from Lefebvre 1999)

Chapter 7

Conclusions and Recommendations for Future Work

7.1 Introduction

The combustion flowfield inside a can-type gas turbine combustor has been simulated numerically with a three dimensional model with detailed representation of the combustor geometries and boundary conditions. The predicted combustion flowfields were validated against the results from the literature, as expected, there are limitations and inaccuracies present in the modeling. Nonetheless, the results have confirmed the validity of the infinitely fast chemistry turbulence combustion models in conjunction with the Lagrangian discrete fuel injection model for non-premixed combustion simulation.

Various issues concerning the CFD simulation for gas turbine combustion have been investigated in the current study, conclusions are drawn upon these investigations, and recommendations are suggested for future research.

7.2 Conclusions

The conclusions of the current study of CFD combustion simulation of the Allison 250 gas turbine combustor are summarized as follows:

- The use of unstructured grids is essential. The important features and detailed geometries of the combustor could be retained in meshing the solid model, and the mesh density could be refined conveniently with grid adaption methods. From the grid independent study, it was concluded that the grid density of 296 000 is sufficient to obtain a grid independent solution.
- The investigation of the effects of turbulence intensity with the $k-\varepsilon$ model revealed that the requirements of high turbulence at the inlet boundary is critical for combustor design to obtain a desired pattern factor at the combustor outflow. It has also been shown that the turbulence intensity of 10 % is sufficient to describe the turbulent flow.
- Comparisons between the predictions with the $k-\varepsilon$ and RSM models confirmed the assumption of isotropic turbulence in the primary zone as the two models predicted a similar flow pattern in this zone. However, the difference in combustion flow predicted at the downstream location near the combustor outlet is a subject for further investigation.
- The predicted flowfield inside the combustor is in good qualitative agreement with the results from the literature.
- In the combustion simulations, it has been shown that detailed specifications of the fluid properties are critical in combustion simulations as the use of constant value fluid property results in unrealistic temperature prediction.

- The infinitely fast chemistry combustion models are able to provide qualitative predictions of the combustion outlet temperature. Comparisons between the flowfields predicted with the different combustion models, especially the Eddy Dissipation combustion model, revealed the tendency of the models to over predict combustion temperature, especially within the combustion zone.
- The improvements to the EDM as described in the literature have been investigated. It showed that the tuning of the modeling constant is useful to yield prediction that is more in line with known data. Nonetheless, the improvements with the implementations of Arrhenius reaction rate and two-step global reaction are not realized. The reasons for the disagreement could be the application of the complex working fuel and the complex combustor injections system in the current simulations. Nonetheless, various important combustion flow features have been observed that are in qualitative agreement with the investigations in the literature and are closely related to the assumptions made in these models.
- The predicted trajectory and evaporation of the liquid droplets are closely related to the observations in the literature, where the larger droplets with high momentum remained in their trajectory and the smaller droplets were drawn by the continuous stream. The stochastic modeling of the droplets trajectory yielded no significant improvement over the representation of fuel spray injection with 100 discrete injections.
- To accurately estimate the liner wall temperature, the effect of convective heat transfer is required. In this study, the predicted liner wall temperature is below the allowable temperature of the material only when accounting for convective heat transfer.
- Also shown in this study is that the prediction of NO_x emission is dominated by the thermal NO mechanism, and the effect of partial equilibrium O atom is significant in the prediction of NO emission.

7.3 Recommendations for Future Work

The simulations of the combustor not only provided details of the combustion flowfield, but also gave useful information such as the liner wall temperature and NO_x emission, both of which are critical for combustor design.

Although not included in the current study, it would be interesting to include the effect of radiation heat transfer from the combustion zone on the liner wall temperature. Furthermore, the spray size distribution could be varied to study its impact on the temperature flowfield and emission predictions.

With the recently available computing resources, a fully coupled combustor simulation from the compressor discharge to the combustor outlet should be attempted to model the coupled effects of the combustor annulus and combustion zone. The investigations of the combustor with the more advanced combustion models can be realized if a detailed chemistry of diesel fuel is available.

It would be useful to install a combustion test rig at the exit of the combustor and thermocouples along the combustion liner to measure the downstream temperature and pressure, and the liner wall temperature to verify the predictions of the CFD modeling.

References

- Adami P and Martelli F. Computational of 3D Turbulent Not-Premixed Reacting Flows Using an Implicit Unstructured Solver. ASME 2000-GT-0147, 2000.
- Anonymous. FLUENT 6.1 User Manual. FLUENT Inc., 2003.
- Anonymous. Hastelloy X Technical Data. High Temps Metals, Inc., 2003a.
<http://www.hightempmetals.com/techdata/hitempHastXdata.php4> [April 23, 2003]
- Anonymous. Model 250-C20, -C20B, -C20F, -C20J, -C20W, -C20S Operation and Maintenance Manual. Rolls-Royce Allison Publication Department, Publication No. 10W2, 6th ed, 3rd Revision, 1999.
- Anonymous. The Jet Engine. Rolls-Royce, Derby, 1986.
- Babinsky E and Sojka PE. Modeling Drop Size Distributions. Progress in Energy and Combustion Science 28, P. 303-329, 2002.
- Barringer MD, Richard OT, Walter JP, Stitzel SM and Thole KA. Flow Field Simulation of a Gas Turbine Combustor. Transaction of the ASME, Vol. 124, 2002.
- Bilger RW. Future Progress in Turbulent Combustion Research. Progress in Energy and Combustion Science 26, P. 367-380, 2000.
- Bilger RW. Turbulent Diffusion Flames. Annual Reviews Fluid Mechanics, P. 101-135, 1989.
- Brink A, Mueller C, Kilpinen P and Hupa M. Possibilities and Limitations of the Eddy-Break-Up Model. Combustion and Flame, Vol. 123, 2000.
- Brizuela EA and Bilger RW. On the Eddy Break-Up Coefficient. Combustion and Flame, Vol. 104, No.1, P. 208-212, 1996.
- Carl M, Behrendt T, Fleing C, Frodermann M, Heinze J, Hassa C, Meier U, Wolff-Gassmann D, Hohmann S. and Zarzalis N. Experimental and Numerical Investigation of a Planar Combustor Sector at Realistic Operating Conditions. ASME Journal of Engineering for Gas Turbines and Power, Vol. 123, 2001.

- Çengel YA. Heat Transfer: A Practical Approach. McGraw-Hill, New York, 2nd, 2003.
- Chang SL and Zhou CQ. Benefits of CFD Simulation: Computational Fluid Dynamic Simulation as an Aid to System Design and Use. Catalysis and Reactions, 1999.
- Čížek P and Jícha M. Re-Designing Annular Combustor of APU for Better Air Management and Spray Development. ASME 2000-GT-4, 2000.
- Correa SM. A Review of NO_x Formation under Gas-Turbine Combustion Conditions. Combustion Science and Technology, Vol. 87, P. 329-362, 1992.
- Correa SM. Assessment of a Three-Variable Reduced Kinetics Scheme in Prescribed Turbulence. Journal of Propulsion and Power, 1995.
- Crocker DS, Nickolaus D and Smith CE. CFD Modeling Of a Gas Turbine Combustor Form Compressor Exit to Turbine Inlet. ASME Journal of Engineering for Gas Turbine and Power, Vol. 121, 1999.
- De Champlain A, Tsogo J and Kretschmer D. Numerical Simulation of A Gas Turbine Combustor. University Laval, Quebec, 1994.
- Eaton AM, Smoot LD, Hill SC and Eatough CN. Components, Formulations, Solutions, Evaluation, and Application of Comprehensive Combustion Models. Progress in Energy and Combustion Science 25, P. 387-436, 1999.
- Forkel H and Janicka J. Large Eddy Simulation of a Turbulent Hydrogen Diffusion Flame Flow. Turbulence and Combustion 65, P. 163-175, 2000.
- Gran IR, Melaaen MC and Magnussen BF. Numerical Simulation of Local Extinction Effects in Turbulent Combustor Flows of Methane and Air. Process of 25th International Symposium on Combustion, P. 1283-1291, 1994.
- Gordon S and McBride BJ. Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonations. NASA, SP-273, Mar, 1976.
- Gulati A, Tolpadi A, and Vandeusen G. Effect of Dilution Air on the Scalar Flowfield at Combustor Sector Exit. Journal of Propulsion and Power, Vol. 11, No. 6, 1995.
- Guo H., Liu F., Smallwood J., and Matovic D. Numerical Simulation of NO_x Formation in a Model Gas Turbine Combustor. American Flame Research Committee, 2002.

- Held TJ and Mongia HC. Application of a Partially Premixed Laminar Flamelet Model to a Low Emissions Gas Turbine Combustor. ASME 1998 Gas Turbine Paper, 1998.
- Hendrick PC. User Experience with the Allison 250-C20R/1 Turboshift on the Belgian Army Agusta A109. RTO AVT Symposium-Ottawa, 1999.
- Islam AKMS and Hossain M. Prediction of Local Species Concentration of a Turbulent Diffusion Combustion in an Axisymmetric Furnace. Journal of Energy Heat and Mass Transfer, 18, P. 141-161, 1996.
- Jones WP and Whitelaw JH. Calculation Methods for Reacting Turbulent Flows: A Review. Combustion and Flame 48, P. 1-26, 1982.
- Jones WP. Large Eddy Simulation of Turbulent Combustion Process. Computer Physics Communication 147, P. 533-537, 2002.
- Ju Y and Niioka T. Computation of NO_x Emission of a Methane-Air Diffusion Flame in a Two-Dimensional Laminar Jet with Detailed Chemistry. Combustion Theory Modeling 1, 1997.
- Karki KC, Oechsle VL and Mongia HC. A Computational Procedure for Diffuser-Combustor Flow Interaction Analysis. ASME Journal of Engineering for Gas Turbine and Power, Vol. 114, 1992.
- Klose G, Schmehl R, Meier G, Meier R, Koch R, Witting S, Hettel M and Leuckel W. Evaluation Of Advanced Two-Phase Flow And Combustion Models For Predicting Low Emission Combustors. ASME 2000-GT-133, 2000.
- Kuo KK. Principles of Combustion. John Wiley and Sons, New York, 1986.
- Lau JHW. Comparison of PDF and Eddy Dissipation Combustion Models Applied To Propane Jet Flame. Combustion and Flame 102, P. 209-215, 1995.
- Launder BE and Spalding DB, Lectures in Mathematical Models of Turbulence. Academic Press, London, England, 1972.
- Lefebvre AH. Gas Turbine Combustion. McGraw-Hill, Toronto, 1983.

- Lefebvre AH. Gas Turbine Combustion. Taylor and Francis, Philadelphia, 2nd, 1999.
- Libby PA (Editor) and Williams FA (Editor). Turbulent Reacting Flows. Springer-Verlag, Berlin, 1980.
- Libby PA (Editor) and Williams FA (Editor). Turbulent Reacting Flows. Academic Press, 1994.
- Liever PA, Smith CE, Myers GD, Hernandez L and Griffith T. CFD Assessment of a Wet, Low- NO_x Combustion System for a 3MW-Class Industrial Gas Turbine. ASME 1998-GT-292, 1998.
- Ma CY, Mahmud T, Gaskell PH and Hampartsoumian E. Numerical Predictions of a Turbulent Diffusion Flame in a Cylindrical Combustor Using Eddy Dissipation and Flamelet Combustion Models. Proc Instn Mech Engrs, Vol. 213, 1999.
- Maidhof S and Janicka J. Numerical Modeling of Turbine Combustion Chambers. VDI Berichte – Verein Deutscher Ingenieure, N. 1090, P. 129, 1993.
- Magnussen BF and Hjertager BH. On Mathematical Models of Turbulent Combustion with Special Emphasis on Soot Formation and Combustion. 16th International Symposium on Combustion, The Combustion Institute, 1976.
- McGuirk JJ and Spencer A. Coupled and Uncoupled CFD Prediction of the Characteristics of Jets from Combustor Air Admission Ports. ASME 2000-GT-0125, 2000.
- Mellor AM. Design of Modern Turbine Combustors. Academic Press, San Diego, 1990.
- Mongia HC. Combustion Modeling In Design Process Applications and Future Direction. AIAA, 1993.
- Montgomery CJ, Cannon SM, Mawid MA and Sekar B. Reduced Chemical Kinetic Mechanisms for JP-8 Combustion. AIAA 2002-0336, 2000.
- Montgomery CJ, Swensen DA, Harding TV and Bockelie MJ. Automated Creation and Testing Of Reduced Chemical Kinetic Mechanisms. AIAA 2001-3418, 2001.
- Naegeli DW, Dodge LG and Moses CA. The Effect of Fuel Properties and Atomization on Low Temperature Ignition in Gas Turbine Combustors. AGARD, 1991.

- Odgers J and Kretschmer D. Gas Turbine Fuels and Their Influence on Combustion. Abacus Press, Cambridge, 1986.
- Oran ES and Boris JP. Numerical Simulation of Reactive Flow. Cambridge University Press, Cambridge, 2nd, 2001.
- Patankar SV. Numerical Heat Transfer and Fluid Flow. McGraw-Hill, New York, 1980.
- Peters N. Turbulent Combustion. Cambridge University Press, New York, 2000.
- Pitsch H. Extended Flamelet Model for LES of Non-Premixed Combustion. Center of Turbulence Research, Annual Research Briefs, 2000
- Pitsch H, Cha CM and Fedotov S. Flamelet Modeling of Non-Premixed Turbulent Combustion with Local Extinction and Re-Ignition. Combustion Theory Modeling 7, P. 317-332, 2003.
- Pope SB. Computations of Turbulent Combustion: Progress and Challenges. Process of 23rd Int. Symposium on Combustion. P. 591-612, 1990.
- Repp S, Sadiki A, Schneider C, Hinz A, Landefeld T and Janicka J. Prediction of Swirling Confined Diffusion Flame with a Monte Carlo and a Presumed-PDF-Model. International Journal of Heat and Mass Transfer 45, P. 1271-1285, 2002.
- Saravanamuttoo HHH, Rogers GFC and Cohen H. Gas Turbine Theory. Prentice Hall, 5th ed., New York, 2001.
- Spalart P and Allmaras S. A One-Equation Turbulence Model for Aerodynamic Flows. Technical Report AIAA-92-0439, AIAA, 1992.
- Spalding DB. Development of the Eddy-Break-Up Model of Turbulent Combustion. 16th Symposium of Combustion, 1971.
- Spalding DB. The Use of CFD in the Design and Development of Gas Turbine Combustors. CHAM, 1999.
- Su K and Zhou CQ. Numerical Study of Spray Parametric Effects on Gas Turbine Combustion Performance. Intl. Mech. Eng. Congress and Exposition, Heat Transfer Division, HTD-Vol. XX, 1999.

- Tolpadi AK, Aggarwal SK and Mongia HC. An Accurate and Affordable Spray Model for Gas Turbine Combustor Design. Proceedings of ASME TURBOEXPO 2000, 2000-GT-128, 2000.
- Tolpadi AK, Correa SM, Burrus DL and Mongia HC. Monte Carlo Probability Function Method for Gas Turbine Combustor Flowfield Predictions. Journal of Propulsion and Power, Vol. 13, No. 2, 1997.
- Tolpadi AK, Hu IZ, Correa SM and Burrus DL. Coupled Lagrangian Monte Carlo PDF-CFD Computation Of Gas Turbine Combustor Flowfields With Finite-Rate Chemistry. ASME Journal of Engineering for Gas Turbine and Power, Vol. 119, P. 519-526, 1997a.
- Tolpadi AK, Prakash C, Hura H and Mongia HC. Advanced Combustion Code: Overall Description, Prediction Of A Jet Diffusion Flame And Combustor Flowfields. ASME Gas Turbine Paper, 1998.
- Tolpadi AK. Calculation of Two-Phase Flow in Gas Turbine Combustors. Journal of Engineering for Gas Turbine and Power, Vol. 117, 1995.
- Turns SR. An Introduction to Combustion: Concepts and Applications. McGraw-Hill, New York, 2nd, 1996.
- Turns SR. Understanding NO_x Formation in Nonpremixed Flames: Experiments and Modeling. Progress in Energy and Combustion Science, Vol. 21, P. 361-385, 1995.
- Vandormaal JP and Raithby GD. Enhancements of the SIMPLE Method for Predicting Incompressible Fluid Flows. Numerical Heat Transfer, 7, P. 147-163, 1984.
- Veynante D and Vervisch L. Turbulent Combustion Modeling. Progress in Energy and Combustion Science 28, P. 193-266, 2002.
- Viskanta R. Overview of Convection and Radiation in High Temperature Gas Flows. International Journal of Engineering Science 36, P. 1677-1699, 1998.
- Volkov DV, Belokin AA, Lyubimov DA, Zakharov VM and Opdyke GJ. Flamelet Model of NO_x in A Diffusion Flame Combustor. ASME Journal of Engineering for Gas Turbine and Power, Vol. 123, 2001.
- Wendt JF, Anderson JD, Degrez G and Dick E. Computational Fluid Dynamics: An Introduction. Springer-Verlag, New York, 2nd, 1996.

Wilcox DC. Turbulence Modeling for CFD. DCW Industries, La Canada, California, 1998.

Xia JL, Yadigaroglu G, Liu YS, Schmidli J and Smith BL. Numerical and Experimental Study of Swirling Flow in a Model Combustor. *Int. J. Heat Mass Transfer*, Vol. 41, No. 11, P. 1485-1497, 1998.

Yakhot V and Orszag SA. Renormalization Group Analysis of Turbulence: I. Basic Theory. *Journal of Science Computing*, 1(1), P. 1-51, 1986.

Zamuner B, Gilbank P, Bissières D and Berat C. Numerical Simulation of the Reactive Two-Phase Flow in a Kerosene/Air Tubular Combustor. *Aerospace Science and Technology* 6, P. 521-529, 2002.

Zarzalís N, Ripplinger T, Hohmann S, Hettel M, Merkle K, Leuckel W, Klose G, Meier R, Koch R, Witting S, Carl M, Behrendt T, Hassa C, Meier U, Lückerrath R and Stricker W. Low-NOX Combustor Development Pursued within the Scope of the Engine 3E German National Research Program in a Cooperative Effort among Engine Manufacturer MTU, University of Karlsruhe and DLR German Aerospace Research Center. *Aerospace Science and Technology* 6, P. 531-544, 2002.

Appendix A

Liner Geometry

The dimensions of the outline of combustor liner are shown in Figure A.1. The cooling slots are 0.25 cm in width, and the injection port is 0.5 cm in depth and 1.6 cm in diameter.

Figure A. 1. Combustor Liner Geometry

The distributions of the holes are shown in Figure A.2, noted that the combustor is symmetry in xz-plane and xy-plane with the origin at the beginning of the centerline of the combustor, as shown with the labels Figure A.2.

Three Hole A, seven Hole C and a Hole D are found on each side of the xz-plane and three Hole B are found on each side of the xy-plane. The angles between Hole A are 36° with respect to the x-axis in the yz-plane, 25° for Hole B and 18.4° for Hole C.

Figure A. 2. Layout of Liner Injection Holes

The axisymmetry profile of the turbine disk shield (Figure A.3) in xy-plane is measured as:

Table A.1. Geometry Profile of Turbine Disk Shield

x (cm)	0	1.538	3.076	4.614	6.152	6.513
y (cm)	4.071	3.89	3.709	3.347	2.171	1.266

Figure A. 3. Geometry of Turbine Disk Shield

The injection slots are distributed evenly on the dome wall with 0.5 cm away from the side of the dome wall as shown in Figure A.4. Since the wall thickness is not included in the model, the cut outs on the dome wall are 4.95 cm in length, 1 cm in width and 0.1 cm in depth to represent the injection Plane 1 to Plane 5. It should be noted that the injection Plane 3 is 0.15 cm wide.

Figure A. 4. Geometry of Dome-Swirler Slots

Appendix B

Lookup Table Preparation

Two different methods are used for the definitions of the diesel fuel, the ultimate analysis and the empirical definition. Based on ultimate analysis, diesel fuel contains 86 % mass fraction of carbon and 14 % mass fraction of hydrogen (Odgers and Kretschmer 1986), the empirical definition of diesel fuel is based on the chemistry composition of $C_{10.8}H_{18.7}$ (Turns 1996). The thermochemistry lookup tables include 12 species for the definitions of the diesel fuel based on ultimate analysis and include 13 species for empirical definition.

Table B.1. Lookup Table Species

Ultimate Analysis	Empirically Defined
$C(s)$	$C(s)$
CO	C
CO_2	CO
CH_4	CO_2
H	CH_4
H_2	H
H_2O	H_2
$H_2O(l)$	H_2O
N_2	$H_2O(l)$
OH	N_2
O_2	OH
O	O_2
-	O

The oxidizer is defined with 21 % mole fraction of O_2 and 79 % of N_2 in the lookup table calculation. The radicals O , H , and OH are included for dissociation effect, CO and H_2 are included for dissociation effect, CH_4 and $C(s)$ are included for hydrocarbon reaction.

Appendix C

Convective Heat Transfer Coefficient of Liner Walls

The method suggested by Çengel (2003) for tube annulus was applied to estimate the convective heat transfer coefficient, h , of the combustor liner wall. As the inner and outer heat transfer coefficients are approximately same for fully turbulent flow, the combustor annulus can be treated as duct with hydraulic diameter calculated from the inner and outer annulus diameter of 0.18 m and 0.155 m respectively as:

$$D_h = D_o - D_i = 0.025 \text{ m}$$

The Nusselt number can be calculated from turbulent flow relation given as:

$$\text{Nu} = \frac{(f/8)(\text{Re} - 1000)\text{Pr}}{1 + 12.7(f/8)^{0.5}(\text{Pr}^{2/3} - 1)}$$

Where Reynolds number, Re , and Prandtl number, Pr are determined from:

$$\text{Re}_D = \frac{\rho u D_h}{\mu}$$

$$\text{Pr} = \frac{\mu C_p}{k}$$

The friction factor, f , can be determined assuming fully developed turbulent flow with the expression:

$$f = 0.184 \text{Re}^{-0.2}$$

Given with the combustor annulus temperature equal to the compressor discharges air temperature of 577 K (304 °C), the properties of air are given as (sourced Çengel, 2003):

Table C. 1. Combustor Annulus Air Properties

Density, ρ (kg/m ³)	0.6158
Specific Heat, c_p (J/kgK)	1044
Thermal Conductivity, k (W/mK)	0.04418
Dynamic Viscosity, μ (kg/ms)	2.934×10^{-5}
Prandtl Number, Pr	0.6935

Given the engine mass flow rate, $\dot{m}$, of 1.7 kg/s, and the liner annulus cross sectional area of $A = \pi(D_o^2 - D_i^2)/4 = 0.0066 \text{ m}^2$, the velocity of the annulus airflow is:

$$u = \frac{\dot{m}}{\rho A} = 420 \text{ (m/s)}$$

The values for Re, f , and Nu can be calculated and are summarized as follows:

Table C. 2. Estimated Parameters for Convective Heat Transfer Calculations

Re_D	220519
f	5.4×10^{-6}
Nu	340

With the correction factor for the Nu of:

$$F = 0.86 \left(\frac{D_i}{D_o} \right)^{-0.16}$$

$$Nu = \frac{hD_h}{k}$$

$$h = \frac{Nu k}{D_h}$$

Table C. 3. Estimated Convective Heat Transfer Coefficient for Liner Wall

Correction Factor, F	0.88
Corrected Nusselt Number, $Nu \times F$	299
Heat Transfer Coefficient, h (W/m ² K)	529

Appendix D

NO_x Prediction Conversions

The NO emissions in parts per million by volume (ppmv) at the combustor outlet are written based on the mixture fractions including the species N_2 , O_2 , H_2O and CO_2 determined in the simulations at the combustor outlet.

NO ppmv (dry basic) is computed as:

$$NO \text{ ppm} = \frac{NO \text{ mole fraction}}{1 - H_2O \text{ mole fraction}}$$

where

$$NO \text{ mole fraction} = \frac{NO \text{ mass fraction} \times M_{\text{mixture}}}{30}$$

and the mixture molecular weight, M_{mixture} , is:

$$M_{\text{mixture}} = \frac{1}{\sum_k \frac{\text{mass fraction}}{M_k}}$$

The correction formula for the expression of ppmv referenced to 15 % oxygen is written as (Lefebvre 1999):

$$NO \text{ ppmv}_{\text{ref 15\% oxygen}} = \frac{5.9 \times NO \text{ ppmv}}{20.9 - O_2 \text{ mole fraction}}$$