Stochastic Modelling of Turbulent Combustion for Design Optimization of Gas Turbine Combustors

by

Mohammed Ali Mehanna Ismail, B.Sc., M.Eng.

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the Faculty of Graduate Studies and Research
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Doctor of Philosophy

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submitted by **Mohammed Ali Mehanna Ismail, B.Sc., M.Eng.**

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the degree of Doctor of Philosophy

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Abstract

The present work covers the development and the implementation of an efficient algorithm for the design optimization of gas turbine combustors. The purpose is to explore the possibilities and indicate constructive suggestions for optimization techniques as alternative methods for designing gas turbine combustors. The algorithm is general to the extent that no constraints are imposed on the combustion phenomena or on the combustor configuration.

The optimization problem is broken down into two elementary problems: the first is the optimum search algorithm, and the second is the turbulent combustion model used to determine the combustor performance parameters. These performance parameters constitute the objective and physical constraints in the optimization problem formulation. The examination of both turbulent combustion phenomena and the gas turbine design process suggests that the turbulent combustion model represents a crucial part of the optimization algorithm. The basic requirements needed for a turbulent combustion model to be successfully used in a practical optimization algorithm are discussed. In principle, the combustion model should comply with the conflicting requirements of high fidelity, robustness and computational efficiency. To that end, the problem of turbulent combustion is discussed and the current state of the art of turbulent combustion modelling is reviewed. According to this review, turbulent combustion models based on the composition PDF transport equation are found to be good candidates for application in the present context. However, these models are computationally expensive.

To overcome this difficulty, two different models based on the composition PDF transport equation were developed: an improved Lagrangian Monte Carlo composition PDF algorithm and the generalized stochastic reactor model. Improvements in the Lagrangian Monte Carlo composition PDF model performance and its computational efficiency were achieved through the implementation of time splitting, variable stochastic fluid particle

mass control, and a second order time accurate (predictor-corrector) scheme used for solving the stochastic differential equations governing the particles evolution. The model compared well against experimental data found in the literature for two different configurations: bluff body and swirl stabilized combustors.

The generalized stochastic reactor is a newly developed model. This model relies on the generalization of the concept of the classical stochastic reactor theory in the sense that it accounts for both finite micro- and macro-mixing processes. The generalized stochastic reactor model is essentially a PDF formulation governed by the transport equation of a volume-averaged PDF over the reactor volume. An improvement to the model performance was achieved by the introduction of turbulence mixing rate bias in selecting particle pairs for mixing in the modified Curl mixing mechanism. The model compared well against measurement obtained from the published experiments on bluff body and swirl stabilized combustors.

Finally, elements and applications of the integrated design optimization algorithm for gas turbine combustors were presented. The integrated design optimization algorithm is comprised of the improved Lagrangian Monte Carlo composition PDF model as an evaluator of the objective function and the genetic algorithms as the optimum search algorithm. Applications of the optimization algorithm were considered in terms of minimization of an axi-symmetric combustor emissions (NO and CO concentrations). The optimization of the objective function was obtained over the course of changing the swirl vane angle and the side wall expansion angle of an axi-symmetric combustor as design variables. Parametric analysis and optimization examples demonstrated the effectiveness and practicality of the optimization algorithm in finding credible optimal geometry in reasonable time despite using modest computational facility.

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(Then say: "provide us with your proof if you are truthful.")

-Qura'an Chapter (2), Verse (111)

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Nomenclature

<i>Symbol</i>	<i>Meaning</i>	<i>Units</i>
A	pre-exponential constant	$[kmol\ m\ sec\ K]$
A	Area	$[m^2]$
A_1, A_2	Random variable with uniform distribution	$[-]$
a	Speed of sound	$[m\ sec^{-1}]$
b_{po}	Weight of the particle contribution to point (o)	$[-]$
C	Progress variable	$[-]$
C_{EBU}	Eddy break up model constant	$[-]$
C_μ	Turbulence model constant	$[-]$
C_θ	Mixing model constant	$[-]$
D	Diffusion coefficient	$[m^2\ sec^{-1}]$
d	Diameter	$[m]$
f	Number of molecules distribution function	$[-]$
f	Residence time distribution function	$[-]$

G	Non-reacting scalar	$[-]$
g	Body force per unit mass	$[m \text{ sec}^{-2}]$
g_i	Constraint function	$[-]$
I	Number of time steps to obtain the final convergence	$[-]$
J^α	Diffusive mass flux vector	$[J \text{ m}^{-2} \text{ sec}^{-1}]$
k	Arrhenius reaction rate constant	$[kmol \text{ m}^{-3} \text{ sec}^{-1}]$
k	Turbulent kinetic energy	$[m^2 \text{ sec}^{-2}]$
k	Boltzman constant	$[J \text{ K}^{-1}]$
L	Turbulence integral length scale	$[m]$
L	Random forces per unit mass	$[N \text{ kg}^{-1}]$
$\mathcal{L}$	Operator	$[-]$
Le	Lewis number	$[-]$
M	Mach Number	$[-]$
m	Mass	$[kg]$
$\dot{m}$	Mass flow rate	$[kg \text{ sec}^{-1}]$
N	Number of degrees of freedom	$[-]$
N_c	Number of cells	$[-]$
N_{CFL}	CFL number (Courant-Fridrichs-Lewy)	$[-]$
N_{cof}	Cut-off number of particles	$[-]$

N_p	Number of particles	$[-]$
N_{pc}	Number of particles in cell	$[-]$
N_s	Number of species	$[-]$
$\mathcal{O}_1$	Convection operator	$[-]$
$\mathcal{O}_2$	Chemical reaction operator	$[-]$
$\mathcal{O}_3$	Mixing operator	$[-]$
p	Pressure	$[N\ m^{-2}]$
P	Probability density function (PDF)	$[-]$
$\wp$	Fine grained PDF	$[-]$
Q	Conditional mean	$[-]$
r	Inertial range length scale	$[m]$
r	Radial location	$[m]$
Re	Reynolds number	$[-]$
S	Number of submoves in global time step Δt	$[-]$
s	Stoichiometric coefficient	$[-]$
S_L	Laminar flame speed	$[m\ sec^{-1}]$
T	Temperature	$[K]$
t	Time	$[sec]$
T_a	Activation energy divided by the universal gas constant	$[k^{-1}]$

U	Velocity	$[m \ sec^{-1}]$
U	Axial velocity component	$[m \ sec^{-1}]$
V	Sample space random variable corresponding to $U(\underline{X}, t)$	$[m \ sec^{-1}]$
V	Radial velocity component	$[m \ sec^{-1}]$
x	Location	$[m]$
W	Angular velocity component	$[m \ sec^{-1}]$
W	Wiener process	$[-]$
W_P	Computational work per particle per time step	$[-]$
$\dot{W}$	Reaction rate	$[kmol \ kg^{-1} \ sec^{-1}]$
w_k	Weight factor	$[-]$
Z	Mixture fraction	$[-]$
Z^*	Sample-space variable corresponding to Z	$[-]$

Greek Symbols

α	Probabilitiy of finding unburned mixture	$[-]$
β	Probabilitiy of finding burned mixture	$[-]$
β	Eddy dissipation model constant	$[-]$
δ	Dirac delta function	$[-]$
ε	Mean rate of energy dissipation	$[m^2 \ sec^{-1}]$
γ	Friction coefficient per unit mass	$[sec^{-1}]$

λ	Taylor length scale	$[m]$
μ	Viscosity coefficient	$[kg\ m^{-1}\ sec^{-1}]$
ν	Kinematic viscosity coefficient	$[m^2\ sec^{-1}]$
Ω	Space angle between the relative velocities	$[rad]$
ω	Turbulent frequency	$[sec^{-1}]$
ω_{mix}	Mixing frequency	$[sec^{-1}]$
ω_{Φ}	Turbulent mixing frequency	$[sec^{-1}]$
Φ	Mass fraction	$[kg\ kg^{-1}]$
ϕ	Dependent variable	$[kg\ kg^{-1}]$
Ψ	Sample space variable corresponding to $\Phi(X, t)$	$[kg\ kg^{-1}]$
ρ	Density	$[kg\ m^{-3}]$
σ_{Φ}	Schmidt number	$[-]$
τ	Turbulence dissipation time scale	$[sec]$
τ_h	Heat release factor	$[-]$
τ_r	Average residence time	$[sec]$
τ_{ij}	Stress tensor	$[N\ m^{-2}]$
τ_{Φ}	Scalar fluctuations dissipation time scale	$[sec]$
η	Standardized Gaussian random variables	$[-]$
ζ	Kolmogorov length scale	$[m]$

$\forall$	Volume	$[m^3]$
-----------	--------	---------

Subscripts

av	Average
b	Burned
c	Corrector
c	Cell
$conv$	Conventional scheme
$coll$	Collision
e	Effective
f	Fuel
i, j, k	Indices
in	Inlet
imp	Improved scheme
L	Lagrangian
l	Laminar
l	Local value
o	Oxidizer
o	Reference value
p	Particle

p	Predictor value
r	Reactor
st	Stoichiometric
t	Turbulent
α	species α

Superscripts

k	Global time
l	Local time
$*$	Arbitrary point
$.$	Rate
$'$	Fluctuations
$''$	Mass weighted fluctuations

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Chapter 1

Introduction

The process of engineering design can be formulated in a general way (i.e., without reference to specific process or design parameters) as an optimization problem. That is, the ultimate goal of an engineer is to design a system which operates to minimize a certain cost and/or maximize a certain gain. This cost or gain measure, in design optimization terminology, is referred to as an objective function.

However, formulating an engineering design process in such a simple way is unsatisfactory. Usually, one is confronted with conflicting demands imposed on the system “performance measure parameters”. An attempt to improve one of these parameters is likely to lead to the deterioration of other parameters. For example, for a gas turbine combustor, reduction of nitrogen oxides (NO_x) emissions by operating the combustor at a lower reaction zone temperature could have an adverse effect on combustion stability as well as on emissions of carbon monoxide (CO) and unburned hydrocarbons.

In addition, the search for geometrical and configurational parameters that comply with the conflicting performance requirements is not free of other types of constraints, sometimes stringent ones. Referring to our previous example in gas turbine combustors, dimensions, weight, and operational life time are general and permanent requirements that

lead to less freedom for the designer and a narrower range of feasible design.

This suggests that one has to observe not only an objective function, but also other performance measures which are expected to vary in the course of changing the design control parameters. One way the optimization problem can be formulated (though, not in the most general way) is as follows: Change design control parameter, within certain specified range, in search for maximum/minimum value of a certain objective. Simultaneously, make sure that a set of well-chosen performance measure parameters are kept within recommended limits. More abstractly, it can be written as,

Minimize/Maximize

$$\text{Objective} = f(\text{geometrical \& physical parameters})$$

subjected to constraints on:

$$g_i(\text{geometrical \& physical parameters})$$

$$i = 1, 2, \dots, N \tag{1.1}$$

where N is the number of geometrical and physical constraints.

In terms of our previous example, the objective corresponds to minimizing NO_x emissions. Constraints are imposed on the maximum value of CO and unburned hydrocarbons. Other constraints can be imposed on proper combustion stability measures. This objective may be obtained in the course of changing geometrical parameters (dimensions, swirl number, number of primary zone holes, and so on) and physical parameters (fuel-to-air ratio, cooling air mass flow rate, and so on), within proper limits usually estimated from

previous experience. We will call the latter set of parameters, design control parameters or independent variables.

Now, we may break down the problem represented by Equation 1.1 into two elementary questions. The first is the question of evaluating the objective function and other performance measures included as functions of the independent variables (design control variables). The second question amounts to the search for the optimum value of this objective (assuming it exists). This simple breakdown allows one to draw some general conclusions

The first conclusion is that the problem of optimization is usually of an iterative nature. That is, one can calculate the objective function and then use its value to drive the design control parameters in the direction which is thought to lead to optimum design. This process continues until a specified convergence criterion is met.

The second conclusion to be drawn is that the output of the optimization process is controlled in the first place by the nature of the objective function. In other words, in solving an optimization problem, one cannot get more or higher quality information than what is contained in the objective function. Let us illustrate this point with two examples.

In the first example, one wants to find the minimum value of the analytical function $f(x) = ax^2 + b$, for any real x . Here, the process of evaluating the objective function is trivial arithmetics. Thus, one may assert that the quality of the optimum solution is practically dependent on the performance of the optimization scheme.

As a second example, we return to the problem of gas turbine combustor design. In this example, the engineer seeks a set of combustor design control parameters that would give minimum NO_x emissions while keeping CO below certain limits. Clearly, this example is of a different nature than the first one. The main difference lies in the evaluation and the nature of the objective and constraints.

In dealing with a complicated and non-linear phenomenon such as turbulent combus-

tion, the functional relation that determines the numerical value of the objective function for each corresponding choice of design control parameters is not given in an explicit form. Moreover, the extreme complexity of such a phenomenon prohibits a priori prediction of the qualitative shape of this functional relation except for a narrow range of working conditions and design parameters. The problem of turbulent combustion is discussed in the next chapter where sources of difficulty in solving turbulent combustion flow are highlighted.

For now, we continue our discussion on the problem of optimization of gas turbine combustors. We arrived at the conclusion that obtaining an optimum solution is dependent, in the first place, on the quality of the solution of the turbulent combustion system. Once this solution has been achieved, the problem is shifted to finding an optimum value for some objective function under some constraints.

The question to be put forward is this: based on the previous discussion, can we derive basic requirements, first on the turbulent combustion model and second, on the optimization method, which may be necessary for constructing a scheme capable of handling the problem of combustor optimization in its general form.

First, we consider the turbulent combustion model. Obviously, we would like to exclude a class of models that are based on semi-empirical arguments and experimental correlations. These models are designed and tested for specific conditions and lack universality. This contradicts the optimization philosophy. As it is the case in an optimization scheme, one usually does not know in advance what the final result will look like.

We shall also insist that the combustion model, inserted in the optimization algorithm, should be able to account for the physical phenomena correctly, at least in a qualitative manner. The bottom line is to be able to guide the optimization scheme towards an optimum point for a wide range of operating conditions.

Also, the combustion model should be sensitive enough to small changes in the design control parameters. For example, in chemical reactors theory, the combustor is represented

by a network of reactors (Essenhigh, 1971). The reactor dimensions are defined in terms of reactor volume. Such a model would not be sensitive to changing both the reactor cross-sectional area and length simultaneously as the reactor volume may remain unchanged.

Other requirements on the turbulent combustion model can be deduced directly from the nature of the optimization scheme. The model should be computationally inexpensive and robust. The robustness originates from the fact that, during the optimization process, the scheme explores a whole domain of points in the design control parameters space. Consequently, the combustion model should be able to deal efficiently with a wide range of initial conditions and configurations. The requirements on the combustion model to be economical is of paramount importance and may introduce severe constraints. This originates from the fact that optimization is an iterative process. For example, if the optimum solution converges in 100 iterations, this simply means that we are solving the combustion system 100 times. As economy, generally speaking, conflicts with accuracy, this conflict is magnified here.

Considering the requirements on the optimization method, a primary issue one can put forward is that it should be able to handle functional relations, not only of a non-linear type but also with a large number of continuous or discrete variables, as is the case of gas turbine combustors. The optimization method should be efficient in finding optimum solution in a reasonable time. Also, the optimization method should be suitable for exploring relatively new problems such as the one at hand. For example, the optimization algorithm should not be trapped by a local minimum/maximum of the objective function.

1.1 Motivation

Recently, there has been an increasing demand for improved performance and reduced emissions of the next generation of gas turbine combustors. On the other hand, designers

of gas turbine combustors are confronted with conflicting requirements, which call for improved design methods. These conflicting requirements can be addressed through the application of optimization methods as an alternative to conventional design procedures.

To the author's knowledge, very few works exist in the literature concerning design optimization of gas turbine combustors (Despiere et al., 1997; Correa and Overton, 1988; and Borghi, 1974). Moreover, these works are generally of a semi-empirical character. In Correa and Overton (1988) and Borghi (1974), the classical stirred reactors theory was implemented as an evaluator of the objective function. This may be considered as a generalization of Bragg criterion (Essenhigh, 1971). Despiere et al. (1997) implemented a semi-empirical design model with the constrained equilibrium model for combustion.

The use of either empiricism or oversimplified models for evaluating the objective function and the physical constraints hinders the real power of the optimization procedures. The potential behind the use of optimization methods for gas turbine combustors motivates the present work as the beginning of a research program devoted to this subject.

1.2 Objectives and Tasks

The main objectives of the present work are to suggest, construct and implement an efficient algorithm for solving the problem of gas turbine combustor optimization in its general form. The purpose is to explore the possibilities of using optimization techniques as alternative tools for designing gas turbine combustors and to come up with constructive recommendations for possible improvements. The specific tasks necessary to accomplish this objective are described below.

1.2.1 Formulation and Construction of Turbulent Combustion Models

On surveying the theories of turbulent combustion (Chapter 2), the Lagrangian Monte Carlo probability density function (PDF) method is found to be the most appropriate method for implementation in an optimization scheme. However, the conventional PDF method suffers from a serious disadvantage; it is expensive from the computation point of view. This violates one of the major requirements for a turbulent combustion method to be used in an optimization scheme.

To address these shortcomings in the current PDF methods, two models were developed for the analysis of gas turbine combustors. The first model was an improved Lagrangian Monte Carlo algorithm for solving the composition PDF transport equation. In this algorithm, special care was given to the numerical method (Monte Carlo). The improvement in the model performance was mainly achieved through the implementation of time splitting, variable particle mass, and second order time accurate (predictor-corrector) scheme for the stochastic differential equations governing the evolution of fluid particles. These strategies lead to an improvement in the model accuracy and robustness while reducing the computation cost of a numerical solution (Kannenberg and Boyd, 2000).

The second model proposed in the present work is what we call the generalized stochastic reactor model. This newly developed model can be thought of as a generalization of the classical stochastic reactor theory or as a simplified composition PDF model. That is, the model employs the concept of dividing the combustor into regions, each called a generalized stochastic reactor. However, unlike the classical stochastic reactors that assume infinite macro-mixing, the generalized model accounts for both finite macro- and micro-mixing.

These two models (the improved Lagrangian Monte Carlo composition PDF algorithm

and the generalized stochastic reactor model) are developed specifically to meet the requirements of robustness, accuracy, and economy, which are essential for the design optimization algorithm.

1.2.2 Models Coding and Evaluation

A Fortran code was written for implementing each of the two proposed combustion models. Both codes have some modules in common. For example, a Fortran algorithm (DVODE), (Brown et al., 1989) to solve a system of stiff and non-stiff ordinary differential equations is used to solve the chemical kinetics in both codes. Also, a finite volume algorithm developed by Lilley and Rhode (1982), is used for solving the turbulent flow field.

The two models are evaluated and verified against experimental data for two different configurations: bluff body and swirl stabilized combustors. Based on this evaluation, one of the two models is selected for the design optimization scheme.

1.2.3 Optimization Scheme

This objective includes several minor tasks, as follows:

- (i) Formulation of the design optimization problem.
- (ii) Selection and implementation of an appropriate optimization method.
- (iii) Optimization algorithm integrity and coding. Specifically, the genetic algorithms method is chosen for solving the optimization problem as it is found appropriate for relatively newly explored problems. The method is integrated with the developed turbulent combustion model and applied to a premixed axi-symmetric combustor. Different, yet simple, objective functions are used for the purpose of evaluating the

optimization scheme. For example, an objective is chosen to minimize the NO_x emissions. In another example the objective is chosen to minimize CO emissions.

1.3 Outline of the Dissertation

The problem of gas turbine combustor optimization is considered in the present work. Two turbulent combustion models are proposed for the design optimization algorithm. The first model is an improved Lagrangian composition PDF algorithm. The second is a generalization of the stochastic reactor model. Eventually, using one of these two models, the design optimization scheme is applied to an axi-symmetric premixed swirl stabilized combustor. In Chapter 2, we first discuss the problem of turbulent combustion both on the theoretical and applied level. Next, based on a survey of the turbulent combustion models for both premixed and diffusion flames, a conclusion is drawn on the general framework of the combustion models proposed for the design optimization.

In Chapter 3, the theory and modelling of the PDF transport approach is discussed. Both the theory and modelling are introduced in a manner which emphasizes the stochastic nature of the approach. An attempt is made to establish a link between the well developed stochastic methods in statistical mechanics and those developed for the PDF transport equation. Assumptions beyond the modelling and the closure approximations are discussed in some details.

In Chapter 4, an improved Lagrangian composition PDF algorithm is developed. The procedures of integrating the stiff chemical kinetics equations are considered. The model is evaluated by comparison to experimental data of premixed Methane combustion in two different configurations: bluff body stabilized and swirl stabilized combustors.

In Chapter 5, the generalized stochastic reactor model is developed. The governing equations are derived and the solution algorithm is discussed. This model is also evaluated

by comparison to the same experimental works as in Chapter 4. Finally, a conclusion is drawn to choose one of the two models developed in Chapters 4 and 5, to be used in the design optimization procedures.

In Chapter 6, some applications of the design optimization algorithm to gas turbine combustors are considered. Finally, in Chapter 7, conclusions and generalizations are outlined.

Chapter 2

Survey of Turbulent Combustion Models

In the present chapter the methods of turbulent combustion are reviewed for both pre-mixed and diffusion flames. Based on this review, an approach is advocated for modelling a gas turbine combustor in a design optimization scheme. But first, the problem of turbulent combustion is briefly discussed in the hope that it will guide us in the selection of the candidate model.

2.1 The Problem of Turbulent Combustion

In this section, aspects and difficulties associated with the theory of turbulent combustion are discussed. Due to the complexity of this subject, it is broken down into four separate phenomena. They are organized in hierarchical order, as shown in Figure 2.1.

Moving in the direction of a higher level of complexity, some sources of difficulty are added to the overall problem. Beginning with the least complex level, the problem of turbulent flow is considered. At the next level, we discuss the phenomena of turbulent

Figure 2.1: Order of complexity in the problem of turbulent combustion.

passive scalar where the focus is on turbulent scalar transport and mixing. The next level of complexity is the turbulent reactive flow without heat release, where attention is given solely to the effect of turbulence on reaction rates. Finally, the effect of heat release on turbulence is presented under the subtitle of the problem of turbulent combustion.

2.1.1 The Problem of Turbulent Flow

In many places, the problem of turbulence is referred to as the last great unsolved problem in classical physics (Balescu and Senatorski, 1970). By this, it is meant that there is no pure theoretical solution has been derived from first principles. Nevertheless, there are many phenomenological theories where an empiricism (Launder and Spalding, 1971) or hypothesis, based on experimental observations, enters the theory at some stage (McComb, 1990).

By increasing Reynolds number, the fluid flow experience a transition from laminar to turbulent conditions. Generally speaking, in turbulence analysis we differentiate between two phenomena: the transition phenomenon and the fully developed turbulence phenomenon. Transition into turbulence may be described as a stability problem. However, here we are only interested in fully developed turbulence as this is the case in the gas turbine combustion chamber.

The Navier-Stokes equation is a non-linear equation. The non-linearity is caused by

the convection term. Moreover, the Navier-Stokes equation possesses another property that distinguishes it from many other non-linear equations in physics. That is, upon non-dimensionalizing the equation, the non-linear term is multiplied by the Reynolds number. By definition, increasing the Reynolds number causes the relative magnitude of the non-linear (convection or inertial) term to increase and the linear dissipative term to decrease. In other words, the non-linearity becomes more significant by increasing the Reynolds number. If a small parameter exist, this would have allowed for an approximation of the solution of the non-linear equation by perturbation methods or asymptotic expansion in terms of this small parameter (Hinch, 1991).

Direct numerical simulation at a high Reynolds number is possible at the theoretical level. Landau and Lifshitz (1959) used a dimensional argument to estimate the number of degrees of freedom of turbulence. To get a satisfactory description of turbulent flow, one must use a grid resolution of a scale given by the Kolmogorov length scale (the smallest turbulence scale),

$$\zeta \approx \left(\frac{\nu^3}{\varepsilon}\right)^{\frac{1}{4}} \quad (2.1)$$

where ν is the kinematic viscosity and ε is the mean dissipation rate of turbulence energy. Therefore, the number of grid points in a cubic volume with one side dimension of the characteristic length scale L is,

$$N \approx \left(\frac{L}{\zeta}\right)^3 \approx Re^{\frac{9}{4}} \quad (2.2)$$

That is, the number of degrees of freedom increases as the term, $Re^{\frac{9}{4}}$ increases. Consequently, it is impractical to give a detailed description of the velocity field at high Reynolds

number.

Another alternative is to look for a statistical description of the velocity field, i.e., to adopt a statistical approach. Here, the velocity is considered to be a random variable.

In a statistical sense, turbulence is a non-equilibrium phenomenon. If it is left to itself, without maintenance (for example by shear), it will decay with time. Also, as previously explained, turbulence is a system with a large number of degrees of freedom interacting with one another. This interaction is caused by the non-linearity and can be seen by Fourier transform as an interaction between Fourier modes¹. Another property that distinguishes turbulent flow is that it is a highly dissipative system. This dissipation may be studied in terms of turbulence decay.

Production of turbulence, non-linear redistribution of energy between degrees of freedom and dissipation of this energy, are three mechanisms that represent the foundations for the statistical theories. Generally speaking, one theory differs from the other based on the assumption of how these mechanisms work and how they are inter-related.

An interesting description of the statistical problem of turbulent flow is given by Heisenberg (1948). In his own words, “As soon as one puts energy into liquid without friction, this energy will be distributed among all degrees of freedom, and what finally results is a certain equilibrium distribution, corresponding to the Maxwellian distribution in gases and found by Kolmogorov, Onsager and V. Weizsaecher. It is the viscosity that reduces the number of degrees of freedom, since it damps, very quickly, in the every small eddies... turbulence is an essentially statistical problem... since it is a problem of distribution of energy among a very large number of degrees of freedom. Just as in Maxwell theory, this problem can be solved without going into any details of the mechanical motion, so it can be solved here by simple considerations of similarity.”

The great scientist suggests that turbulent energy is an integral of motion (meaning a

¹The Fourier transform provides a natural tool to visualize the degrees of freedom in a continuum and therefore turbulence can be easily seen as a many-body problem.

constant of motion) that cascades from large eddies into smaller ones. Also, he points out another important property of statistical systems of a very large number and interacting degrees of freedom. These systems (in the course of interaction between degrees of freedom) tend to forget about the initial conditions and develop a universal distribution. This is explained by the fact that interaction introduces elements of equipartition and randomness. In this context it is useful to think of collisions of billiard balls. Each collision will act to transfer kinetic energy from the ball that possesses higher kinetic energy to the ball with lower level of kinetic energy. Thus, equipartition will develop. Also, in a certain sense, these collisions introduce an element of randomness to the motion.

Interaction in terms of turbulence eddies was discussed by McComb (1990). He pointed out that “the interaction of two eddies can be decomposed into (a) the convection of one by the other and (b) the shearing of one by the other. While the first type of interaction...is not dynamically significant, the second effect results in the internal distortion of the eddies with the transfer of energy to a smaller size of disturbance”. That is, for the interaction between two eddies to be dynamically relevant, it has to be between two eddies that do not differ significantly in size. Since eddies of similar size are closely located when represented in the wavelength space, McComb concluded that the non-linear interaction is to some degree local in wave number space. In other words, large eddies carry smaller ones without distorting them. This points to the Kolmogorov theory of local isotropy.

The ideas in the previous paragraph have been treated in a quantitative manner by Kolmogorov (1941a, 1941b) in his elegant theory of local isotropy. A detailed review of Kolmogorov’s work was introduced by Batchelor (1947) and recently in a book by Frisch (1995). Kolmogorov adapted the cascade picture. Turbulence production occurs on large scale eddies (integral scale L) while dissipation occurs on the smallest scale (Kolmogorov scale ζ). At sufficiently large Reynolds number, there is an inertial range r such that,

$$\zeta \ll r \ll L \quad (2.3)$$

where there is no production or dissipation, and energy is just transferred to smaller eddies by the action of non-linear inertia.

It is evident that the characteristics of large-scale turbulent motions may not change considerably at distance of the order (r) . Assuming that (r) is small enough compared with the integral length scale. Therefore the relative velocity at two closely located points provides a proper description of small scale fluctuations. The relative velocity in direction (i) can be written as,

$$\Delta u_i = u_i(x + r) - u_i(x) \quad (2.4)$$

Without going into details, employing two similarity hypotheses, Kolmogorov showed that at a very high Reynolds number there exists a range of scales $\zeta \ll r \ll L$, in which the structure function can be written as,

$$\langle |\Delta u_i|^n \rangle = K_n \langle \varepsilon \rangle r^{\frac{n}{3}} \quad (2.5)$$

where K_n is a universal constant and $\langle \varepsilon \rangle$ is the average of the rate of energy dissipation. This distribution is universal, in the sense that it does not depend on the flow configuration or how the turbulence was produced.

Shortly after this theory was introduced, Landau and Lifshitz (1959) noted that Equation 2.5 did not take into account the fact that $\langle \varepsilon \rangle$, when averaged over a period in the order of the time scale of large eddies, will give different values for different flows. That is,

the large scale eddies, which are dependent on the turbulence production (flow type), will affect the distribution of the structure function of the small eddies. This is known as intermittency. Intermittency was also observed experimentally by Batchelor and Townsend (1949). It is manifested by deviation of the flatness factor of the velocity derivatives from the corresponding Gaussian value. An important implication of intermittency is that it reduces the universality of the small scale statistics. The flow conditions have some effect (likely small) on the small scale statistical properties.

One may ask what is the relevance of Kolmogorov theory, since the governing equations can be handled directly without a priori knowledge of the equilibrium distribution. However, knowledge about the equilibrium distribution (if it exists) by itself is important as it provides means for a better understanding of the mechanism of interaction and evolution of the random field of such a complicated phenomenon. It also provides a strong test for any theory of modelling turbulent flow. That is, one may ask, under the condition of a very high Reynolds number, does the theory produce the same structure function distribution for the inertial range. Moreover, a new theory can be built by enforcing the system to produce such an equilibrium distribution (for example, Langevin-type equation for turbulence (Haworth and Pope, 1986)). In fact, the intent in finding equilibrium distribution explains the special attention given to limit theorems such as the central limit theorem and the law of large numbers in the application of the probability theory to statistical systems.

2.1.2 The Problem of Turbulent Scalar Transport and Mixing

Consider Φ , a passive scalar such that it does not affect the turbulence characteristics. Experimentally, this may be obtained by slightly increasing the flow. In this case, the kinematics of the passive scalar are governed by the convection diffusion equation,

$$\frac{\partial \Phi}{\partial t} + U_i \frac{\partial \Phi}{\partial x_i} = D \nabla^2 \Phi \quad (2.6)$$

where D is the molecular diffusivity and U_i is the velocity. We ask, knowing the statistical properties of the velocity field at all the times and the statistical properties of the scalar field only at the initial time, what are the statistical properties of the scalar field at any later time. Equation 2.6, possesses a clear, pleasant character; it is a linear partial differential equation. Saffman (1969) pointed out that despite the linearity of Equation 2.6, it represents a subtle problem from the mathematical point of view. This is attributed to the existence of random coefficient (the velocity random variable, U_i).

Equations governing the statistical quantities can be derived from Equation 2.6, either in terms of hierarchy of moments or the probability density function (PDF) of the scalar. For example, upon deriving an equation for the mean, $\langle \Phi \rangle$, a term representing turbulent flux, $\frac{\partial \langle \Phi u_i' \rangle}{\partial x_i}$, appears which is unknown and requires modelling (Tavoularis, 2002). Here, u_i' are the velocity fluctuations in direction i , and $\langle \rangle$ implies ensemble averaging.

Similarly, an equation for the scalar variance $\langle \Phi'^2 \rangle$ can be derived starting with Equation 2.6. For simplicity, let us write the equation for the scalar variance in the case of homogeneous isotropic turbulence. It is assumed that the scalar fluctuation field is homogeneous as well as jointly homogeneous with the velocity and pressure fields. Also, the initial mean scalar field is initially uniform (Tavoularis, 2002),

$$\frac{\partial \langle \Phi'^2 \rangle}{\partial t} = -2D \langle \frac{\partial \Phi'}{\partial x_i} \frac{\partial \Phi'}{\partial x_i} \rangle \quad (2.7)$$

The term on the right-hand side of this equation is quadratic (meaning always non-negative) with a negative sign. This suggests that the role of this term is to work on reducing the variance of the scalar as time passes. In other words, this term will function in a way that decreases the fluctuations around the scalar mean value and consequently causes the effect of mixing. This is deduced directly from the definition of the state of perfect mixing, where all the fluctuations around the mean have died out.

Clearly, the term on the right-hand side of Equation 2.7 is unknown and requires modelling. This term is usually called the mean of the rate of fluctuation dissipation. This term plays a significant role in the theory of turbulent mixing as well as the theory of turbulent combustion. This is concluded from the simple fact that combustion is a chemical reaction. For a chemical reaction to develop, there must be direct molecular contact or collision or mixing. In turn, molecular mixing or contact is indicated by the dissipation of the smallest continuum scale in turbulence (Kolmogorov scale). This dissipation is quantitatively estimated by the rate of scalar fluctuations dissipation.

Warhaft (2000) pointed out that there is a certain division between the way engineers and physicists approach the subject of turbulent passive scalar. Engineers are likely concerned with problems of more applied nature such as the scalar flux variation and the quality of mixing process. Physicists have concentrated on questions of a more academic nature. The questions of universal behaviour of small scale (Sreenivasan, 1991), intermittency (Warhaft, 2000), the shape of the scalar PDF (Tavoularis and Corrsin, 1981; Ferchichi and Tavoularis, 2002), and many other questions have been a matter of extensive research on experimental (Ferchichi and Tavoularis 2002), analytical (Shraiman and Siggia, 1994; Sainai and Yakhot 1989) and numerical levels (Eswaran and Pope 1988).

This distinction between the interests of engineers and physicists is rather superficial. Both approaches are intimately connected. Let us illustrate this important point with some examples.

In the first example, the question of the single point PDF shape is considered. It is believed that the shape of the scalar PDF in homogeneous field is Gaussian. This is supported by the earlier experimental work by Tavoularis and Corrsin (1981), and recently by a more refined experiment by Ferchichi and Tavoularis (2002). Also, on a theoretical level, this is supported by a common belief that there is a possibility for the application of the central limit theorem. The linearity of Equation 2.6 implies superposition, and

together with the central limit theorem, indicates a rough picture of Gaussian distribution of the scalar. One may think of it this way: the scalar random variable, after a long period of time, is a superposition of incremental effects at earlier times. If these increments (accumulations) are independent, then Gaussian distribution is immediately implied ². For engineering applications, the condition of Gaussian distribution of the scalar random variable in homogeneous field is used directly in turbulent mixing modelling (*cf.* Chapter 3). An example is the mapping closure model proposed for modelling turbulent mixing by Chen et al. (1989). In this case, the unclosed mixing term which arises in the composition PDF transport equation is modelled as a non-linear mapping of Gaussian reference field in a way to ensure that the initial PDF shape relaxes to a Gaussian distribution in a sufficiently long time.

As a second example, the consequences of the question of the universal behaviour (local isotropy) of the dissipation scale as well as intermittency in engineering applications are considered. Warhaft (2000) pointed out that the issues of both intermittency and anisotropy are closely related. Both are manifested in considering higher order statistical moments. The question of the universal behaviour of the scalar small scale has been reviewed thoroughly by Sreenivasan (1991). In summary, the ideas of the Kolmogorov theory of local isotropy were extended by Obukhov (1949) and Corrsin (1951) to the theory of turbulent passive scalar. However, experimental evidence suggests that the local isotropy hypothesis may not be a natural concept in turbulent scalar (at least for Reynolds numbers of practical interest) (Sreenivasan, 1991; Warhaft, 2000).

Concerning intermittency, Mydlarski and Warhaft (1998) pointed out that the inertial range of the scalar field showed a higher level of intermittency than in the velocity field. Moreover, scalar intermittency may take place in the absence of velocity intermittency (*i.e.*, when the velocity field is strictly Gaussian). This also was suggested by the direct nu-

²The author knows no theoretical proof for this point. Therefore, there may be some risk in confirming this argument. However, there is more than one reason to make this argument an acceptable one.

merical simulation (Holzer and Siggia, 1994). Again, these ideas are impressed directly in the engineering applications. For example, Chomiak (1976) and Magnussen et al. (1976), exploited the fact that scalar dissipation is concentrated in a small volume fraction in the fluid (intermittent behaviour). They introduced the eddy dissipation model for turbulent diffusion combustion. Simply puts, a chemical reaction occurs when reactants are mixed on a molecular level. This molecular mixing is associated with the process of scalar dissipation. Consequently, they proposed that the mean reaction rate is proportional to the volume fraction occupied by small scale structure (*cf.* Section 2.2.2a)

This discussion suggests an interesting fact. That is, despite the linearity of the passive scalar equation, the scalar and velocity fields do not behave in a similar manner. Arguments which are acceptable for the latter may not be naturally extended to the former. A nice comment concerning this matter is given by Sreenivasan (1991): “It is believed that non-trivial universality in systems with many degrees of freedom manifests itself because of non-linearity.” He probably meant that the linearity of the scalar equation is the cause of its distinctive behaviour.

2.1.3 The Problem of Turbulent Reactive Flows

The problem of turbulent reactive flow is retained by solely recovering the reaction rate term in Equation 2.6. A subtle problem arises when attempting to derive the equations governing the statistical moments behaviour for a turbulent reactive flow. The major difficulty lies in the fact that the chemical source term is highly non-linear (usually an exponential multiplied by a polynomial) function of temperature and sometimes species concentrations. This difficulties has been explained, first, by Pratt (1976) using Taylor series expansion. But first, the Favre averaging procedures will be considered.

Some difficulties arise in using Reynolds-averaging procedures with turbulent flames and may be explained by a simple example. Consider the application of Reynolds-averaging

procedures to the continuity equation is the case of variable density flow,

$$\frac{\partial \langle \rho \rangle}{\partial t} + \frac{\partial}{\partial x_i} (\langle \rho U_i \rangle + \langle \rho' U_i' \rangle) = 0 \quad (2.8)$$

Compared to the case of constant density flow, it is found that there is an extra term which appears in Equation 2.8. This term is due to the correlation between velocity and density fluctuations. It is an unknown term and has to be modelled. Unknown terms arising from the density fluctuations can be avoided by employing Favre-averaging procedures. Consider a quantity Q , which may be decomposed to,

$$Q = \tilde{Q} + Q'' \quad (2.9)$$

where,

$$\tilde{Q} = \frac{\langle \rho Q \rangle}{\langle \rho \rangle} \quad (2.10)$$

and,

$$\tilde{Q}'' = \frac{\langle \rho (Q - \tilde{Q}) \rangle}{\langle \rho \rangle} = 0 \quad (2.11)$$

Employing Favre-averaging procedures to the continuity equation, we have,

$$\frac{\partial \langle \rho \rangle}{\partial t} + \frac{\partial \langle \rho \rangle \tilde{U}_i}{\partial x_i} = 0 \quad (2.12)$$

Where the unknown term due to the density fluctuations disappeared and Equation 5.7 takes the form of a constant density, Reynolds-averaged continuity equation. Employing the Favre-averaging procedures, other averaged conservation equations, in the case of turbulent flames, can be written in a way identical to the corresponding Reynolds-averaged

equations for constant density flow. Nevertheless, upon solving the Favre-averaged conservation equations, one expects a Favre-averaged results. Consequently, care should be taken in confirming such results with experimental data. This is explained by the fact that many experimental techniques measure time-averaged quantities. Under certain circumstances, the difference between the time and Favre-averaged quantities may be significant. Unfortunately, there is no simple way to estimate time-averaged quantities from the Favre-averaged ones. In such case, one has to model the unknown density correlations. A discussion on this problem was considered by Bilger (1975).

Back to the series expansion of the reaction term, consider a simple irreversible reaction between fuel (f) and oxidizer (o),

where s is the stoichiometric coefficient and p is the product. The fuel mass reaction rate $\dot{W}_f$ is expressed in Arrhenius form as,

$$\dot{W}_f = -AT^b \Phi_f \Phi_o \exp\left(-\frac{T_a}{T}\right) \quad (2.13)$$

where A is the pre-exponential constant, T_a is the activation energy divided by the universal gas constant and T is the temperature. Φ_f and Φ_o are the fuel and oxygen mass fractions respectively. In expanding the mean reaction rate as a Taylor series (Pratt, 1976; Borghi, 1988), we have,

$$\exp\left(-\frac{T_a}{T}\right) = \exp\left(-\frac{T_a}{\bar{T}}\right) \left(1 + \sum_{n=1}^{+\infty} P_n \left(\frac{T'^n}{\bar{T}^n}\right)\right) \quad (2.14)$$

and,

$$T^b = \tilde{T}^b \left(1 + \sum_{n=1}^{+\infty} Q_n \left(\frac{T''^n}{\tilde{T}^n} \right) \right) \quad (2.15)$$

P_n and Q_n are given by,

$$P_n = \sum_{k=1}^n (-1)^{(n-k)} \frac{(n-1)!}{(n-k)![(k-1)!]^2 k} \left(\frac{T_a}{\tilde{T}} \right)^k \quad (2.16)$$

and,

$$Q_n = \frac{b(b+1) \dots (b+n-1)}{n!} \quad (2.17)$$

The mean reaction rate $\tilde{W}_f$ can be written as,

$$\begin{aligned} \tilde{W}_f = & -A\tilde{T}^b \tilde{\Phi}_f \tilde{\Phi}_o \exp\left(-\frac{T_a}{\tilde{T}}\right) \left[1 + \frac{\Phi_f'' \Phi_o''}{\tilde{\Phi}_f \tilde{\Phi}_o} + (P_1 + Q_1) \left(\frac{\Phi_f'' T''}{\tilde{\Phi}_f \tilde{T}} + \frac{\Phi_o'' T''}{\tilde{\Phi}_o \tilde{T}} \right) \right. \\ & \left. + (P_2 + Q_2 + P_1 Q_1) \left(\frac{\Phi_f'' T''^2}{\tilde{\Phi}_f \tilde{T}^2} + \frac{\Phi_o'' T''^2}{\tilde{\Phi}_o \tilde{T}^2} \right) + \dots \right] \end{aligned} \quad (2.18)$$

Equation 2.18 contains several unknown correlations that have to be modelled. Moreover, in applying Taylor series analysis to a realistic chemical reaction, more correlations will be encountered and the closure problem becomes formidably complicated. Pratt (1976) used this analysis in order to indicate that the straightforward application of moment method to the problem of turbulent reactive flow is far from being adequate.

2.1.4 The Problem of Turbulent Combustion

The effect of combustion on turbulence is retained by considering the effect of the heat released on turbulence. Bray et al. (1981) pointed out that, among all the aspects of turbulent combustion, this is possibly the least studied one. The apparent reason for that stems from the fact that turbulence by itself is a complicated phenomenon. Consequently,

Figure 2.2: Schematic diagram of a steady one-dimensional premixed turbulent flame.

an attempt to study the modification of turbulence by heat release from combustion will be even more complicated. Also, because several and distinct effects result from a single action, which is the heat release by combustion, it is experimentally difficult to isolate these effects and to study each of them one at a time.

Hence, it is not surprising that there is as yet no general theory, which covers this problem. However, one may attempt to estimate what the influence of adding a large amount of heat in a thin zone on the local distribution of fluid properties will be. Then, with the help of experimental observations, one may attempt to determine how the variations in these properties will affect both the turbulence and turbulent scalar transport.

Let us direct our discussion to a simple example. Consider a planar normally propagating premixed flame, as shown in Figure 2.2. The density of premixed reactants is ρ_u (where the subscript u stands for unburned gases). The reactants move, with respect to a frame of reference fixed to the flame zone, with the flame speed. Due to the effect of heat released, the density of the products is much lower than the density of reactants. The density of the hot products is denoted by ρ_b (where the subscript b stands for burned gases).

For a thin flame zone, it is reasonable to assume that the pressure is nearly constant across the flame. We have,

$$\rho \approx \frac{1}{T} \quad (2.19)$$

and,

$$\nu \approx T^2 \quad (2.20)$$

where T is the temperature and ν is the kinematic viscosity. Thus the heat released may have the following direct effects on the fluid (Bray, 1979):

1. The density of the high temperature products will be much less than the density of unburned reactants. Under the effect of the same force, two different mass will experience two different rates of change of velocity (Newton's second law). In the case in hand, the force action is caused by the pressure gradient, the reactants are the heavier mass, and the products are the lighter mass. Since the reactants and products accelerate in different proportions, this leads to the creation a relative velocity between them. It will be seen later that this pressure-density interaction will affect both turbulent production and turbulent scalar transport.
2. According to Equation 2.20 molecular viscosity will increase in burned products. A typical ratio between the molecular viscosity of products to that of reactants is 10 (Pope, 1987). Consequently, Reynolds number, $\frac{UL}{\nu}$ will decrease in the products downstream.
3. Heat release also produces large rates of mean strain, significantly larger than the mean strain rate arising in constant density flow (Libby and Williams, 1981).

These effects give rise to the three relevant mechanisms that are specific to turbulence and turbulent transport properties in the case of turbulent combustion flow:

- (i) Counter-gradient diffusion (Libby and Bray, 1981).
- (ii) Turbulent kinetic energy production (Bray, 1975; Bray et al., 1981).
- (iii) Significant increment in differential diffusion effect (Libby and Williams, 1981).

Mechanisms (i) and (iii) amount to modifying the turbulent scalar transport while mechanism (ii) amounts to modifying the turbulence itself.

Let us discuss first the counter-gradient diffusion. As previously explained, due to the pressure gradient, a relative velocity will be created between the reactants and products. In other words, the products will move faster than the reactants. For an observer in a frame of reference fixed to the products, the reactants will be seen as moving from the products in violation to the usual gradient diffusion process (Anand and Pope, 1987). For a turbulent combustion model to be successful in detecting counter-gradient diffusion, the common modelling of turbulent flux by gradient closure should be avoided. Examples of models that avoid gradient closure for turbulent flux are the modified Bray-Moss-Libby model, (Bray et al., 1981), and the joint-velocity composition PDF models (Anand and Pope, 1987)³. Although detecting counter-gradient diffusion is an interesting test for turbulent premixed combustion models, its quantitative importance for practical applications has not been confirmed (Borghi, 1988).

The second issue to be discussed in the present context is the effect of combustion on modifying turbulence kinetic energy production. Also, here we confine our discussion to turbulent premixed flames. Experimental evidence indicates that there is a significant increase in turbulent kinetic energy production accompanying turbulent combustion (Bray

³In composition PDF, a gradient closure is usually used for modelling the turbulent scalar flux and accordingly, this model does not detect this phenomenon.

et al., 1981). In the case of variable density flow, in addition to the well established mechanisms affecting turbulent kinetic energy (diffusion, production and dissipation) in the constant density flow, additional effects were observed and are summarized here (Borghi, 1988):

- (i) The mean pressure produces a significant effect in the case of a large amount of heat release. This term originates from the interaction between the mean pressure gradient and density variations. This interaction ceases to exist in the case of constant density flow (Bray et al., 1981). It was previously shown that this interaction may lead to counter-gradient diffusion when considering the turbulent scalar transport.
- (ii) The decrease in Reynolds number by increasing the temperature may cause a suppression of turbulence or relaminarization effect (Borghi, 1988).

Borghi (1988) pointed out that combustion can have other indirect effects on the flow field. In this context, Figure 2.3 is of interest as it shows a comparison of the boundaries of the core of an isothermal jet (no combustion) to the flame boundaries in the case of combustion. The flame forward boundary is located much closer to the tube inlet than is the inner boundary of the jet core. Similar effects will be shown in Chapter 4, when considering the computed velocity-distribution in confined swirling flow.

The third and last mechanism to be discussed is the differential diffusion phenomenon. Usually, molecular diffusion is neglected compared to the turbulent diffusion. The high temperature products leads to lower Reynolds number as previously explained. This means that molecular transport may be significant compared to the turbulent one. Consequently, the differential diffusion, due to unequal diffusion coefficients, may have significant effects and should be taken into consideration.

Figure 2.3: Flame contours for combustion of propane air in Bunsen burner. Dashed lines are isothermal jet core while solid lines are flame boundaries (from Kuzentsov and Sabel'nikov (1990)).

2.2 Survey of Turbulent Combustion Models

In general, the processes of turbulent combustion may be classified as premixed or diffusion (non-premixed) combustion. Examples for systems operating under premixed conditions are spark ignition engines and to modern stationary gas turbines. Examples for systems operating under diffusion combustion conditions are diesel engines and aero-propulsion gas turbines (Peters, 2000).

Each type of combustion has its own advantages and disadvantages which stem from the nature of the combustion process. In diffusion combustion, the fuel and oxidizer are initially separated. Both are introduced into the combustion chamber where they are allowed to mix and burn. Therefore, the mixing in this case occurs on the interface surface between fuel and oxidizer. Moreover, mixing occurs naturally by diffusion between fuel and oxidizer where there is no control over local equivalence ratios. In other words, the main

control over the equivalence ratio is a global one, while the mixing between fuel and oxidizer occurs locally in a stoichiometric ratio. This causes a high level of local temperature. Since the rate of formation of the thermal NO_x is very sensitive to temperature, this leads to a higher level of NO_x emissions. Nevertheless, this type of combustion enjoys wide stability limits and is found in aero-propulsion gas turbines.

In premixed combustion, fuel and oxidizer are initially allowed to mix down to the molecular level with a specified equivalence ratio. In the case of a lean mixture, stoichiometric interfaces cannot form. Consequently, the associated high level of local temperature does not occur. This allows for a considerable reduction of NO_x emissions. However, premixed flames suffer from the serious disadvantage of the possibility of occurrence of flashback and auto-ignition.

To construct a theory of turbulent combustion one must consider the coupling between two different phenomenon: turbulence and chemical reactions. Both phenomena experience a wide range time and length scales. This cause a difficulty in the application of the powerful scale separation assumptions. Once a scale separation approximation is pursued, the two phenomena can be treated in sequence, one at a time, and the problem is greatly simplified. Therefore, simplifying assumptions have to be introduced to remove this coupling and to simplify the solution procedures. Here, some of the pervasive approximations in combustion theory are briefly discussed.

The first approximation is the fast chemistry assumption. This approximation relies on the existence of time scale separation between the chemical kinetics and the turbulent mixing. Practical combustion systems usually operate at high temperature level. High temperatures accelerate the combustion process and reduce the chemistry time scale. Consequently, combustion may be assumed to be controlled by the slower process, which in this case is the turbulent mixing. In other words, for the combustion process to advance, mixing should occur first. An immediate implication of this assumption is that chemical

kinetics at high temperature regions can be expressed in terms of turbulent mixing parameters. Examples of models that employ this assumption are the eddy break up model and the eddy dissipation model.

Another characteristic of combustion systems which leads to a powerful approximation, is based on length scales comparison in contrast to the previous argument which relies on the comparison between time scales. This approximation is usually referred to as the laminar flamelet. In the laminar flamelet limit, combustion is assumed to proceed in a very thin zone of length scale smaller than the smallest turbulence length scale. this assumption is supported by the fact that the temperature attains a very high level inside the reaction zone. Therefore, it can be assumed that the reaction in this zone is not influenced by the turbulent fluctuations. That is, this reaction is governed by the laminar flame theory. This is a very powerful approximation as the solution of the problem of turbulent combustion proceeds in two steps: first, the location of the very thin reaction zone, and second, the solution of the combustion inside this thin zone using the simple laminar combustion theories. These two steps are reflected in the mathematical simplification of the turbulent combustion problem. The first stage (determination of the reaction zone), is represented by a partial differential equation without a source term, i.e., the chemistry is absent. In the second stage (determination of the temperature and chemistry distributions inside the reaction zone), the chemical kinetics is represented by ordinary differential equations.

The gross feature of diffusion flame is that most of the reaction occurs in a narrow zone, as shown in Figure 2.4. The structure of premixed flame is shown in Figure 2.5. Clearly, it includes two main zones: a chemically inactive preheat zone, followed by a reaction zone of a smaller width.

This justifies the laminar flamelet assumption. A surface can be assumed to be attached to the reaction zone. Once the location of this surface is defined, one can proceed in the second stage of determining the scalar distribution in the reaction zone attached to this

Figure 2.4: Schematic representation of diffusion flame (adapted from Kuo (1986)).

surface.

Another important kind of approximation, which is frequently used in many combustion models, is the assumed shape PDF. It has been pointed out that the failure of the moment methods in turbulent combustion analysis is mainly due to the inherent difficulty of treating the chemical source term. On the other hand, the PDF method is able to treat the chemical source term exactly, without the need for modelling. In principle, the PDF function can be determined by solving the transport equation governing the PDF evolution. This is referred to as the PDF transport equation approach which must be distinguished from the the pre-assumed PDF approach. For the former, there is no a priori assumption concerning the shape of the PDF distribution. For the latter, the shape of the PDF distribution is assumed in advance. This pre-assumed distribution is usually written in terms of two unknown parameters and consequently, the problem of determining the PDF function is reduced to solving two equations for the statistical moments.

In the following subsections, some of the theories of turbulent combustion will be

Figure 2.5: Schematic representation of premixed flame (adapted from Kuo (1986)).

briefly reviewed for both diffusion and premixed flames. These methods are shown in the diagrammatic representation in Figure 2.6. First we start by reviewing the models for premixed flames, then models for diffusion flames. The PDF transport method will be reviewed separately because it is a general method and can be applied directly to both premixed and diffusion flames without modifications.

Before surveying the models of the turbulent premixed and diffusion flames, two new variables that are used for describing the diffusion and premixed flames must be defined. These are the mixture fraction and the progress variable. Consider a diffusion flame with an irreversible single step chemical reaction between fuel and oxidizer,

Figure 2.6: Schematic diagram for the models of premixed and diffusion turbulent combustion.

where s is the stoichiometric coefficient. Assuming that both fuel and oxidizer have equal diffusivity, a Schwab-Zeldovich (conserved scalar) variable can be defined such that the chemical source term is removed from the mass transport equation for this variable (Kuo, 1986). Then the mixture fraction (Z) is the normalized value of this conserved scalar such that it is equal to one in the fuel stream and zero in the oxidant stream. The mixture fraction follows the balance equation,

$$\frac{\partial \rho Z}{\partial t} + \underline{U} \cdot \nabla(\rho Z) = \nabla \cdot (\rho D \nabla Z) \quad (2.21)$$

where the underscore denotes a vector. For premixed combustion, the flame may be described using a progress variable C , such that $C = 0$ in the fresh gases and $C = 1$ in the fully burnt ones. Considering irreversible simple chemical reaction,

The progress variable may be defined either as a reduced temperature or reduced mass fraction,

$$C = \frac{T - T_u}{T_b - T_u} \quad (2.22)$$

or

$$C = \frac{\Phi_f - \Phi_f^u}{\Phi_f^b - \Phi_f^u} \quad (2.23)$$

where T , T_u and T_b are respectively the local, the unburnt gases and the burnt gases temperature. Φ_f , Φ_f^u and Φ_f^b are respectively the local, unburnt gases and burnt gases fuel mass fractions. Assuming a unity Lewis number (molecular and thermal diffusivity are equal), without heat losses and compressibility effect, the two definitions are equivalent and mass transfer and energy equations can be written in the same form,

$$\frac{\partial \rho C}{\partial t} + \underline{U} \cdot \nabla(\rho C) = \nabla \cdot (\rho D \nabla C) + \rho \dot{W} \quad (2.24)$$

2.2.1 Turbulent Premixed Combustion Models

2.2.1a Eddy Break up Model

It was previously explained that most practical combustion systems operate at high temperature, consequently, fast chemistry assumption can be employed. That is, the ad-

vancement of the chemical reaction is essentially controlled by turbulent mixing (Spalding, 1971). The higher the turbulence time scale, the lower the mixing effectiveness and the production rate of the chemical species. Therefore, the mean reaction rate is assumed to be inversely proportional to the turbulence time scale ($\frac{\varepsilon}{k}$). According the eddy break up model, introduced first by Spalding (1971), the mean reaction rate of products is calculated as,

$$\langle \dot{W} \rangle_p = \min \{ \dot{W}_p, -C_{EBU} \langle \rho \rangle \frac{\tilde{\varepsilon}}{k} (\widetilde{\Phi_p''^2})^{\frac{1}{2}} \} \quad (2.25)$$

where $\widetilde{\Phi_p''^2}$ is the variance of the product mass fraction and C_{EBU} is a model constant. Equation 2.25 reflects the fact that in the case of slow chemistry (cold flow conditions or *NO* formation) the combustion is controlled by the rate of chemical reaction rather than turbulent mixing. The eddy break up model can be considered as a semi-phenomenological model. This is manifested by the existence of an empirical parameter C_{EBU} which has to be tuned depending on the flow conditions (Peters, 2000).

2.2.1b Premixed Flamelet Model Based on G Equation

It has been previously explained that the solution to the question of turbulent combustion can proceed in two steps. The first is the determination of the reaction zone location and the second is the solution of the laminar reactive flow problem inside this reaction zone. This criterion is shown in Figure 2.7. In the first step the chemical kinetics is not important, while in the second step the turbulence characteristics are not directly linked the chemical reactions.

Flamelet models for premixed combustion can be formulated in terms of either the progress variable or what is called the level set or *G* equation. An example of the first is the Bray-Moss-Libby model, and it will be discussed separately in the following subsection.

Figure 2.7: Turbulent premixed flame propagation in flamelet regime. The flame structure is essentially a one-dimensional premixed laminar flame (from Haworth (2003)).

Here the models based on the G equation are briefly reviewed. This kind of model is explained in great detail in a recent book by Peters (2000).

Consider a non-reacting scalar G . Since G is non-reacting, the scalar transport equation will contain no source term. An equation G can be derived by considering an iso-scalar surface,

$$G(\underline{X}, t) = G_o \quad (2.26)$$

A possible choice of the iso-scalar surface is such that it lies on the surface separating the unburnt mixture from the flame, as shown in Figure 2.8. An equation for the iso-scalar can be derived,

$$\frac{\partial G}{\partial t} + \underline{U} \cdot \nabla G = S_L |\nabla G| \quad (2.27)$$

where $\underline{U}$ is the flow velocity at the flame front and S_L is the flame speed. This equation was first derived first by Williams (1985). It may be noted that the flame speed S_L is assumed to be known all over the entire flow field. In deriving Equation 2.27, it was

Figure 2.8: A schematic representation of the flame front as an iso-scalar surface $G(\underline{X}, t) = G_0$ (adapted from Peters (2000)).

assumed that the thickness of the flame is smaller than the Kolmogorov scale.

At this point, it is important to remember that the purpose of solving the G Equation 2.27 is to be able to define the surfaces to which the thin reaction zones are attached. In other words, we are working on the first of the two steps to the flamelet approach. Therefore, we ask the question: how can we use Equation 2.27 to determine the location of the flame surface (the surface to which the thin reaction zone is attached). Usually, a pre-assumed PDF, $P(G; \underline{X}, t)$ for the scalar G (Wirth and Peters, 1993), is used for calculating the first two moments of G , the mean and variance, as,

$$\langle G(\underline{X}, t) \rangle = \int G P(G; \underline{X}, t) dG \quad (2.28)$$

$$\langle G'^2(\underline{X}, t) \rangle = \int (G - \langle G \rangle)^2 P(G; \underline{X}, t) dG \quad (2.29)$$

The equations for these two moments are modelled and solved. Assuming that the shape of the pre-assumed PDF depends on two parameters, these two parameters can be

specified from the solution of the equation of the mean and the variance. Once $P(G; X, t)$ is known, the flame surface G_o can be found by,

$$P(G_o; X, t) = \int_{-\infty}^{\infty} \delta(G - G_o) P(G; X, t) dG \quad (2.30)$$

Once the statistical properties of the flame surface are found, the next step is to solve for chemical kinetics. This is done by first deriving a flamelet equation for premixed combustion (Peters, 2000),

$$\rho S_L |\nabla G| \frac{\partial \Phi_i}{\partial G} = \frac{d}{dG} \left(\rho D_i |\nabla G|^2 \frac{d\Phi_i}{dG} \right) + \rho W_i \quad (2.31)$$

This equation allows for solving the chemical kinetics and consequently, the determination of the concentrations and temperature distribution in the thin reaction zone attached to the iso-scalar surface. Note that Equation 2.31 can be obtained by coordinate transformation of reactive scalar (Φ_i) transport equation from the physical to the G space. In addition, simplifying assumptions concerning the geometry of the flame front are made. For example, similar to the boundary layer approximation when the curvature of the reaction zone is much larger than its thickness, the derivatives in the direction of the tangents to the flame front surface can be ignored.

Because of mathematical and conceptual difficulties, there have been few attempts to use the flamelet-based G equation for practical application (Peters, 2000).

2.2.1c Bray-Moss-Libby Model

Detailed measurements indicate that a premixed combustion in most practical systems of interest occurs in thin zones that are strongly distorted by turbulent fluctuations. In this case, (Kuzentsov and Sabel'nikov, 1990) stated that "the temperature profile involves

Figure 2.9: Oscillogram of temperature fluctuations in the combustion of homogeneous mixture (from Kuzentsov and Sabel'nikov (1990)).

Figure 2.10: Frozen position of the flame front. Test conditions are the same as in Figure 2.9 (from Kuzentsov and Sabel'nikov (1990)).

a succession of pulses of nearly rectangular form, approximately with the same amplitude but different duration.” . This is illustrated in the oscillogram of temperature fluctuations in Figure 2.9. The corresponding physical structure of the flame surface as function of time is illustrated in Figure 2.10.

Considering the progress variable as previously defined, Figure 2.11 is an idealization for the measurements shown in Figure 2.9. According to this idealization, the progress variable is considered as a discontinuous function in the form of pulses of different durations. Moreover, its value assumes one of two states, either 1 (fully burnt) or 0 (unburnt). Zero probability is assigned to the event of the intermediate state (as a first approximation). The later assumption is equivalent to the assumption of infinitely fast chemistry. One can write the probability density function as (Bray and Moss, 1977),

$$P(C; \underline{X}, t) = \alpha(\underline{X}, t)\delta(C) + \beta(\underline{X}, t)\delta(1 - C) \quad (2.32)$$

Figure 2.11: Intermittency between fresh and fully burnt gases at given location in the reaction zone. This signal corresponds to a bimodal ($C = 0$ and $C = 1$) probability density function (adopted from Kuzentsov and Sabel'nikov (1990)).

Figure 2.12: The pre-assumed PDF of the progress variable in the BML model (adopted from Peters (2000)).

where α and β are the probabilities of finding unburnt and burnt mixture, respectively, at location X and time t .

Equation 2.32 may be considered as an example the flamelet approximation in which the flame surface is defined by the progress variable of value one. This surface is the reaction zone or the flamelet. Also, Equation 2.32 is an example of a priori or pre-assumed PDF shape. The bimodal representation of the PDF of the progress variable given by Equation 2.32 is represented in Figure 2.12.

To determine the PDF function, one needs to know $\alpha(X, t)$ and $\beta(X, t)$. Integration of

Equation 2.32 from $C = 0$ to $C = 1$ yield the condition,

$$\alpha(\underline{X}, t) + \beta(\underline{X}, t) = 1 \quad (2.33)$$

With some manipulation (Libby, 1985), and assuming constant pressure and adiabatic conditions it can be shown that,

$$\alpha = \frac{1 - \tilde{C}}{1 + \tau_h \tilde{C}} \quad (2.34)$$

and

$$\beta = \frac{(1 + \tau_h) \tilde{C}}{1 + \tau_h \tilde{C}} \quad (2.35)$$

where $\tilde{C}$ is the Favre average progress variable and τ_h is the reaction heat release factor, defined by,

$$\tau_h = \frac{\rho_u}{\rho_b} - 1 = \frac{T_b}{T_u} - 1 \quad (2.36)$$

The right-hand side arises from the equation of state, assuming constant pressure and constant molecular weight. The values of τ_h (heat release factor) are fixed for a given chemical reaction and assumed to be known. Therefore, α and β can be used to calculate the PDF distribution.

An important feature of the Bray-Moss-Libby (BML) model is that the gradient diffusion closure is avoided and therefore, the model is able to capture the counter-gradient transport (Libby, 1980). In addition to the assumption of infinitely fast chemistry, another shortcoming of this model is the requirement of a priori knowledge of the heat release factor (Pope, 1987).

2.2.2 Turbulent Diffusion Combustion Models

2.2.2a Eddy Dissipation Model

The immediate application of the eddy break up model to non-premixed combustion is far from being accurate. That is, the model does not take into account the fact that the turbulent diffusion flame has a distinctive character which is different from premixed flames. In diffusion flames, there is an additional limitation which should be added. This limitation can be expressed by the fact that combustion in diffusion flames is conditional on the possibility of finding a stoichiometric mixture at a certain point in the flow field.

The eddy dissipation model proposed by Magnussen et al. (1976) may be considered as a modification to the eddy break up model in order to be able to handle the case of diffusion flames. Magnussen et al. (1976) incorporated some modifications, originally proposed by Chomiak (1976), which allow the application of their model to diffusion flames.

The starting point is the fact that the fine structures in turbulence are responsible for the dissipation of turbulence within these structures. Therefore, within these fine structures, one can assume that the reactants are mixed at the molecular scale. These regions, which are occupied by fine structures, are believed to be vortex tubes with a characteristic dimension of the same magnitude as the Kolmogorov scale, as shown in Figure 2.13. This dissipative region (vortex tubes) may be considered as well-stirred reactors placed in a chemically inert background (Chomiak, 1976).

Therefore, it is essential to know the volume fraction occupied by fine structures, or alternatively, the mass transferred between the bulk fluid and fine structures. For nearly isotropic turbulence, this was estimated by Magnussen et al. (1976) as,

$$\dot{m} = 23.6(\nu \frac{\varepsilon}{k^2})^{\frac{1}{4}} \frac{\varepsilon}{k} \quad (2.37)$$

Figure 2.13: Model of a region of concentrated vorticity. λ is the Taylor length scale and ζ is the Kolmogorov length scale (from Chomiak (1976)).

However, not all the fine structures will be sufficiently heated to react. The fraction of the fine structures (f) which react can be assumed to be proportional to the ratio of the concentration of reacted fuel and the total fuel concentration. Thus the fuel burning rate is calculated as,

$$\langle \rho \dot{W} \rangle = 23.6 \langle \rho \rangle \left(\frac{\nu \varepsilon}{k^2} \right)^{\frac{1}{4}} f \frac{\varepsilon}{k} \min \left(\tilde{\Phi}_f, \frac{\tilde{\Phi}_o}{s}, \beta \frac{\tilde{\Phi}_p}{(1+s)} \right) \quad (2.38)$$

where β is an adjustable parameter of the model. Φ_f, Φ_o, Φ_p are the mixture fractions of the fuel, oxygen and product, respectively. s is the stoichiometric coefficient. Recently, application of the eddy dissipation model to practical combustion systems was evaluated by Brink et al. (2000).

As is the case in the eddy break up model, the eddy dissipation model exhibits a dependence of the mean reaction rate on turbulence characteristics. Also, it may be considered as a semi-phenomenological model in the sense that the empirical parameter β requires tuning.

2.2.2b Diffusion Flamelet Model

The concept of laminar flamelet for diffusion flames is similar in many aspects to that of premixed ones. An obvious choice for a scalar variable which does not see the chemical source term is the mixture fraction Z . This is similar to the non-reactive scalar G used in premixed combustion. The equation governing such a scalar field is given by (Peters, 2000),

$$\frac{\partial \rho Z}{\partial t} + \underline{U} \cdot \nabla(\rho Z) = \nabla \cdot (\rho D \nabla Z) \quad (2.39)$$

According to the flamelet hypothesis, the only purpose of solving this equation is to determine a flamelet surface (a surface on which a thin reaction zone is attached). For diffusion flames, this surface can be found on the boundary separating the fuel and oxidizer. On this surface, the fuel and oxidizer mix by diffusion in a stoichiometric ratio. Therefore, the flamelet surface can be diagnosed by the stoichiometric surface condition,

$$Z(X, t) = Z_{st} \quad (2.40)$$

The flamelet equation (unsteady flamelet) is written as (Peters, 2000),

$$\rho \frac{\partial \Phi_i}{\partial t} = \frac{\rho}{Le_i} \frac{\varepsilon_Z}{2} \frac{\partial^2 \Phi_i}{\partial Z^2} + \rho W_i \quad (2.41)$$

Le_i is the Lewis number. Z is non-dimensionalized with respect to Z_{st} and ε_Z is the scalar dissipation rate defined by,

$$\varepsilon_Z = 2D|\nabla Z|^2 \quad (2.42)$$

It may be noted that Equation 2.41 is written in mixture fraction space, i.e., the mixture

Figure 2.14: Surface of stoichiometric mixture in turbulent jet diffusion flame (adapted from Peters (2000)).

fraction is the independent variable. It can be obtained by transformation of the coordinates from the physical space to the mixture fraction space, as shown in Figure 2.14.

Usually, the unsteady flamelet is used to simulate transient phenomena such as ignition. A steady flamelet model can be obtained by removing the time derivative from Equation 2.41. In deriving the flamelet Equation 2.41 it supposed that the mixing field dominates in the direction normal to the flame surface. Therefore, the derivatives in the tangential directions may be ignored. Again, these assumptions are very similar to the boundary layer transport assumptions.

2.2.2c Conditional Moment Closure Model

Conditional moments differ from conventional moments in that they are taken only for those members of the whole ensemble which comply with a specified condition. Conditional statistics have already been extensively used in turbulence intermittency (Kuzentsov and Sabel'nickov, 1990). The conditional moment closure was independently introduced by Klimenko (1990) and Bilger (1993) for diffusion flames. However, before reviewing this class of models, it is convenient to introduce mathematical tools necessary for the advancement of the discussion.

Let X and Y be random variables. The expected value of X for a given $Y = y$, where

Figure 2.15: Conditional averages of reactant concentration conditioned on mixture fraction in a reacting scalar mixing layer at different normalized distances from the layer center (adapted from Bilger (1993)).

y is a sample space variable corresponding to Y , is defined as,

$$E(X|Y = y) = \int x \frac{P(x, y)}{P(y)} dx \quad (2.43)$$

where $P(x, y)$ is the joint probability distribution of X and Y . An example of measurements of a conditional mean mole fraction of reactant concentration, conditional on mixture fraction and normalized by its unmixed value in a mixing layer is given in Figure 2.15 (Bilger, 1993). Such a conditional expectation is the basic quantity calculated in the conditional moment closure method.

However, when one is basically interested in conventional expectations or means. This

can be calculated from the conditional one as (Feller, 1968),

$$\begin{aligned} E(E(X|Y = y)) &= \int E(X|Y = y)P(y)dy \\ &= E(X) \end{aligned} \tag{2.44}$$

In that sense, the entire curve in Figure 2.15, for continuous range of conditions of mixture fraction, represents only one point of conventional average or expectation.

Let Φ_i be a mass fraction of species i . In turbulent flow, $\Phi_i(\underline{X}, t)$ is a random variable where $\underline{X}$ is the spatial coordinate vector. Let Z be a mixture fraction such that it assumes a value of unity in the fuel stream and zero in the oxidant stream. The mixture fraction is also a random variable. We define Z^* as a sample-space variable corresponding to Z . The conditional average of $\Phi(\underline{X}, t)$, conditional on the associated value of $Z(\underline{X}, t)$ being equal to a chosen value Z^* , is $Q(Z^*, \underline{X}, t)$, where,

$$\begin{aligned} Q(Z^*, \underline{X}, t) &\equiv \langle \Phi(\underline{X}, t) | Z(\underline{X}) = Z^* \rangle \\ &\equiv \langle \Phi | Z^* \rangle \end{aligned} \tag{2.45}$$

The angular brackets denote an ensemble average and the vertical bar indicates that this average is conditional on,

$$Z(\underline{X}, t) = Z^*(\underline{X}, t) \tag{2.46}$$

That is, only those members of the whole ensemble that meet this condition are included in the average.

The task is to derive a governing equation for the conditional average $Q(Z^*, \underline{X}, t)$

starting from the instantaneous transport equation of the scalar. While Klimenko (1990) derived this equation starting from the PDF transport equation, Bilger (1993) used a decomposition similar to the one used in the moment methods.

Assuming constant density, the derived equation for the conditional average Q is written as,

$$\begin{aligned} \frac{\partial Q}{\partial t} = & -\langle U_i | Z^* \rangle \frac{\partial Q}{\partial x_i} \\ & + \langle \dot{W} | Z^* \rangle + D_i \langle \nabla Z \cdot \nabla Z | Z^* \rangle \frac{\partial^2 Q}{\partial Z^{*2}} \\ & + e_Q + e_y \end{aligned} \quad (2.47)$$

U_i represents the velocity components while $\dot{W}$ is the reaction rate. e_Q represents molecular along with differential diffusion effects conditioned on $Z = Z^*$, while e_y represents the effect of conditional turbulent flux. The last two terms are estimated to be small in comparison to other terms in the turbulence equation (Bilger, 1993). The first three terms on the right-hand side of Equation 2.47 are not closed and require closure. They represent the effect of convective transport, chemical source term and turbulent mixing, respectively. Before discussing the proposed closures for Equation 2.47, first, the solution methodology for this equation will be outlined.

Essentially, the unknown variable in this equation is the conditional mean Q_i of species i . However, the quantity of real interest is the conventional mean which may be estimated from the former using Equation 2.44. This is usually done by numerical integration. Therefore, Equation 2.47 is determined M times for N species. The M times represents M values for the conditional mixture fraction. These M values are integrated numerically in order to compute one point of the conventional average.

Returning to the closure of Equation 2.47, the conditional mean velocity is usually replaced by conventional mean velocity (Peters, 2000). The second term representing the reaction rate is of special interest. Based on detailed experimental data of the reacting scalar mixing layer (Bilger et al., 1991), the contribution of the conditional fluctuations to the conditional mean reaction rate was found to be small compared to the contribution of the conditional mean. This justifies the following expression,

$$\langle \dot{W} | Z^* \rangle = \dot{W}(\langle \Phi | Z^* \rangle) \quad (2.48)$$

That is, the mean of the conditional reaction rate is equal to the reaction rate of the conditional mean (Bilger, 1993). Application of Equation 2.48 to the conventional average is far from being reasonable, as previously shown in Section 2.1.3.

The last term which needs closure is the conditional scalar dissipation representing the effect of turbulent mixing. This is the third term on the right-hand side of Equation 2.47. Usually this term is closed using mixing models similar to the ones used in the PDF transport equation, as will be discussed in the next chapter.

Finally, it is noted that the conditional moment closure model is not yet widely used in practical applications of turbulent combustion. Peters (2000) noted that it is necessary to obtain benefits of higher moment closure (e.g., conditional variance) for the conditional moment closure to be an alternative combustion model rather than a conceptual one.

2.2.3 PDF Transport Method

The PDF method usually refers to an approach where a PDF transport equation is solved. In that, it is different from the pre-assumed shape PDF method; the PDF shape is not specified in advance and is revealed by solving the PDF transport equation. The theory of the PDF transport equation has been treated thoroughly by Pope (1985) and

Borghi (1988).

As the theory and modelling of the PDF transport equation will be considered in latter chapters, the focus here will be on the general characteristic and the application of the PDF method in practical combustion systems.

In principle, a joint PDF transport equation can be written for any number of dependent variables at any number of points (one point PDF, two points joint PDF, and so on). However, two kinds of PDF transport equations are found in practice: the single point joint velocity composition PDF and the single point composition PDF.

Additional information regarding time and length scales for turbulence must be supplied, in the case of a single point-single time formulation. This is because these two scales represent a difference or relative measure and require two points of statistical description. Turbulence length and time scales can be obtained from usual turbulent models such as $(k-\varepsilon)$ or $(k-\omega)$ or the Reynolds stress model. This explains the fact that the conventional moment methods for the turbulent flow are usually combined with the PDF method in what is called hybrid methods.

In a joint velocity-composition PDF formulation, one usually solves for the joint PDF distribution of velocity and scalar. Once this distribution is obtained, both the velocity PDF distribution and the scalar PDF distribution can be derived from the joint distribution. Also, any higher moments of velocity or scalar or combined moments can be calculated at a single point. On the other hand, in a composition PDF, one usually solves for the PDF distribution of the multiple scalar at a single point. The joint velocity-composition PDF contains more information than the composition PDF. It also has the advantage of the turbulent diffusion term being closed. This removes the need for the modelling of turbulent diffusion, which is usually done employing gradient closure. Therefore, the joint velocity-composition can detect the counter-gradient diffusion phenomenon in premixed combustion (Anand and Pope, 1987). However, the solution of the joint

velocity-composition PDF is complicated compared to the composition PDF (Haworth and El Tahery, 1991).

For the purpose of the discussion, it is useful to consider, as an example, the composition PDF transport equation for a single scalar Φ and constant density flow,

$$\begin{aligned} \frac{\partial P(\Psi; \underline{X}, t)}{\partial t} + \frac{\partial}{\partial \Psi} \left(P(\Psi; \underline{X}, t) \frac{\dot{W}}{\rho} \right) = & - \frac{\partial}{\partial x_j} \int V_j P(\underline{V}, \Psi; \underline{X}, t) d\underline{V} \\ & - D \frac{\partial}{\partial \Psi} \lim_{\underline{X}_j^* \rightarrow \underline{X}_j} \frac{\partial^2}{\partial x_j^* \partial x_j} \int \Psi^* P(\Psi, \Psi^*; \underline{X}, \underline{X}^*, t) d\Psi^* \end{aligned} \quad (2.49)$$

where Ψ is the sample space variable corresponding to the scalar random variable $\Phi(\underline{X}, t)$. $\underline{V}$ is the sample space vector corresponding to the random velocity vector $\underline{U}(\underline{X}, t)$. $\dot{W}$ is the reaction rate. $\underline{X}^*$ is an arbitrary point different from $\underline{X}$. Ψ^* is the sample space variable corresponding to $\Phi(\underline{X}^*, t)$. D is the molecular diffusion coefficient. Equation 2.49 is an evolution equation for the single scalar PDF $P(\Psi; \underline{X}, t)$. The reaction term (the second term on the left-hand side) is closed and needs no modelling. This is a distinguished advantage which makes the PDF method superior to moment methods in turbulent reactive flow.

The two terms on the right-hand side represent turbulent diffusion and mixing, respectively. The first term contains the joint PDF distribution for the velocity and the scalar. The second term contains the joint PDF for the scalar at two points $\underline{X}$ and $\underline{X}^*$. Since Equation 2.49 governs the evolution of the PDF of the scalar Φ at a single point, clearly both terms represent a closure problem. Modelling of the turbulent diffusion and mixing terms will be considered in detail in Chapter 3.

In addition to the exact representation of the chemical reaction term, the PDF method possesses other advantages. No assumption is made regarding the local PDF shape. Also, the formulation and modelling are introduced without reference to the type of combustion

mechanism (premixed or diffusion). In that sense, the method is general and can be applied to both premixed and diffusion combustion without the need for modification. In fact, the only difference lies in the input flow composition.

The main shortcoming of the PDF method lies in the difficult problem of modelling the turbulent mixing term. Consider, for example, the case when chemistry is fast compared to turbulent mixing. In this case, chemistry takes place in a thin layer. This results in steep local gradients of the reacting scalars, which makes most of the closure assumptions applied to the turbulent mixing questionable. Unfortunately, most of the models available for closure assume, more or less, some forms of smoothly varying function. This point may explain the motivation behind recent efforts to develop a hybrid PDF-flamelet model (Haworth, 2000), as the flamelet model amounts to detecting the local steep variations in the reaction zone.

For the composition PDF, the dimensions of the PDF transport equation are $N_s + 1$, where N_s is the number of species. Regarding the joint velocity-composition PDF, it is $N_s + 4$, where three velocity components add extra dimensions. Due to the high dimensionality of the PDF transport equation, the application of finite difference (finite volume) techniques encounter difficulty. This is evident from early attempts at solving the composition PDF transport equation using the finite difference method (Bywater, 1982; Kollman and Janicka, 1982) and explained by the fact that the memory requirements increase exponentially with the dimensions of the PDF (Pope, 1985).

Instead, a Monte Carlo simulation may be used for solving the PDF transport equation. The essence of the Monte Carlo technique is to simulate the stochastic process of the flow with the evolution of a large number of particles. The advantage of a Monte Carlo simulation over the finite difference method is that the memory requirements are in linear proportion to the number of the PDF dimensions (Pope, 1985).

The main drawback of the Monte Carlo approach is that it suffers from a statistical

error. It will be shown later that this error is inversely proportional to the square root of number of particles in the ensemble. To decrease the statistical error, the number of particles per cell should increase. In that sense, the PDF method is computationally more expensive compared to moments methods. Table 2.1 contains figures of the number of particles per cell used in practical applications. As shown in the table, that an average number of around 100 particles per cells is used in typical simulations.

In general, transport of physical quantities can either be formulated from an Eulerian or a Lagrangian point of view. These two approaches are reflected in the Monte Carlo simulation of the PDF evolution. With the Eulerian approach, the location of a particle within the cell is irrelevant. That is the particles represent directly field quantities. Transportation of the PDF takes place by replacing a randomly chosen number of particles by particles from the adjacent cells. In the Lagrangian approach, the fluid flow is represented by stochastic particles. The particle does not belong to a certain cell. Rather, it evolves according to the governing stochastic differential equations. These stochastic differential equations govern the evolution of random variables and are equivalent to the PDF transport equation. The mass of the stochastic particle and its other properties are allowed to vary in the course of the particle movement.

Mobus et al. (2001) compared the Eulerian approach to the Lagrangian approach and found the Lagrangian approach is preferred. In general, the Lagrangian Monte Carlo method does not suffer numerical diffusion such as the one encountered in the Eulerian method. It also requires a smaller number of particles to reach the same accuracy level as the Eulerian approach. However, the implementation of the Lagrangian approach is more complicated than the Eulerian approach.

Table 2.1: Examples of the application of PDF method.

Reference	Particles/Cell	PDF Type	Monte Carlo Method	Application
Hsu (1991)	1000	Composition	Eulerian	· H_2 - F_2 diffusion flame.
Tsai and Fox (1994)	50	Velocity-composition	Lagrangian	· Isothermal reaction in a single-jet reactor.
Noreen et al. (1997)	100	Velocity-composition	Lagrangian	· Modelling of natural gas diffusion flame.
Carmen and Feikama (1998)	1000	Composition	Lagrangian	· Spark ignition of premixed Methane. · 1-D spherically symmetric domain.
Cannon et al. (1999)	98	Velocity-composition	Lagrangian	· Bluff body stabilized premixed Methane flame. · The chemistry is solved using in situ adaptive tabulation.
Subramanian and Haworth (2000)	up to 80	Composition	Lagrangian	· Modelling of internal combustion engine. · Turbulent flow solver with deformed mesh.
Xu and Pope (2000)	100	Velocity-composition	Lagrangian	· Prediction of local extinction in piloted premixed Methane jet flame. · 16 steps mechanism using in situ adaptive tabulation
Fueyo et al. (2000)	200	Composition	Lagrangian	· Bluff body stabilized premixed Methane flame. · Comparison of different turbulence models. · Comparison of different reduced chemical mechanisms.

2.3 Summary and Candidate Approach

The purpose of the survey of the turbulent combustion models is to select a method suitable for the application in an optimization scheme. The rule for preferring one method over the other is established by the general requirements stated in Chapter 1, for a combustion model to be used in a design optimization scheme. These requirements may be summarized as high fidelity and computational efficiency.

Models which rely on the assumption of infinitely fast chemistry, such as the eddy break up and Bray-Moss-Libby models for premixed and the eddy dissipation model for diffusion combustion, are excluded. This is because these models fail in predicting emissions such as those of *CO* and *NO*. The reaction mechanisms responsible for *CO* and *NO* are generally slow. Therefore, a combustion model which employs the assumption of infinitely fast chemistry would be questionable in predicting emissions. Considering the evermore stringent regulations, it is hard to imagine an optimization method for gas turbine combustors design which excludes the possibility to minimize emissions.

The models capable of treating finite rate chemistry-finite rate turbulent mixing are the conditional moment closure, the laminar flamelet and the PDF transport models. The conditional moment closure models are the most recently developed and there has so far been few applications of these models to actual combustion systems. Also, the extension of this models to premixed flow is still in its infancy.

Flamelet models employ an attractive concept; the thin reaction zones are detected first, then the combustion in these zones is modelled using laminar flame theory. However, by doing so we implicitly admit that the reaction zone length scale is smaller than even the smallest scale in turbulence (the Kolmogorov scale). In other words, the internal structure of the reaction zone is not influenced by the turbulence fluctuations of the small eddies. This could be true for fast reactions such as fuel oxidizing reactions. However, this is not

be the case for slow reactions.

PDF models have the advantage of treating the chemical reactions exactly and without approximation. This is a remarkable characteristic of these models over the other turbulent combustion models. Also, the PDF models are broad in the sense that they may be applied to both premixed and diffusion flames. In addition, there is no a priori imposed restriction on the PDF shape. The latter is also an attractive property from the physics point of view. On the other hand, the PDF method is expensive from a computational point of view because methods that employ particles simulation usually suffer a statistical error, which is slowly reduced by increasing the number of particles. The use of a large number of particles for simulating the combustion process is then necessary. In fact, as will be seen in chapters 4 and 5, some of the efforts in the present work are devoted to developing models based on the PDF approach which require lower computational time and capacity. These developed models may be considered as attractive candidates for a gas turbine combustor design optimization algorithm.

Chapter 3

Theory and Modelling

3.1 Introduction

Turbulent reactive flow is governed by the equations of continuity, the Navier-Stokes equation, the equations of scalar transport, the energy equation and the equation of state. These equations govern the instantaneous behaviour of the flow variables. It has been shown in Chapter 1 that a direct numerical solution of these equations is theoretically possible but not practical. The argument introduced then was based on the estimation of the number of degrees of freedom (Landau and Lifshitz, 1959), and accordingly, the required computational resolution. It was pointed out that the impractical application of the direct numerical simulation is mainly due to the required computational capacity.

However, the computational cost may not be the only objection to direct simulation. The exceedingly large amount of data generated and even the nature of these data may not be of practical interest. Likely, an engineer is not interested in an instantaneous picture of the flow.

Also, the initial and boundary conditions, in reality, are known only in a statistical sense. There are always hidden parameters. For example, these hidden parameters may

be due to interaction with the background medium or any other activity. In this case, one has to smoothen out the data obtained from direct numerical simulation by averaging. It would be more elegant and even practical if one could construct a theory that requires only the knowledge of the statistical properties of the initial and boundary conditions and consequently reveals the solution in terms of statistical properties. In short, a statistical approach is adapted.¹

The statistical methods for turbulent flow can be generally classified into probabilistic and moment formulations. This classification is rather artificial since both methods can be shown to be mathematically equivalent. The probability density function associated with certain random variable (if it is known) can be used to construct an infinite hierarchy of moments, such as mean, variance, and so on. Vice-versa, if one has complete information of moments, a probability distribution can be constructed in what is called the moment problem (Van Kampen, 1992). For the reasons mentioned in Chapter 2, the probability density formulation is advantageous for turbulent combustion and the present discussion will henceforth be confined to this type of formulation.

Pursuing a probabilistic formulation simply amounts to answering this question: starting with the transport equations that govern the instantaneous behaviour of the state of the flow system, derive a transport equation that governs the joint probability density function of a set of random variables which completely define the state of that system. The derivation of the PDF transport equation will be discussed in the first part of this chapter, specifically, the PDF equation of a single point-single time scalar random variable. The remainder of this chapter will be devoted to the theoretical modelling of this equation.

¹Ironically, the required resolution for direct numerical simulation is estimated by a statistical argument.

3.2 Composition Probability Density Function Transport Equation

3.2.1 Low Mach Number Flow

The assumption of a low Mach number flow in gas turbine combustors is a reasonable one. In fact, low flow speed is required for flame stability and pressure losses considerations. The Mach number usually ranges from 0.1 to 0.2 inside the gas turbine combustors (Lefebvre, 1987). Technically, a low Mach number flow refers to a class of flow that experiences appreciable change of density due to the addition of a substantial amount of heat. As such, it differs from the density change at a higher Mach number ($M > 0.3$), in which the variation of density is due to the compressibility effect. Merkle and Choi (1986) considered this type of flow in detail.

Consider a gas mixture composed of N_s species, where, $\sigma - 1 = N_s$. The species mass fraction is $\Phi_\alpha(\underline{X}, t)$ and $\alpha = 1, 2, \dots, \sigma - 1$. The specific enthalpy is denoted by Φ_σ . These notations are used in such a way that mass fraction and enthalpy can be written in a common form. The pressure is $p(\underline{X}, t)$ and the velocity vector is denoted by $\underline{U}(\underline{X}, t)$. The conservation equations of mass, momentum, chemical species and enthalpy can be written as (Pope, 1985),

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho U_i) = 0 \quad (3.1)$$

$$\rho \frac{DU_j}{Dt} = \frac{\partial \tau_{ij}}{\partial x_i} - \frac{\partial p}{\partial x_j} + \rho g_j \quad (3.2)$$

$$\rho \frac{D\Phi_\alpha}{Dt} = \frac{\partial J_i^\alpha}{\partial x_i} + \rho S_\alpha \quad \alpha = 1, 2, \dots, \sigma \quad (3.3)$$

where the total derivative is,

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + U_i \frac{\partial}{\partial x_i} \quad (3.4)$$

where g_j is the body force (per unit mass) in the x_j direction. τ_{ij} is the sum of the viscous and viscous-diffusive stress tensors (Williams, 1965). S_α ($\alpha = 1, 2, \dots, \sigma - 1$) is the mass rate of addition of species α due to reaction. J_i^α ($\alpha = 1, 2, \dots, \sigma - 1$) is the diffusive mass flux vector of species α . J_i^σ ($\alpha = \sigma$) is the specific energy flux vector due to molecular transport. S_σ ($\alpha = \sigma$) is the source of specific enthalpy. We have,

$$S_\alpha = S_\alpha(\Phi, p) \quad \alpha = 1, 2, \dots, \sigma - 1 \quad (3.5)$$

where Φ is the set of scalars. Together, with the equation of state,

$$\rho = \rho(\Phi, p) \quad (3.6)$$

where ρ is the mixture density. The isothermal non-reactive flow Equations 3.1 and 3.2 are coupled with the thermochemical Equations 3.3, 3.5, and 3.6 through pressure and density. The introduction of a low Mach number assumption will be shown to remove the pressure coupling as follows,

$$p(X, t) = p_o(t) + \Delta p(X, t) \quad (3.7)$$

where $p_o(t)$ is the reference pressure and Δp refers to the pressure variations. Therefore, the pressure gradient can be written as,

$$\frac{\partial p}{\partial x_i} = \frac{\partial}{\partial x_i}(p_o(t) + \Delta p(X, t)) = \frac{\partial \Delta p}{\partial x_i} \quad (3.8)$$

Employing Taylor series expansion of the equation of state, 3.6, around $p_o(t)$,

$$\rho(\Phi, p) = \rho(\Phi, p_o) \left\{ 1 + \frac{p_o}{\rho} \frac{\partial \rho}{\partial p} \frac{\Delta p}{p_o} + \dots \right\} \quad (3.9)$$

$\frac{\Delta p}{p_o}$ can be estimated as,

$$\Delta p \approx \rho U^2 \approx M^2(\rho a^2) \quad (3.10)$$

U is the characteristic (reference) velocity inside the combustor and a is the speed of sound.

$$a = \sqrt{\frac{\gamma p_o}{\rho}} \quad (3.11)$$

Therefore,

$$\frac{\Delta p}{p_o} \approx M^2 \quad (3.12)$$

At low Mach number, $\frac{\Delta p}{p_o}$ is small compared to unity. Therefore, Equation 3.9 can be written as,

$$\rho = \rho(\Phi, p_o) \quad (3.13)$$

Similarly,

$$S_\alpha = S_\alpha(\Phi, p_o) \quad \alpha = 1, 2, \dots, \sigma - 1 \quad (3.14)$$

Employing similar assumptions, it can be shown that,

$$S_\alpha = (\Phi, p_o, \frac{dp_o}{dt}) \quad \alpha = \sigma \quad (3.15)$$

In gas turbines (unlike internal combustion engines) p_o does not vary significantly with time. Therefore,

$$S_\alpha = S_\alpha(\Phi, p_o) \quad \alpha = \sigma \quad (3.16)$$

However, the momentum equation assumes no dependence on p_o . Therefore, the assumption of low Mach number removes the pressure coupling, so we can write,

$$\rho = \rho(\Phi) \quad (3.17)$$

$$S_\alpha = S_\alpha(\Phi) \quad \alpha = 1, 2, \dots, \sigma \quad (3.18)$$

3.2.2 Probability Density Functional

For simplicity, assume a two-dimensional flow with physical boundaries $0 < x < a$ and $0 < y < b$, as shown in Figure 3.1. Suppose that the physical domain is covered by $N \times N$ discrete points. Assume that the state of the system is described in terms of the scalar random variable $\Phi(x_n, y_n)$, where x_n and y_n are coordinates of an arbitrary point (n). Therefore, to specify the state of the system completely at time(t), one needs to know the value $\Phi(x_n, y_n)$ for all the points $N \times N$, simultaneously at that time. However, this is not the only way to describe the state of the system. Instead of the two-dimensional system (Figure 3.1) in which the state of the system is represented by $N \times N$ points, one can

Figure 3.1: Two-dimensional flow domain.

construct $N \times N$ coordinate system in which the state of the system at hand is described by only one point. Eventually, each one of the $N \times N$ coordinates represents the range of all possible values that the variable Φ can assume at point (n) . This new coordinate system is called phase space and its coordinate variables will be denoted by Ψ . It is easy to show that when the state of the system changes as a function of time, it will be represented as a path or trajectory in the phase space, as illustrated in Figure 3.2.

Each point on this trajectory represents the state of the flow system at a given time while the initial point, where the trajectory starts, represents the initial conditions of the system at time t_0 . If the initial state of the system deviated slightly, the evolution of the system will follow another trajectory. Furthermore, trajectories must not intersect, this follows from the uniqueness of solution.

Representation of the flow domain by a discrete number of $(N \times N)$ points is an approximation. In reality, the domain is continuous and described by an infinite number of points. Mathematically, this can be obtained by starting with a discrete representation and then taking the limits when $N \rightarrow \infty$. The corresponding phase space coordinate system is composed of an infinite number of coordinates, $\Psi(x_1, y_1), \Psi(x_2, y_2) \dots \Psi(x_N, y_N)$ and

Figure 3.2: Representation of the time evolution of the flow system in the phase space coordinate system.

$N \rightarrow \infty$.

By developing the phase space coordinate system, the statistical element can be introduced in a straightforward manner. At this point, let us assume that the initial conditions are not precisely known. That is to say, our knowledge of the initial conditions are in terms of some statistical property rather than an instantaneous one. Whatever the reason for the lack of precise knowledge of the initial conditions, it is irrelevant to our procedures and should not affect the final conclusions.

In that case, the initial conditions will be represented by a finite region in the phase space. Moreover, this region is precisely defined by the statistical properties at hand. Let us illustrate this point with a simple example. Assume two variables a and b , such that $1 \leq a \leq 4$ and $6 \leq b \leq 8$. It is assumed also that all that is known about a and b is their arithmetic average, say 5. Therefore, acceptable combinations of a and b are (2,8), (4,6), (3,7), (2.1, 7.9), and so on. In fact, there are infinite number of combinations. The combination (1.5, 8.5) is not permissible. Clearly, the possible values of a and b can be represented in phase space a^*b^* , as shown in Figure 3.3. All the points on the thick line are defined by constraints on both arithmetic averages and a, b ranges.

Figure 3.3: Phase space representation of combinations of random variables a and b .

It may be possible now to draw some conclusions. A set of initial conditions (instantaneous) that is compatible with some specified statistical properties (say, averages) are equivalent to the observer, who is only interested in statistical quantities. One way of expressing this idea mathematically is to attach certain weights to all the possible instantaneous states.

For example, a weight zero is given to states that do not match the statistical constraints, while equal weights are given to the states that are compatible with this constraint. Such a set of weighted points is called an ensemble. Furthermore, it may be noted that by giving a priori equal weights to each compatible (instantaneous) state, then the influence of these (instantaneous) states on the monitored statistical properties is uniquely determined by its frequency of occurrence. This gives the required link with the theory of probability.

Consider for simplicity a one-dimensional flow. In phase space representation, there is an infinite number of coordinates $\Psi(x_1), \Psi(x_1), \dots, \Psi(x_N)$ and $N \rightarrow \infty$. Assume that our weight function is $P(\Psi(x_1), \Psi(x_1), \dots, \Psi(x_N), t)$. In the limit $N \rightarrow \infty$, it is written as (Beran, 1968),

$$P(\Psi(x_1), \Psi(x_1), \dots, \Psi(x_N), t) = P[\Psi(x), t] \quad N \rightarrow \infty \quad (3.19)$$

$P[\Psi(x), t]$ is called a functional (in the sense of Volterra (1959)).

A functional is a quantity which depends on all the infinite number of values which a function $\Psi(x)$ takes at some interval $a \leq x \leq b$. Then the average of an arbitrary function of the instantaneous states $F(\Psi(x_1), \Psi(x_1), \dots, \Psi(x_N), t)$ and $N \rightarrow \infty$, is calculated as,

$$\langle F \rangle = \int_{\Omega} F(\Psi) dP[\Psi(x), t] \quad (3.20)$$

The integral is over the whole phase space. Equation 3.20 can be easily derived starting by the definition of the average and considering a discrete number of points. Then, when the number of points tends to infinity, the summation is replaced by an integral. If $P[\Psi(x), t]$ is non-negative and furthermore, is normalized such that,

$$\int_{\Omega} dP[\Psi(x), t] = 1 \quad (3.21)$$

Then, it is a probability density functional. Starting with the probability density functional and the notion of phase space, together with the turbulent flow equations, a transport equation governing the functional probability density can be derived. This has first been done by Hopf (1952).

Hopf considered a single time probability density functional for the velocity random variable. This has been generalized by Lewis and Kraichnan (1962) for multi-times distribution. The Hopf technique was applied by Dopazo and O'Brien (1974) to derive a functional probability formalism for the turbulent reactive flow.

Due to the extreme complexity of the probability functional equations, it is sufficient for

our purpose to discuss its characteristics and importance without going into mathematical details.

First, the probability density functional equation is closed and linear. It is equivalent to the Liouville equation in classical mechanics (Foias et al., 1987). Therefore, it can be written in the general form,

$$\frac{\partial}{\partial t} P[\Psi(x), t] = \mathcal{L} P[\Psi(x), t] \quad (3.22)$$

where $\mathcal{L}$ is a complicated operator.²

In spite of the fact that Equation 3.22 is linear and closed, there is no known closed form solution to this type of equation. However, the functional formulation is still useful in many ways. It can be used to derive reduced probability distributions such as the single point PDF and the joint two points PDF. Also, a compact formal solution for Equation 3.22 in terms of the operator, $\mathcal{L}$, can be obtained. This solution is formal in the sense that it is not amenable to calculations since it is a function of the operator $\mathcal{L}$. However, this formal solution can be used as a starting point for some powerful techniques such as projection operators (Zwanzing, 2000). Zwanzing and others have used the projection operators technique to derive a generalized Langevin equation for different stochastic systems. However, these techniques are not widely used in turbulent reactive flow. This may be attributed to the extreme complexity of the problem.

3.2.3 Single Point Composition PDF Transport Equation

Lundgren (1967) derived a hierarchy of reduced probability density functions for turbulent flow random field. This hierarchy is similar to the Bogliubov-Born-Green-Kirkwood-

²For a specific form of the operator ($\mathcal{L}$), compare Equation 3.22 to Equation 15 in Dopazo and O'Brien (1974).

Yvon (BBGKY) hierarchy in statistical mechanics (Balescu, 1975). Later, Dopazo and O'Brien (1974) derived reduced PDF equations for turbulent reactive flow. In practice, only single point PDF is amenable to a solution. Higher order distributions lead to extreme complexity.

One simple way to derive the PDF transport equation is to define a fine grained PDF,

$$\wp(\Psi; \underline{X}, t) = \delta(\Phi(\underline{X}, t) - \Psi) \quad (3.23)$$

This is a dirac delta function. $\underline{X}$ is a position vector in physical space, $\Phi(\underline{X}, t)$ is the scalar random variable and Ψ is the corresponding sample space independent variable. One can think of a fine-grained PDF as a filter. It singles out all members of the ensemble except the realized one. Therefore, its role is to give a probability density representation of each single realization of the random field. By definition, one point PDF of the scalar $\Phi(\underline{X}, t)$ can be calculated as,

$$P(\Psi; \underline{X}, t) = \langle \delta(\Phi(\underline{X}, t) - \Psi) \rangle \quad (3.24)$$

while a joint PDF for velocity $\underline{U}(\underline{X}, t)$ and scalar $\Phi(\underline{X}, t)$ can be written as,

$$P(\underline{V}, \Psi; \underline{X}, t) = \langle \delta(\underline{U}(\underline{X}, t) - \underline{V}) \delta(\Phi(\underline{X}, t) - \Psi) \rangle \quad (3.25)$$

where $\underline{V}$ is the sample space random variable corresponding to $\underline{U}(\underline{X}, t)$. As an example, we derive the PDF equation for constant density, constant diffusivity and single species reactive field. The scalar transport equation for this flow is written as,

$$\frac{\partial \Phi}{\partial t} + U_j \frac{\partial \Phi}{\partial x_j} = D \frac{\partial^2 \Phi}{\partial x_j \partial x_j} + \dot{W} \quad (3.26)$$

where D is the diffusivity coefficient and $\dot{W}$, the rate of production of species i .

The functional dependence in Equation 3.26 is to be understood on space and time.

The time derivative of $\wp(\Psi; X, t)$ is calculated as,

$$\begin{aligned} \frac{\partial \wp}{\partial t} &= \frac{\partial \delta(\Phi - \Psi)}{\partial t} \\ &= \frac{\partial \delta(\Phi - \Psi)}{\partial \Phi} \cdot \frac{\partial \Phi}{\partial t} \\ &= -\frac{\partial \delta(\Phi - \Psi)}{\partial \Psi} \cdot \frac{\partial \Phi}{\partial t} \\ &= -\frac{\partial \wp}{\partial \Psi} \cdot \frac{\partial \Phi}{\partial t} \end{aligned} \quad (3.27)$$

Substituting $\frac{\partial \Phi}{\partial t}$ from Equation 3.26, we arrive at,

$$\frac{\partial \wp}{\partial t} = U_j \frac{\partial \wp}{\partial \Psi} \frac{\partial \Phi}{\partial x_j} - D \frac{\partial \wp}{\partial \Psi} \frac{\partial^2 \Phi}{\partial x_j \partial x_j} - \frac{\partial \wp}{\partial \Psi} \dot{W} \quad (3.28)$$

Further manipulation of Equation 3.28 leads to

$$\frac{\partial \wp}{\partial t} = -U_j \frac{\partial \wp}{\partial \Phi} \frac{\partial \Phi}{\partial x_j} - D \frac{\partial}{\partial \Psi} \left(\wp \frac{\partial^2 \Phi}{\partial x_j \partial x_j} \right) - \frac{\partial}{\partial \Psi} (\wp \dot{W}) \quad (3.29)$$

Therefore,

$$\frac{\partial \wp}{\partial t} + \frac{\partial}{\partial \Psi} (\wp \dot{W}) = -U_j \frac{\partial \wp}{\partial x_j} - D \frac{\partial}{\partial \Psi} \left(\wp \frac{\partial^2 \Phi}{\partial x_j \partial x_j} \right) \quad (3.30)$$

The last term on the right-hand side of Equation 3.30 can be further manipulated as follows,

$$\begin{aligned}
\frac{\partial^2 \wp}{\partial x_j \partial x_j} &= \frac{\partial}{\partial x_j} \left(\frac{\partial \wp}{\partial x_j} \right) \\
&= \frac{\partial}{\partial x_j} \left(\frac{\partial \wp}{\partial \Phi} \cdot \frac{\partial \Phi}{\partial x_j} \right) \\
&= \left(\frac{\partial}{\partial x_j} \left(-\frac{\partial \wp}{\partial \Psi} \right) \right) \left(\frac{\partial \Phi}{\partial x_j} \right) + \left(\frac{\partial^2 \Phi}{\partial x_j \partial x_j} \right) \left(-\frac{\partial \wp}{\partial \Psi} \right) \\
&= \frac{\partial}{\partial \Phi} \left(-\frac{\partial \wp}{\partial \Psi} \right) \left(\frac{\partial \Phi}{\partial x_j} \right) \left(\frac{\partial \Phi}{\partial x_j} \right) - \frac{\partial}{\partial \Psi} \left(\wp \frac{\partial^2 \Phi}{\partial x_j \partial x_j} \right) \\
&= \frac{\partial^2}{\partial \Psi^2} \left(\left(\frac{\partial \Phi}{\partial x_j} \right)^2 \wp \right) - \frac{\partial}{\partial \Psi} \left(\wp \frac{\partial^2 \Phi}{\partial x_j \partial x_j} \right) \tag{3.31}
\end{aligned}$$

Therefore,

$$-\frac{\partial}{\partial \Psi} \left(\wp \frac{\partial^2 \Phi}{\partial x_j \partial x_j} \right) = \frac{\partial^2 \wp}{\partial x_j \partial x_j} - \frac{\partial^2}{\partial \Psi^2} \left(\left(\frac{\partial \Phi}{\partial x_j} \right)^2 \wp \right) \tag{3.32}$$

Substituting in Equation 3.30, we obtain,

$$\frac{\partial \wp}{\partial t} + \frac{\partial}{\partial \Psi} (\wp \dot{W}) = -U_j \frac{\partial \wp}{\partial x_j} + D \frac{\partial^2 \wp}{\partial x_j \partial x_j} - D \frac{\partial^2}{\partial \Psi^2} \left(\left(\frac{\partial \Phi}{\partial x_j} \right)^2 \wp \right) \tag{3.33}$$

Equations 3.30 and 3.33 are equivalent. However, Equation 3.33 may be preferred whenever molecular transport (represented by the second term on the right-hand side) is neglected compared to the turbulent mixing term (the last term on the right-hand side). Taking the ensemble average of Equations 3.30 and 3.33 leads to the transport equation of the PDF,

$P(\Psi; \underline{X}, t)$,

$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial \Psi} (P\dot{W}) = -\frac{\partial}{\partial x_j} \langle U_j \wp \rangle - D \frac{\partial}{\partial \Psi} \left\langle \wp \frac{\partial^2 \Phi}{\partial x_j \partial x_j} \right\rangle \quad (3.34)$$

and,

$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial \Psi} (P\dot{W}) = -\frac{\partial}{\partial x_j} \langle U_j \wp \rangle + D \frac{\partial^2 P}{\partial x_j \partial x_j} - D \frac{\partial^2}{\partial \Psi^2} \left\langle \left(\frac{\partial \Phi}{\partial x_j} \right)^2 \wp \right\rangle \quad (3.35)$$

In both Equations 3.34 and 3.35, the first and last term on the right-hand side are unknown and require modelling.

The hierarchical nature of the reduced PDF equations is not clear in Equations 3.34 and 3.35. An alternative formulation which emphasizes this characteristic can also be derived. Let us consider, for example, the unknown term “ $D \frac{\partial}{\partial \Psi} \left\langle \frac{\partial^2 \Phi}{\partial x_j \partial x_j} \wp \right\rangle$ ”, noting that,

$$\int \delta(\Phi(\underline{X}, t) - \Psi^*) d\Psi^* = 1 \quad (3.36)$$

where $\underline{X}^*$ is an arbitrary point different from $\underline{X}$, and Ψ^* is the sample space variable corresponding to $\Phi(\underline{X}^*, t)$. We can thus write,

$$\begin{aligned}
D \frac{\partial}{\partial \Psi} \left\langle \frac{\partial^2 \Phi(\underline{X}, t)}{\partial x_j \partial x_j} \varphi \right\rangle &= D \frac{\partial}{\partial \Psi} \left\langle \frac{\partial^2 \Phi(\underline{X}, t)}{\partial x_j \partial x_j} \delta(\Phi(\underline{X}, t) - \Psi) \right\rangle \int \delta(\Phi(\underline{X}^*, t) - \Psi^*) d\Psi^* \\
&= D \frac{\partial}{\partial \Psi} \lim_{x_j^* \rightarrow x_j} \frac{\partial^2}{\partial x_j^* \partial x_j^*} \int \langle \Phi(\underline{X}^*, t) \delta(\Phi(\underline{X}, t) - \Psi) \\
&\quad \times \delta(\Phi(\underline{X}^*, t) - \Psi^*) \rangle d\Psi^* \\
&= D \frac{\partial}{\partial \Psi} \lim_{x_j^* \rightarrow x_j} \frac{\partial^2}{\partial x_j^* \partial x_j^*} \int \Psi^* P(\Psi, \Psi^*; \underline{X}, \underline{X}^*, t) d\Psi^* \quad (3.37)
\end{aligned}$$

With similar treatment of the first term on the right-hand side of Equation 3.34, the PDF transport equation can be written as,

$$\begin{aligned}
\frac{\partial P(\Psi; \underline{X}, t)}{\partial t} + \frac{\partial}{\partial \Psi} (P(\Psi; \underline{X}, t) \dot{W}) &= - \frac{\partial}{\partial x_j} \int V_j P(\underline{V}, \Psi; \underline{X}, t) d\underline{V} \\
&\quad - D \frac{\partial}{\partial \Psi} \lim_{x_j^* \rightarrow x_j} \frac{\partial^2}{\partial x_j^* \partial x_j^*} \int \Psi^* P(\Psi, \Psi^*; \underline{X}, \underline{X}^*, t) d\Psi^* \quad (3.38)
\end{aligned}$$

where $\underline{V}$ is the sample space variable corresponding to the velocity random variable $\underline{U}$ at point $\underline{X}$. The hierarchy of unclosed PDF equations is obvious in Equation 3.38. The transport equation of the single point PDF of the scalar random variable contains terms with higher order distributions. The first term on the right-hand side contains a joint velocity-scalar PDF. The second on the right-hand side contains a two point scalar PDF distribution. Therefore, more PDF transport equations are required for the higher order PDF distributions. Consequently, the hierarchy continues.

Equation 3.38 is a balance equation for the single point PDF of the scalar random

variable. The first term on the left-hand side is the unsteady term. The second term on the left-hand side is the reaction term. It represents a convection in the phase space and it is closed. This closed term demonstrates the power of the PDF formulation in turbulent reactive flow. The first term on the right-hand side represents convection in the physical space $\underline{X}$, i.e., due to flow motion. It can be further written as a summation of mean and turbulent convection. The latter may be seen as an unclosed turbulent diffusion flux,

$$\begin{aligned} \frac{\partial}{\partial x_j} \int V_j P(\underline{V}, \Psi; \underline{X}, t) d\underline{V} &= \frac{\partial}{\partial x_j} (\langle U_j \rangle P(\Psi; \underline{X}, t)) \\ &+ \frac{\partial}{\partial x_j} \int (V_j - \langle U_j \rangle) P(\underline{V}, \Psi; \underline{X}, t) d\underline{V} \end{aligned} \quad (3.39)$$

The last term on the right-hand side of Equation 3.39 is due to the correlation between velocity fluctuation and scalar. In Equation 3.38, the last term on the right-hand side is a mixing term, meaning it is responsible for the dissipation of the scalar fluctuations. It is also unclosed as it contains two point PDF distribution.

Equation 3.38 can be easily generalized into the case of three-dimensional, variable density, variable diffusivity and multiple reactive species. Moreover, it is written for Favre-averaged PDF³. Thus we have,

$$\begin{aligned} \frac{\partial}{\partial t} \langle \rho \rangle \tilde{P}(\underline{\Psi}) + \frac{\partial}{\partial x_j} \langle \rho \rangle \int V_j \tilde{P}(\underline{V}, \underline{\Psi}) d\underline{V} &= - \sum_{i=1}^{Ns+1} \frac{\partial}{\partial \Psi_i} (\langle \rho \rangle \dot{W}_i(\underline{\Psi}) \tilde{P}(\underline{\Psi})) \\ &= - \sum_{i=1}^{Ns+1} \frac{\partial}{\partial \Psi_i} \left[\lim_{x_j^* \rightarrow x_j} \frac{\partial}{\partial x_j^*} \langle \rho \rangle D_i \frac{\partial}{\partial x_j^*} \int \Psi^* \tilde{P}(\Psi^*, \underline{\Psi}) d\Psi^* \right] \end{aligned} \quad (3.40)$$

³For procedures and notations of Favre averaging, refer to Chapter 2.

Here the functional dependence on time and space was omitted for the sake of simplicity.

3.3 Modelling of the Composition PDF Transport Equation

3.3.1 Background

The purpose of this section is to discuss some of the ideas, definitions and techniques that are thought to be helpful in understanding and constructing solvable models for the PDF transport equation.

It was mentioned that a closed statistical description of the turbulent reactive flow in terms of probability density functional is possible. Unfortunately, there is no known closed form solution for this equation. Instead, one must adopt a reduced PDF formulation (such as a single point PDF). An interesting observation can be made here. The term which originates from the highly non-linear reaction is closed. On the other hand, the term which originates from linear diffusion is unclosed (turbulent mixing term).

However, this should not be surprising. That is, when one admits a single point PDF formulation, he is actually isolating each point at a time from the surrounding ones. In so doing, the effect of the surrounding points appears as an unclosed term. Although the reaction term is highly non-linear, it is local in character. This is apparent from the fact that this term does not contain any spatial derivatives. For a similar reason, a diffusion term which contains a spatial derivative (two point process) leads to a closure problem.

The closure problem arising in this context can be looked at as a purely mathematical problem. One wishes to replace the unknown term with an equivalent expression which is a function of the dependent variable and/or its derivatives. In other words, a term which is amenable to calculation. Generally speaking, one may attempt to expand the unknown

term as a summation of a series of canonical distributions, then apply a proper truncation to this series.

An example of this type of work in turbulent scalar transport and mixing was done by Saffman (1969). Following suggestions by Wiener (1938), Saffman expanded the scalar random variable in terms of what is called Wiener-Hermite functionals. The first term in this expansion is Gaussian, while the higher order terms are successively further and further removed from Gaussianity⁴. However, the results of Saffman's work and other similar works are not very encouraging. The lesson is that physical intuition, which simplifies the analysis, is desirable.

As previously mentioned, similar kinds of reduced probability distribution equations arise in the field of statistical mechanics. One of the earliest attempts at constructing and solving such equations was Einstein's treatment of the Brownian motion (Gardiner, 1985). The Brownian motion refers to a small but macroscopic particle immersed in a fluid. Fluid molecules collide with the particle leading to a motion of the particle of random and irregular character.

On the microscopic scale, the complete solution of Brownian particles would consist of solving all the microscopic equations that govern the motion of this particle and the interacting fluid molecules. This is an impossible task. Instead, the very irregular motion (function) can be smoothed out by averaging over a suitable time interval. Equivalently this averaging can be done over an ensemble of particles rather than time averaging. That is to say, one describes this highly irregular motion (large number of variables or microscopic variables) by a smooth motion (reduced number of variables or macroscopic variables). But doing that alone is hardly convenient. One has to account for the ignorance of the smoothed out details. This can be done by introducing the fluctuation terms by which the ignored variables make themselves felt. As a consequence, the macroscopic variables are

⁴Wiener-Hermite expansion is applied directly to the random variable. Probability density distributions can be also expanded, for example, using what is called Gram-Charlier or Edgeworth series.

a stochastic function of time (stochastic process). The art of stochastic modelling lies in how one introduces these fluctuations in such a way that the reduced (simplified) system can properly replace the detailed one.

These concepts first appeared in the treatment of the Brownian motion. For simplicity, assume a one-dimensional Brownian motion. Each impact will cause the particle to jump randomly in (+ve) or (-ve) direction. This model is referred to in the mathematical theory of probability as the random walk model. The k^{th} step displacement of the particle (Δx_k) is assumed to be a Markovian process. This means that the probability of the particle performing displacement (Δx_k) in the k^{th} step does not depend on the history of its previous steps. The validity of this assumption can be reasonably supported by a suitable choice of the time scale (Δt) for which (Δx_k) is to be observed. In this case, the chosen time scale should be very small compared to the observation time of the particle motion but sufficiently large so that the two successive displacements are independent of each other. Einstein derived an equation governing the probability distribution of the position of the particle,

$$\frac{\partial P(x; t)}{\partial t} = D \frac{\partial^2 P(x; t)}{\partial x^2} \quad (3.41)$$

where D is the diffusion coefficient and is connected to the microscopic jumps of the particle (Δx) through,

$$D = \frac{\langle (\Delta x)^2 \rangle}{2\Delta t} \quad (3.42)$$

Note that Equation 3.41 is closed with respect to the probability distribution $P(x; t)$. The effect of fluctuations is solely introduced by the diffusion coefficients. Because D is assumed to be known in advance, and not derived from the theory, it is referred to as a phenomenological theory.

Equation 3.41 is a special case of what is known in the theory of stochastic process as a Fokker-Planck equation,

$$\frac{\partial P(y; t)}{\partial t} = -\frac{\partial}{\partial y}(A(y)P(y; t)) + \frac{1}{2}\frac{\partial^2}{\partial y^2}(B(y)P(y; t)) \quad (3.43)$$

where the first term on the right-hand side is called a drift term and the second term on the right-hand side is called the fluctuation term. $A(y)$ and $B(y)$ are arbitrary functions of y and are called drift and diffusion coefficients, respectively.

In using the Fokker-Planck equation for modelling fluctuating variables, the problem is reduced to finding $A(y)$ and $B(y)$. Usually $A(y)$ is determined from the macroscopic (deterministic) part of the motion. $B(y)$ is determined from the fluctuating part of the motion, usually introduced by the diffusion coefficient. Later, we will use this equation in modelling the turbulent flux term in the PDF transport equation. The Fokker-Planck equation was used by Fox (1992; 1994) for modelling the turbulent mixing term in the PDF transport equation. The theory of the Fokker-Planck equation is covered in a book by Risken (1989).

An alternative and more direct method for the Brownian motion was introduced by Langevin (1908). In this method, one deals directly with the equation of motion rather than the PDF equation (Fokker-Planck for example). The fluctuations are introduced by adding a random or noise term to the equation of motion. Let us consider, for example, a Brownian particle moving in a fluid. Newton's second law can be written as,

$$\dot{v} = -\gamma v + L(t) \quad (3.44)$$

The left-hand side is the acceleration per unit mass of the particle. v is the velocity and

γ is the friction coefficient between the particle and the fluid. $(-\gamma v)$ is the friction force affecting the particle during its motion. $L(t)$ are irregular or random forces which are not fully known. However, they represent the fluctuating forces due to molecular collisions with the particle. Some postulates can be made about $L(t)$,

$$\langle L(t) \rangle = 0 \quad (3.45)$$

This follows from the assumption that $L(t)$ is purely random. Moreover, $L(t)$ is caused by collisions of the particles with the molecules of the surrounding fluids. These collisions can be assumed to be instantaneous. In addition, if two successive collisions can be assumed to be independent, then the autocorrelation function of the random force can be written as,

$$\langle L(t)L(t') \rangle = \Gamma \delta(t - t') \quad (3.46)$$

where Γ is a constant representing the strength of collision. If Γ is specified, then the first moment (Equation 3.45) and the second moment (Equation 3.46) are completely specified. Γ can be found by solving the differential Equation 3.44 for $v(t)$, then applying the condition,

$$\lim_{t \rightarrow \infty} \langle v(t)^2 \rangle = kT \quad (3.47)$$

where T is the average temperature of the molecules and k is the Boltzman constant. This condition follows from the kinetic theory; the molecular mean velocity must have the equilibrium distribution given by Equation 3.47.

Langevin Equation 3.44, together with Equation 3.46, can be shown to be equivalent to the Fokker-Planck equation of the form:

$$\frac{\partial P(v; t)}{\partial t} = \gamma \frac{\partial}{\partial v} v P(v; t) + \frac{\Gamma}{2} \frac{\partial^2 P(v; t)}{\partial v^2} \quad (3.48)$$

Application of the Langevin approach in turbulent flow was first proposed by Landau and Lifshitz (1959). Later, it was applied by Chung (1969) for modelling the turbulent flow particles motion (Langrangian approach) in turbulent reactive flow. In an analogy to the equilibrium distribution given for Brownian particle by kinetic theorem, Chung used Kolmogorov structure functions for small scale as an equilibrium distribution. Thus, in both cases, Brownian motion and turbulent flow, the Langevin equation is written in such a way as to give an equilibrium distribution in the limit of long time. Haworth and Pope (1986) used what is called the generalized Langevin equation, derived first by Zwanzig (1961), to model turbulent Langrangian motion of fluid particles. The generalized Langevin equation includes memory effect and therefore can be applied to the more general non-Markovian process. The application of the generalized Langevin equation to general turbulent flow encounters extreme complications such that simplifying assumptions have to be introduced (Pope, 1994). The Langevin approach was also used by Valino and Dopazo (1991) to model the unclosed turbulent mixing term in the PDF equation.

The introduction of Langevin equation has led to what is known in the mathematical literature as the stochastic differential equation. Here, we briefly discuss some features of this class of differential equations as it will be used extensively in modelling turbulent combustion in latter chapters. Consider the non-linear Langevin equation,

$$\dot{v} = A(v) + C(v)L(t) \quad (3.49)$$

where the autocorrelation function of $L(t)$ is given by Equation 3.46. That is, the autocorrelation of $L(t)$ is a Dirac delta function. This idealization of the autocorrelation leads to some mathematical difficulties. $L(t)$ itself can be seen as a sequence of delta peaks arriving

at random times. It is usually called white noise. Therefore, in considering the coefficient $C(v)$, one is confronted with a dilemma: at which value of v should $C(v)$ be evaluated. In other words, should $C(v)$ be determined before the jump of the delta function or after the jump or as their mean value. In fact, different interpretations have been proposed to the stochastic differential Equation 3.49.

As one would expect, each interpretation leads to a slightly different equivalent Fokker-Planck equation. In the present work, we adopt what is called *Ito* interpretation or *Ito* calculus or sometimes the stochastic differential equation. According to *Ito*, the appropriate value of v is the one before the arrival of the delta peak (Arnold, 1974). By integrating Equation 3.49 with *Ito* interpretation,

$$v(t + \Delta t) - v(t) = A(v(t))\Delta t + C(v(t)) \int_t^{t+\Delta t} L(t')dt' \quad (3.50)$$

This equation is usually written in differential form as,

$$dv = A(v)dt + C(v)dW(t) \quad (3.51)$$

This is a stochastic differential equation for the process v . The process v defined by Equation 3.51 is called a diffusion process and it is a Markovian process. W is called the Wiener process. It is a Gaussian process, which means that it is completely defined by the first and second order statistics. Moreover, it is an additive process or alternatively, a process with independent increments. The Wiener process is an example of a “nowhere differentiable” process.

Before proceeding to discuss more stochastic models of the reduced PDF equation, we summarize some important features of both the Langevin and Fokker-Planck approaches. In both the Langevin and Fokker-Planck equations, the many-body problem is reduced to one body problem. That is, the coupling or interaction is removed. This removal is substi-

tuted so that the stochastic fluctuations will lead the body under consideration to reveal “a priori” known equilibrium distribution in the long time behaviour. If the Fokker-Planck equation is used, this equilibrium distribution is introduced through the diffusion coefficient. If the Langevin equation is used, this equilibrium distribution is introduced directly through the equilibrium distribution which is also known as the fluctuation dissipation theorem.

Another approach of more fundamental character worth highlighting is the Boltzman equation (Balescu, 1975). It is the first closed equation for the distribution function of position and velocity of molecules in dilute gases. Let $f(\underline{X}, \underline{v}, t)d\underline{X}d\underline{v}$ be the number of molecules in the volume element $d\underline{X}d\underline{v}$ of velocity and position space (phase space). $\underline{X}$ and $\underline{v}$ are three-dimensional vectors. Assuming zero external force field, the Boltzman equation is written as,

$$\frac{\partial f}{\partial t}(\underline{X}, \underline{v}; t) + \underline{v} \cdot \nabla f(\underline{X}, \underline{v}; t) = \left(\frac{\partial f}{\partial t} \right)_{coll} \quad (3.52)$$

where the collision operator is written as,

$$\left(\frac{\partial f}{\partial t} \right)_{coll} = \int d\underline{v}_1 \int d\Omega |\underline{v} - \underline{v}_1| \sigma(\underline{v}, \underline{v}_1 | \underline{v}', \underline{v}'_1) [f(\underline{X}, \underline{v}'; t) f(\underline{X}, \underline{v}'_1; t) - f(\underline{X}, \underline{v}; t) f(\underline{X}, \underline{v}_1; t)] \quad (3.53)$$

$\sigma(\underline{v}, \underline{v}_1 | \underline{v}', \underline{v}'_1)$ is called the differential scattering cross section and depends on the nature of collision (Landau and Lifshitz, 1976). $\underline{v}, \underline{v}_1$ and $\underline{v}', \underline{v}'_1$ are the velocities of the two colliding molecules before and after collision. Ω is the space angle between the relative velocities $\underline{v} - \underline{v}_1$ and $\underline{v}' - \underline{v}'_1$. Equation 3.52 is closed but it is non-linear. The non-linearity is apparent in the expression of the collision operator given by Equation 3.53. To arrive at this form of this important operator, one considers solving the classical problem of two-body collision

(two-body problem).

Assuming two molecules of equal masses, the conservation of momentum and energy is applied,

$$\boldsymbol{v} + \boldsymbol{v}_1 = \boldsymbol{v}' + \boldsymbol{v}'_1 \quad (3.54)$$

$$||\boldsymbol{v}||^2 + ||\boldsymbol{v}_1||^2 = ||\boldsymbol{v}'||^2 + ||\boldsymbol{v}'_1||^2 \quad (3.55)$$

Equations 3.54 and 3.55 are four equations with six unknowns. In order to solve for the remaining unknowns, one has to assume a law of interaction (Landau and Lifshitz, 1976).

It is particularly interesting to compare some important features of the techniques used in modelling the Fokker-Planck and Langevin equations, on one hand, and the Boltzman equation, on the other. In the Boltzman equation, no information is requested for equilibrium distribution (long time behaviour) nor for the diffusion coefficient. The only ad-hoc argument introduced in the Boltzman equation is the law of interaction between the colliding particles. In turn, this law of interaction can be estimated by considering a simple problem to which the results are known. In that sense, the Boltzman equation is a more powerful and honest approach than Langevin and Fokker-Planck equations. However, on using the Boltzman equation, a price is paid in the form of the non-linearity of this equation and the arbitrariness in specifying the law of interaction.

Again, there exists a particular class of models used in closing the scalar PDF transport equation in turbulent reactive flow which has relied heavily on this form of the Boltzman collision operator. There is a striking similarity between what is called coalescence dispersion mixing model (sometimes called Curl mixing model) and the collision operator in the kinetic equation (Curl, 1963; Kattan and Adler, 1972). The Curl model and its modification will be discussed in detail later. For now, it is sufficient to point out that

the Curl model amounts to modelling the mixing process by collisions. During these non-physical or imaginary collisions, particles exchange their concentrations and temperatures according to a pre-assumed law of interaction.

So far, we have encountered a strong resemblance between the stochastic models in statistical mechanics and the closure approximations of PDF transport equation of the turbulent scalar. Naturally, this raises an interesting question about the credibility of extending these techniques for modelling turbulent combustion. In other words, are the circumstances that guarantee the success of these models in statistical mechanics still relevant to turbulent reactive flow. Here we should emphasize the fact that this extension is by no means straightforward (McComb, 1990). When extending these models to turbulent reactive flow, difficulties will be encountered.

For example, it is possible to find a time scale separation in the statistical treatment of molecular motion. In dilute gases, the collision time scale is small compared to the time between collisions. In this case, the ratio of the two time scales is a small parameter. This allows series expansion and truncation in terms of the power of the small parameter.

That is not the case with turbulent reactive flow. There is always a cascade of time and length scales and consequently, there is no clear scale separation between them. This observation was made in the early years of treating turbulence. Taylor (1921), in his treatment of turbulent diffusion, adapted a Lagrangian picture of the fluid particles. In other words, the diffusion results from random and turbulent motion. Taylor raises the question of the possibilities of extending the statistical mechanics methods to the turbulent diffusion at the start of his article: “It has been shown by the author⁵ and others that turbulent motion is capable of diffusing heat and other diffusible properties through the interior of a fluid in much the same way that molecular agitation gives rise to molecular diffusion. In the case of molecular diffusion, the relationship between the rate of diffusion

⁵“eddy motion in the atmosphere,” Phil. Trans. 1915

and the molecular constants is known; a large part of the kinetic theory is devoted to this question. On the other hand, nothing appears to be known regarding the relationship between constants which might be used to determine any particular type of turbulent motion and its diffusing power”.

In fact, Taylor used what he called a random flight model for modelling Lagrangian motion of fluid particles. This is a random walk model. However, in his model, Taylor introduced the Lagrangian time correlation coefficient. It is a correlation between the turbulent velocities of the same fluid particle at two different times. The introduction of this correlation coefficient manifests the non-Markovian character of the turbulent flow motion because it introduces the effect of the particle motion history (or memory effects) on the particle motion in the future.

There can also be conceptual difficulties associated with extending statistical mechanics techniques into turbulence. For example, there is an obvious analogy between the Boltzman collision operator and the Curl mixing model. For the former, when applied to gas molecules, a collision is a real physical process and its meaning is well defined. This is not the case for the Curl mixing model. The modelling of the mixing process in terms of the collision mechanism is conceptual rather than physical. That is, the mixing process is a continuous process and not a discrete one.

3.3.2 Lagrangian Versus Eulerian PDF

For reasons outlined in Chapter 2, the Lagrangian approach is used in the present work. In other things, the Lagrangian description of the turbulent reactive flow provides a natural means for describing the mixing process, specifically in particles interaction models (for example, Curl mixing model). From the modelling point of view, the Lagrangian description of the fluid particles motion provides a convenient framework for using methods of stochastic differential equations, as explained in the preceding subsection.

A Lagrangian description of turbulent flow is essentially implemented by following the motion of a marked particle at $t = 0$. First, we define what is meant by a fluid particle. Here, a fluid particle refers to every volume of the fluid having linear dimensions which are very large compared to the average distance between molecules. Therefore, for such volumes, it is possible to speak of their velocity and remain within the framework of continuous medium. Nevertheless, the particle dimensions are so small that the volume and pressure inside the fluid particle may be considered nearly constant (Monin and Yaglom, 1971).

The path of a marked particle is described by its position at different times, and marked by its conditions at the beginning of the motion. The position of a particle at time t is the vector $\underline{X}_L(\underline{X}_o, t)$. It turns out that the velocity at time t is the vector $\underline{U}_L[\underline{X}_L(\underline{X}_o, t), t]$, and the composition is $\Phi_L[\underline{X}_L(\underline{X}_o, t), t]$. The connection between the Lagrangian $\underline{X}_L$ and $\underline{U}_L$ and the Eulerian description $\underline{U}$ and $\underline{X}$ is given by,

$$\underline{U}(\underline{X}, t) = \frac{\partial \underline{X}_L(\underline{X}_o, t)}{\partial t} \quad (3.56)$$

$$\underline{X} = \underline{X}_L(\underline{X}_o, t) \quad (3.57)$$

with the initial condition,

$$\underline{X}_L(\underline{X}_o, t_o) = \underline{X}_o \quad (3.58)$$

The Lagrangian PDF considered is,

$$P_L(\underline{\Psi}, \underline{X}; t | \underline{\Psi}_o, \underline{X}_o) \quad (3.59)$$

which is a joint PDF of the event,

$$\{\Phi_L(X_o, t) = \Psi, \quad X_L(X_o, t) = X\} \quad (3.60)$$

subjected to the condition,

$$\Phi_L(X_o, t_o) = \Psi(X_o, t_o) \quad (3.61)$$

That is, P_L is the joint PDF of the fluid particle properties at time t , conditional upon their properties at time t_o . It is important to note that in the Lagrangian PDF, X denotes the sample space variable corresponding to $X_L(X_o, t)$, while it is a parameter in the Eulerian PDF.

For variable density flow, the Eulerian PDF is related to the Lagrangian PDF through the relation (Pope, 1985),

$$P(\Psi, X; t) = \int \int P(\Psi_o; X_o, t_o) P_L(\Psi, X; t | \Psi_o, X_o) d\Psi_o dX_o \quad (3.62)$$

where the integration is over all the concentrations and the entire flow domain at t_o . From Equation 3.62, the Lagrangian PDF (P_L) can be interpreted as a transition probability density for the turbulent flow. It determines the transition of the Eulerian PDF from time t_o to time t .

3.3.3 Modelling of Turbulent Diffusion Flux

In the present subsection, the closure for the turbulent diffusion term is derived. Consider for simplicity an incompressible flow. The instantaneous velocity can be written as mean and fluctuating components,

$$U_j = \langle U_j \rangle + u'_j \quad (3.63)$$

The first term on the right-hand side of Equation 3.34 can then be written as,

$$\begin{aligned} \frac{\partial}{\partial x_j} \langle U_j \phi \rangle &= \frac{\partial}{\partial x_j} (\langle U_j \rangle P) + \frac{\partial}{\partial x_j} (\langle u'_j \phi \rangle) \\ &= P \frac{\partial}{\partial x_j} \langle U_j \rangle + \langle U_j \rangle \frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_j} (\langle u'_j \phi \rangle) \\ &= \langle U_j \rangle \frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_j} (\langle u'_j \phi \rangle) \end{aligned} \quad (3.64)$$

The first term on the right-hand side is the convection due to the mean velocity. The second term is the turbulent convection, which may also be seen as a turbulent diffusion flux. Usually, the turbulent diffusion flux is modelled using gradient diffusion closure,

$$\langle u'_j \phi \rangle = -D_t \frac{\partial P}{\partial x_j} \quad (3.65)$$

where D_t is the turbulent diffusion coefficient and,

$$D_t = \frac{\mu_t}{\sigma_\Phi} \quad (3.66)$$

σ_Φ is the turbulent Schmidt number and is taken as 0.7 (Tsai and Fox, 1994). μ_t is the turbulent viscosity and is defined by,

$$\mu_t = C_\mu \langle \rho \rangle \frac{\tilde{k}^2}{\tilde{\epsilon}} \quad (3.67)$$

$\tilde{k}$ is the turbulent kinetic energy, $\tilde{\varepsilon}$ is the turbulent energy dissipation rate and C_μ usually is ascribed a value of 0.09 (Lilley and Rhode, 1982). Substituting Equations 3.64 and 3.65 into the PDF transport Equation 3.34, we have,

$$\frac{\partial P}{\partial t} + \langle U_j \rangle \frac{\partial P}{\partial x_j} - \frac{\partial}{\partial x_j} (D_t \frac{\partial P}{\partial x_j}) = - \frac{\partial}{\partial \Psi} (\dot{W} P) - D \frac{\partial}{\partial \Psi} \left\langle \wp \frac{\partial^2 \Phi}{\partial x_j \partial x_j} \right\rangle \quad (3.68)$$

Equation 3.68 is closed with respect to the turbulent diffusion. From a Lagrangian point of view, this diffusion corresponds to random motion of fluid particles. It is also useful from a numerical point of view to adopt this picture. This can be done by writing the stochastic differential equation corresponding to the evolution Equation 3.68. Since we already assume knowledge of the diffusion coefficient, a stochastic differential equation for the evolution of the position of the stochastic fluid particle can be derived.

Consider the diffusion process $X(t)$. It obeys the stochastic differential equation,

$$dx_j = A_j dt + \sqrt{B} dW_j(t) \quad (3.69)$$

where the increment in Wiener process can be thought of as a Gaussian random variable with a zero mean and a variance dt . The corresponding Fokker-Planck equation can be written as,

$$\frac{\partial P_L}{\partial t} = - \frac{\partial}{\partial x_j} (A_j P_L) + \frac{1}{2} \frac{\partial^2}{\partial x_j \partial x_j} (B P_L) \quad (3.70)$$

where $P_L = P_L(\Psi, \underline{X}; t)$. Note that this is a Lagrangian PDF evolution equation. To determine the coefficients $A_j(\underline{X})$ and $B(\underline{X})$, we have to compare Equation 3.70 with Equation 3.68. However, the first is a Eulerian PDF evolution equation and the second is a Lagrangian PDF evolution equation. Therefore, we have to transform one form into the

other. This can be done using Equation 3.62. However, we may note that the operators in Fokker-Planck Equation 3.70 are independent of t_o , x_o , and Ψ_o . It follows immediately from Equation 3.62 that the Eulerian PDF also evolves according to the same Fokker-Planck equation. Therefore, a comparison can be made directly between Equation 3.70 and Equation 3.68. These two equations should be the same, assuming that the right-hand side of Equation 3.68 is zero. It follows immediately that,

$$A_j = \langle U_j \rangle + \frac{\partial D_t}{\partial x_j} \quad (3.71)$$

and,

$$B = 2D_t \quad (3.72)$$

Therefore, the stochastic differential Equation 3.69 can be written with the new coefficients as,

$$dx_j = \left(\langle U_j \rangle - \frac{\partial D_t}{\partial x_j} \right) dt + \sqrt{2D_t} dW_j(t) \quad (3.73)$$

It is important to note that the stochastic particles governed by Equation 3.73 do not have to be the same as the fluid elements defined in the previous subsection. These particles represent mathematical entities rather than physical ones. The only link between the two types of particles (real fluid particles and stochastic particles) is that their statistical properties are identical. That is to say, the instantaneous paths produced by Equation 3.73 are irrelevant and meaningless until they are used in calculating the statistical distributions of interest. Accordingly, the limits imposed on the real fluid particles by the definition given in the previous subsection, (such as dimensions and so on), cease to exist for the stochastic particles.

3.3.4 Modelling of Turbulent Mixing

3.3.4a General

The last term on the right-hand side of Equations 3.34 or 3.35 is obviously unknown and represents a closure problem. As it is the method for closure approximation, one would like to replace this unknown term by another expression which is amenable to calculations. As a rule, for convenient closure modelling, it is necessary to gather as much information on the role and behaviour of the unclosed term as possible. Generally, this can be achieved by employing physical, mathematical or experimental arguments. Then, one can attempt to construct a model which matches these requirements. Therefore, the first step towards addressing the difficult problem of turbulent mixing modelling is to specify some of these requirements.

For incompressible, constant diffusivity and a statistically homogeneous conserved scalar field without reaction, the composition PDF Equation 3.35 is reduced to,

$$\frac{\partial P}{\partial t} = -D \frac{\partial^2}{\partial \Psi^2} \left\langle \left(\frac{\partial \Phi}{\partial x_j} \right)^2 \wp \right\rangle \quad (3.74)$$

Let,

$$G = D \left\langle \left(\frac{\partial \Phi}{\partial x_j} \right)^2 \wp \right\rangle \quad (3.75)$$

Using the mathematical identity,

$$\int \Psi^m \frac{\partial^n}{\partial \Phi^n} [\wp(\Psi) h(\Psi)] d\Psi = \begin{cases} 0 & m < n \\ (-1)^n \frac{m!}{(m-n)!} \int \Psi^{m-n} \wp(\Psi) h(\Psi) d\Psi & n \leq m \end{cases} \quad (3.76)$$

A direct substitution of $h(\Psi)$ by $(\frac{\partial \Phi}{\partial x_j})^2$ in the case $m = 1$ and $n = 2$ in Equation 3.76, leads to,

$$\int \Psi \frac{\partial^2 G}{\partial \Psi^2} d\Psi = 0 \quad (3.77)$$

and for $m=2$ and $n=2$, it follows that,

$$-\int \Psi^2 \frac{\partial^2 G}{\partial \Psi^2} d\Psi = -2 \int G d\Psi \leq 0 \quad (3.78)$$

The inequality 3.78 follows from the fact that G is composed of a quadratic multiplied by a positive quantity, such that, it is always non-negative.

Equations 3.77 and 3.78 indicate the role of the unclosed term. It causes the scalar variance to decay while keeping the mean conserved. In fact, this is a mixing mechanism. The effect of the mixing term (solely) on the evolution of the scalar PDF and the scalar random variable is shown in Figure 3.4 (Pope, 1979). In this Figure, the PDF is initially composed of two equal delta functions at $\Psi = 0$ and $\Psi = 1$,

$$P(\Psi) = \frac{1}{2}\delta(\Psi) + \frac{1}{2}\delta(1 - \Psi) \quad (3.79)$$

This distribution is realized by a rectangular waveform of the scalar variable $\Phi(x, t)$. It should be noted that the state of complete mixing can be achieved in the limit of very long time under the action of the turbulent mixing term alone.

Some of the known characteristics of the mixing term can be summarized as follows:

1. The mixing term does not influence the mean (Equation 3.77).
2. The mixing term causes the variance $\langle \Phi'^2 \rangle$ to decrease with time (Equation 3.78).
3. The PDF, $P(\Psi; t)$, relaxes to Gaussian in homogeneous field (*cf.* Chapter 2).
4. The mixing term maintains the boundness of the scalar. This fact can be easily deduced from the physics of the mixing process. For example, consider a hot body

Figure 3.4: The evolution of scalar and PDF in homogeneous turbulence (adapted from Pope (1979)).

at temperature T_h in contact with a cold body at temperature T_c . Neither of the two bodies will attain a temperature higher than T_h or lower than T_c . This condition can be expressed mathematically for a scalar Φ ; If at $t = 0$, $(\Phi_{min} \leq \Phi \leq \Phi_{max})$ then, at any time $t > 0$, $(\Phi_{min} \leq \Phi \leq \Phi_{max})$. It was pointed out by Kuzentsov and Sabel'nikov (1990) that the boundness condition is non-trivial as it rules out a wide class of models that violate the boundness principle.

An ideal mixing model should be able to verify these requirements. Another requirement is related to the mixing models used in turbulent reactive flow. The effect of reaction on mixing should be included. However, this requirement is found extremely difficult to be formulated quantitatively and will not be considered here.

According to Equation 3.78, the mixing term causes the variance to decay. On modelling this term, one may wish to construct a model which causes the fluctuations to decay at the same rate as in a real case. Let us rewrite Equation 2.7, which describes the decay of variance in the case of homogenous isotropic turbulence and homogenous scalar fluctuations, in the following form,

$$\frac{\partial \langle \Phi'^2 \rangle}{\partial t} = -\varepsilon_\Phi \quad (3.80)$$

ε_Φ is the mean rate of the scalar fluctuations dissipation, defined as,

$$\varepsilon_\Phi = 2D \langle \nabla \Phi' \cdot \nabla \Phi' \rangle \quad (3.81)$$

The decay time scale of the scalar fluctuations τ_Φ is defined by,

$$\tau_\Phi = \frac{\langle \Phi'^2 \rangle}{\varepsilon_\Phi} \quad (3.82)$$

Following Spalding (1971), τ_Φ is proportional to the time scale of velocity fluctuations τ where,

$$\tau = \frac{k}{\varepsilon} \quad (3.83)$$

k is the turbulence kinetic energy and ε is the dissipation rate. Therefore,

$$\tau_\Phi = \frac{\tau}{C_\Phi} \quad (3.84)$$

C_Φ is usually assumed to take the value 2.0 (Pope, 1985). therefore,

$$\varepsilon_\Phi = C_\Phi \frac{\langle \Phi'^2 \rangle}{\tau} \quad (3.85)$$

Substituting Equation 3.85 in Equation 3.80,

$$\frac{d\langle \Phi'^2 \rangle}{dt} = -C_\Phi \frac{\langle \Phi'^2 \rangle}{\tau} \quad (3.86)$$

$$\frac{d\langle \Phi'^2 \rangle}{dt} = -\omega_\Phi \langle \Phi'^2 \rangle \quad (3.87)$$

where,

$$\omega_\Phi = \frac{C_\Phi}{\tau} = C_\Phi \frac{\varepsilon}{k} \quad (3.88)$$

That is, ω_Φ is the turbulent mixing frequency. Solving the differential Equation 3.87 for the variance with the initial conditions of $\langle \Phi'^2 \rangle_o$ at $t = 0$, we have

$$\langle \Phi'^2 \rangle = \langle \Phi'^2 \rangle_o e^{-\omega t} \quad (3.89)$$

This means that the variance decays exponentially with a time scale of $\frac{\tau}{C_\Phi}$. It should be noted that there is considerable doubt concerning the universality of C_Φ . However, it was found in many shear flow that C_Φ is in the range 1.5:2.5 (Pope, 1985). Therefore, in the absence of a better information about C_Φ , its value will be taken as 2.0 in the present work.

Many models have been suggested for the closure of the turbulent mixing term. However, we shall discuss only two of these models; coalescence dispersion or Curl model and the linear mixing by exchange with the mean. These are the two models considered in the numerical modelling in the present work.

3.3.4b Curl Model

The Curl model or the coalescence dispersion model was first derived by Curl (1963). It was originally intended for interactions of drops in a two-liquid phase chemical reactor. Later, it was adapted by Kattan and Adler (1972), Flagan and Appleton (1974), and Pratt (1976) in what is known as the stochastic reactor theory for modelling turbulent combustion. For his derivation, Curl relied on a combinatorial argument. According to this model, the turbulent scalar is composed of a large number of particles. Each particle carries a certain mass, concentration, and temperature. In a time period Δt , a number of collisions will occur with a certain frequency. This frequency is proportional to the turbulence intensity. Each collision involves two particles and is assumed to be instantaneous. This mechanism for mixing is illustrated in Figure 3.5. Two particles with scalar values $\Phi_p(t)$ and $\Phi_q(t)$ are allowed to mix together, then disperse with new scalar values $\Phi_p(t + \Delta t)$ and $\Phi_q(t + \Delta t)$.

Following Pope (1985) an alternative derivation to the Curl model, which emphasizes

Figure 3.5: Illustration of mixing by collision and dispersion according to Curl model for two particles of equal mass

its stochastic nature, is introduced here. Starting with Curl (1963) hypothesis,

$$\Phi_p(t + \Delta t) = \Phi_q(t + \Delta t) = \frac{1}{2}[\Phi_p(t) + \Phi_q(t)] \quad (3.90)$$

From Equation 3.90, we have,

$$\Phi_p(t + \Delta t) + \Phi_q(t + \Delta t) = \Phi_p(t) + \Phi_q(t) \quad (3.91)$$

Taking the mean,

$$E[\Phi_p(t + \Delta t) + \Phi_q(t + \Delta t)] = E[\Phi_p(t) + \Phi_q(t)] \quad (3.92)$$

which implies that the mean remains unchanged before and after mixing. Starting with the definition of the scalar fluctuations, the following equations are derived,

$$\Phi' = \Phi - \langle \Phi \rangle \quad (3.93)$$

$$\Phi'^2 = \Phi^2 + \langle \Phi \rangle^2 - 2\Phi \langle \Phi \rangle \quad (3.94)$$

$$\begin{aligned}
\langle \Phi'^2 \rangle &= \langle \Phi^2 \rangle + \langle \Phi \rangle^2 - 2\langle \Phi \rangle^2 \\
&= \langle \Phi^2 \rangle - \langle \Phi \rangle^2
\end{aligned} \tag{3.95}$$

Therefore,

$$\langle \Phi'^2(t + \Delta t) \rangle - \langle \Phi'^2(t) \rangle = \langle \Phi^2(t + \Delta t) \rangle - \langle \Phi^2(t) \rangle - \langle \Phi(t + \Delta t) \rangle^2 + \langle \Phi(t) \rangle^2 \tag{3.96}$$

Since the mean remains unchanged according to Equation 3.92, the last two terms on the right-hand side of Equation 3.96 cancel each other out. Thus,

$$\langle \Phi'^2(t + \Delta t) \rangle - \langle \Phi'^2(t) \rangle = \langle \Phi^2(t + \Delta t) \rangle - \langle \Phi^2(t) \rangle \tag{3.97}$$

The right-hand side of Equation 3.97 can be estimated from particle representation as,

$$\langle \Phi^2(t + \Delta t) \rangle - \langle \Phi^2(t) \rangle = \frac{1}{N} E \left\{ \sum_{n=1}^N [\Phi_{(n)}(t + \Delta t)]^2 - \sum_{n=1}^N [\Phi_{(n)}(t)]^2 \right\} \tag{3.98}$$

Then,

$$\langle \Phi'^2(t + \Delta t) \rangle - \langle \Phi'^2(t) \rangle = \frac{1}{N} E \left\{ \sum_{n=1}^N [\Phi_{(n)}(t + \Delta t)]^2 - \sum_{n=1}^N [\Phi_{(n)}(t)]^2 \right\} \tag{3.99}$$

Note that the particles only contribute to the change in the variance whenever they encounter mixing events. The number of mixing events in N particles population during time period Δt is estimated as,

$$N_{mix} = \omega_{mix} N \Delta t \tag{3.100}$$

The summations in Equation 3.99 can be replaced by the estimated number of mixing

events of particle pairs p and q . Using Equations 3.90, 3.91, and 3.100, we obtain,

$$\begin{aligned}\langle \Phi'^2(t + \Delta t) \rangle - \langle \Phi'^2(t) \rangle &= \frac{N_{mix}}{N} E \left\{ [\Phi_p(t + \Delta t)]^2 + [\Phi_q(t + \Delta t)]^2 \right\} \\ &= \omega_{mix} \Delta t E \left\{ -\frac{1}{2} [\Phi_p(t)]^2 - \frac{1}{2} [\Phi_q(t)]^2 + [\Phi_p(t)][\Phi_q(t)] \right\}\end{aligned}\quad (3.101)$$

Since the two particles p and q are selected at random, and using Equation 3.95, we have,

$$E(\Phi_p)^2 = E(\Phi_q)^2 = \langle \Phi^2 \rangle = \langle \Phi'^2 \rangle + \langle \Phi \rangle^2 \quad (3.102)$$

Also, since q and p are independent, then,

$$E\{\Phi_p \Phi_q\} = E(\Phi_p)E(\Phi_q) = \langle \Phi \rangle^2 \quad (3.103)$$

Substituting Equation 3.102 and 3.103 in 3.101,

$$\Delta \Phi'^2(t) = -\omega_{mix} \Delta t \langle \Phi'^2(t) \rangle \quad (3.104)$$

Taking the limits when Δt tends to zero,

$$\frac{\partial}{\partial t} \langle \Phi'^2(t) \rangle = -\omega_{mix} \langle \Phi'^2(t) \rangle \quad (3.105)$$

Comparing Equation 3.105 with Equation 3.87 for the Curl mixing model to produce the correct decay of variance, we arrive at,

$$\omega_{mix} = \omega_{\Phi} \quad (3.106)$$

That is, the mixing frequency in the Curl mixing model is estimated by the turbulent

mixing frequency to produce the correct decay of the variance.

3.3.4c Modified Curl Model

The original Curl model has been studied extensively by Dopazo (1979), Janicka et al. (1979), and Pope (1982). Although the model leaves the mean unchanged and causes the variance to decrease, it was found to exhibit some unrealistic behaviour. In general, the proposed modifications to the Curl model can be classified into two categories:

- (i) post-collision quantitative behaviour of the scalar of the mixed particles.
- (ii) pre-collision selectivity of the mixed particles.

Let us consider the first point. It has been shown independently by Dopazo (1979) and Janicka et al. (1979) that rather than producing continuous distribution as shown in Figure 3.4, the Curl model relaxes the initially segregated binary scalar field into a large number of discontinuous delta functions. Dopazo (1979) and Janicka et al. (1979), both suggested a modification to the Curl model that results in continuous PDF distribution. The modification is essentially applied to the interaction model of the mixing process or, in our previous terminology, the post-collision behaviour. Equation 3.90 is replaced by,

$$\Phi_p(t + \Delta t) = (1 - \alpha)\Phi_p(t) + \frac{1}{2}\alpha(\Phi_p(t) + \Phi_q(t)) \quad (3.107)$$

$$\Phi_q(t + \Delta t) = (1 - \alpha)\Phi_q(t) + \frac{1}{2}\alpha(\Phi_p(t) + \Phi_q(t)) \quad (3.108)$$

The corresponding PDF evolution equation is written as,

$$\frac{dP}{dt} = 2\omega_\phi \int \int P(\Psi_p)P(\Psi_q)K(\Psi, \Psi_p, \Psi_q)d\Psi_p d\Psi_q - 2\omega_\phi P \quad (3.109)$$

where,

Figure 3.6: Long tails deviation from Gaussian distribution.

$$K(\Psi, \Psi_p, \Psi_q) = \int_0^1 A(\alpha) \delta(\Psi - (1 - \alpha)\Psi_p - \frac{1}{2}\alpha(\Psi_p + \Psi_q)) d\alpha \quad (3.110)$$

α is a random variable with continuous PDF. The simplest choice of $A(\alpha)$ was proposed by Janicka et al. (1979),

$$A(\alpha) = 1 \quad (3.111)$$

Now, let us consider the second kind of modification to the Curl model or the modification to the pre-collision selection of the mixed particles. Pope (1982) showed that the modified Curl model by Dopazo (1979) and Janicka et al. (1979), does not relax the PDF to a Gaussian distribution. The PDF exhibits deviation from Gaussian which is revealed by the large deviation of the fourth order moment from the corresponding Gaussian value. In other words, the asymptotic PDF exhibits long tails as illustrated in Figure 3.6.

Pope (1982) proposed a biased selection of the particles to mix, rather than an equal probability of mixing for each particle. The bias in selection depends on the age of the particle. Simply, an age function is attributed to each particle. This function counts the time passed since the particle encountered the last mixing event. The longer this time, the higher the probability of selecting the particle.

Kosaly (1986) studied different expressions for the age distribution in an attempt to improve the model performance. He also argued that this age biased mixing amounts to physical reasoning. Here, we argue that this is not the case. In fact, this age biased mixing modification can be advocated based on a purely mathematical argument. It has been mentioned that this modification was proposed as a remedy for the long tails of the asymptotic PDF. The existence of long tails implies that there are a few particles which experience considerable deviation from the mean. That is, the tails represent rare events which encounter a much different history from that of most of the ensemble elements. Alternatively, the long tails can be explained by the existence of non-exponentially decaying correlations. Both of rare events and non-exponentially decaying correlation may be seen as equivalent. That is, upon mixing of a particle, the time correlation decays very rapidly as the mixing erases the previous particle history. Therefore, age biasing amounts to reducing the number of rare events by assigning them a higher probability of selection. Consequently, long tails will cease to exist.

Finally, we pointed out earlier the similarity between the Curl model and the Boltzman collision operator. Here, we also point out the striking similarity between Pope's improved model (Pope, 1982) and the modified Boltzman collision operator given by Skinner and Wolynes (1980). To the author's knowledge, this similarity has not been mentioned in the mixing models literature.

3.3.4d Linear Mean Square Estimation Mixing Model

The linear mean square estimation model (LMSE) was first proposed by Lundgren (1969), as a closure for the viscous term in the velocity PDF transport equation. Later, the LMSE model was adapted by Dopazo and O'Brien (1974) as a closure for the mixing term. This closure is also referred to as interaction by exchange with the mean (IEM).

To simplify discussion of this model, the mixing term is expressed in terms of the

expectation of the scalar at one point conditional on another neighboring point scalar value. Consider the last term on the right-hand side of Equation 3.38,

$$-D \frac{\partial}{\partial \Psi} \lim_{x_j^* \rightarrow x_j} \frac{\partial^2}{\partial x_j^* \partial x_j^*} \int \Psi^* P(\Psi, \Psi^*; X, X^*, t) d\Psi^* \quad (3.112)$$

For a homogeneous field, one can write 3.112 as,

$$-D \frac{\partial}{\partial \Psi} \lim_{r_j \rightarrow 0} \frac{\partial^2}{\partial r_j \partial r_j} \int \Psi^* P(\Psi, \Psi^*; \mathbf{r}, t) d\Psi^* \quad (3.113)$$

where,

$$r_j = x_j^* - x_j \quad (3.114)$$

Since,

$$P(\Psi, \Psi^*; \mathbf{r}, t) = P(\Psi^* | \Psi; \mathbf{r}, t) P(\Psi; t) \quad (3.115)$$

Then substituting Equation 3.115 in Equation 3.112, the mixing term is written as,

$$\begin{aligned} & -D \frac{\partial}{\partial \Psi} \lim_{r_j \rightarrow 0} \frac{\partial^2}{\partial r_j \partial r_j} \int \Psi^* P(\Psi^* | \Psi; \mathbf{r}, t) P(\Psi; t) d\Psi^* \\ &= -D \frac{\partial}{\partial \Psi} P(\Psi; t) \lim_{r_j \rightarrow 0} \frac{\partial^2}{\partial r_j \partial r_j} \int \Psi^* P(\Psi^* | \Psi; \mathbf{r}, t) d\Psi^* \\ &= -D \frac{\partial}{\partial \Psi} P(\Psi; t) \lim_{r_j \rightarrow 0} \frac{\partial^2}{\partial r_j \partial r_j} \langle \Psi^* | \Psi; \mathbf{r}, t \rangle \end{aligned} \quad (3.116)$$

where, $\langle \Psi^* | \Psi; \mathbf{r}, t \rangle$ stands for the conditional expected value of the random variable Φ^* at location $\mathbf{r}$, given Φ at location zero.

Before introducing the conditional Gaussian hypothesis, we first verify some of the mathematical properties of the joint normal distribution. If (Φ, Φ^*) are two joint normal random variables, then the joint normal PDF can be written in terms of the variances $\langle \Phi'^2 \rangle$, $\langle \Phi^{*'}2 \rangle$ and the correlation coefficient $\rho_{\Phi\Phi^*}$,

$$P(\Psi, \Psi^*) = [4\pi^2 \langle \Phi'^2 \rangle \langle \Phi^{*'}2 \rangle (1 - \rho_{\Phi\Phi^*}^2)]^{-\frac{1}{2}} \exp \left[\frac{1}{2(1 - \rho_{\Phi\Phi^*}^2)} \left(\frac{(\Psi - \langle \Phi \rangle)^2}{\langle \Phi'^2 \rangle} - \frac{2\rho_{\Phi\Phi^*}(\Psi - \langle \Phi \rangle)(\Psi^* - \langle \Phi^* \rangle)}{(\langle \Phi'^2 \rangle \langle \Phi^{*'}2 \rangle)^{\frac{1}{2}}} + \frac{(\Psi^* - \langle \Phi^* \rangle)^2}{\langle \Phi^{*'}2 \rangle} \right) \right] \quad (3.117)$$

where,

$$\rho_{\Phi\Phi^*} = \frac{\langle \Phi' \Phi^{*'} \rangle}{(\langle \Phi'^2 \rangle \langle \Phi^{*'}2 \rangle)^{\frac{1}{2}}} \quad (3.118)$$

It follows that both $P(\Psi)$ and $P(\Psi^*)$ are Gaussian. Moreover, if Φ and Φ^* are uncorrelated, then they are independent. The joint normal distribution also implies the following important property of the conditional mean,

$$\langle \Psi | \Psi^* \rangle = \langle \Phi \rangle + \frac{\langle \Phi' \Phi^{*'} \rangle}{\langle \Phi^{*'}2 \rangle} (\Psi^* - \langle \Phi^* \rangle) \quad (3.119)$$

Finally, it follows also that the conditional PDF $P(\Psi | \Psi^*)$ is Gaussian.

Returning to the LMSE closure, Dopazo and O'Brien (1974) invoked the hypothesis that for a homogenous scalar field, $\langle \Psi^* | \Psi; \mathbf{r}, t \rangle$ is conditionally Gaussian. Thus,

$$\langle \Psi^* | \Psi; \mathbf{r}, t \rangle = \langle \Phi \rangle + \rho(\mathbf{r}, t) (\Psi - \langle \Phi \rangle) \quad (3.120)$$

and,

$$\rho(\mathbf{r}, t) = \frac{\langle (\Psi - \langle \Phi \rangle)(\Psi^* - \langle \Phi^* \rangle) \rangle}{\langle (\Psi - \langle \Phi \rangle)^2 \rangle} = \frac{\langle \Phi' \Phi^{*'} \rangle}{\langle \Phi'^2 \rangle} \quad (3.121)$$

For isotropic turbulence, using Equations 3.116 and 3.120, we arrive at,

$$-\lim_{r_j \rightarrow 0} \frac{\partial^2}{\partial r_j \partial r_j} \langle \Psi^* | \Psi; \mathbf{r}, t \rangle = 3(\Psi - \langle \Phi \rangle) \left(-\frac{\partial^2 \rho(\mathbf{r}, t)}{\partial r^2} \right)_{r=0} \quad (3.122)$$

Taylor micro-scale of the scalar fluctuations is defined as,

$$\lambda = \frac{2}{\left(-\frac{\partial^2 \rho(\mathbf{r}, t)}{\partial r^2} \right)_{r=0}} \quad (3.123)$$

This scalar fluctuations time scale has to be provided in order for the LMSE closure to be complete. This can be done by assuming a relation between the scalar fluctuations time scale and the turbulence time scale as was done in the previous section. Therefore, by substituting in the PDF evolution equation while considering the effect of mixing term, we have,

$$\frac{\partial P(\Psi; \underline{X}, t)}{\partial t} = \frac{1}{2} \frac{C_\Phi}{\tau} \frac{\partial}{\partial \Psi} (\Psi - \langle \Phi \rangle) P(\Psi; \underline{X}, t) \quad (3.124)$$

The LMSE mixing model is used extensively in practical applications due to its simplicity. It is a deterministic model, as can be seen in Equation 3.124. This is also apparent in the corresponding equation of the evolution of the scalar random variable,

$$\frac{\partial \Phi}{\partial t} = -\frac{1}{2\tau} C_\Phi (\Psi - \langle \Phi \rangle) \quad (3.125)$$

Implicitly, Equation 3.125 indicates that the rate of change of the random variable Φ depends solely on its linearized state. Since the model is deterministic, implicitly this also implies once equilibrium is approached, no other deviations from this equilibrium arise in

the system⁶.

Dopazo and O'Brien (1974) argued that the conditionally Gaussian hypothesis given by Equation 3.120 is physically sound. As $\underline{r} \rightarrow 0$, the correlation coefficient tends to one and,

$$\langle \Psi^* | \Psi; 0, t \rangle = \Phi(t) \quad (3.126)$$

Considering the other extreme, when $\underline{r} \rightarrow \infty$ the correlation coefficient tends to zero and,

$$\langle \Psi^* | \Psi; \infty, t \rangle = \langle \Phi(t) \rangle \quad (3.127)$$

That is, the expected value of the scalar at X^* is independent of Φ at X , given that X^* is far from X .

On the other hand, the LMSE model suffers from unsatisfactory behaviour. Starting from initial PDF rather than Gaussian distribution, the model preserves the shape of the initial PDF (O'Brien, 1981). For example, starting with a double delta function as initial conditions, there is no relaxation to Gaussian. Instead, the delta functions will remain and continue moving towards each other. This can be illustrated by considering the general solution for Equation 3.124,

$$P(\Psi, t) = \frac{f(t + \ln(\Psi - \langle \Phi \rangle))}{(\Psi - \langle \Phi \rangle)} \quad (3.128)$$

where the specific form of the function f is determined by the initial conditions $P(\Psi; t)$. It is clear from this equation that the shape of the PDF, determined by the initial conditions, is scaled in a linear manner. In other words, the LMSE model relaxes the PDF while

⁶This point can be made clearer if the LMSE model is compared with the corresponding Langevin model. In the Langevin model, there is a fluctuation term which always drives the system to fluctuate around the mean. However the conventional Langevin violates the condition of boundness of the scalar and cannot be used in modelling the mixing term.

preserving its shape (Correa, 1995).

Finally, we note that Kosaly (1986) has been able to derive the LMSE, starting with the Curl model. He simply employed a series expansion and truncation to the collision term.

Chapter 4

Numerical Modelling and Evaluation: Lagrangian Composition PDF Model

In the present chapter, the development and numerical solution for the composition PDF model using Lagrangian Monte Carlo method with time splitting and variable particle mass is presented. The model is implemented using a hybrid finite volume-Monte Carlo method. This is illustrated by the schematic diagram shown in Figure 4.1.

The Favre-averaged Navier Stokes equation is modelled by the $(k-\epsilon)$ turbulence model. The averaged momentum equation, the turbulent kinetic energy and rate of energy dissipation transport equations, when subjected to appropriate boundary conditions, are solved using the finite volume method. The mean velocity, pressure and turbulence quantities are passed to the PDF Monte Carlo method.

The Favre-averaged composition PDF transport equation, with appropriate initial and boundary conditions, is modelled using a stochastic Lagrangian Monte Carlo approach. This also includes solving for the chemical kinetics. Chemical kinetics are modelled using a global reaction mechanism for Methane combustion with seven species, including *CO*

Figure 4.1: Hybrid finite volume-Monte Carlo scheme for turbulent combustion.

and NO . Integration of chemical kinetics is undertaken using a scheme for solving stiff ordinary differential equations (DVODE), (Brown et al., 1979).

For a chosen time step, the density, concentration and temperature are calculated using the Monte Carlo method. The new calculated density, together with the updated viscosity, are passed to the finite volume module, where the mean velocity field is solved using the finite volume method and the flow parameters are passed to the Monte Carlo module again. These procedures are repeated until a specified convergence criterion is met. In the present work, the convergence of NO mean concentrations is monitored as an indicator for the convergence of the solution as it is the slowest dependent variable to converge. Consequently, convergence criterion is met when NO concentrations reach a steady state.

4.1 Turbulent Flow Modelling and Simulation

The modelled Favre-averaged Navier Stokes equation, together with the continuity equation and two transport equations for turbulent kinetic energy and energy dissipation, constitute what is known as $(k - \varepsilon)$ model. These equations are written in a cylindrical coordinate system for axi-symmetric flow in terms of general dependent variable ϕ as,

$$\frac{1}{r} \left[\frac{\partial}{\partial x} (\langle \rho \rangle \tilde{U} r \phi) + \frac{\partial}{\partial r} (\langle \rho \rangle \tilde{V} r \phi) - \frac{\partial}{\partial x} \left(r \Gamma_\phi \frac{\partial \phi}{\partial x} \right) - \frac{\partial}{\partial r} \left(r \Gamma_\phi \frac{\partial \phi}{\partial r} \right) \right] = S_\phi \quad (4.1)$$

For $\phi = 1$, the continuity equation is retrieved. For $\phi = U, V, W$ (three velocity components), the momentum equations are retrieved. For $\phi = k, \varepsilon$, the turbulent two transport equations are retrieved. The forms of the source term S_ϕ are given in Table 4.1.

Certain quantities given in Table 4.1 are defined as follows,

$$S_U = \frac{\partial}{\partial x} \left(\mu_e \frac{\partial \tilde{U}}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \mu_e \frac{\partial \tilde{V}}{\partial x} \right) \quad (4.2)$$

Table 4.1: The form of the source term in the general equation for ϕ

ϕ	S_ϕ
$\tilde{U}$	$-\frac{\partial \langle P \rangle}{\partial x} + S_U$
$\tilde{V}$	$-\frac{\langle P \rangle}{\partial r} + \frac{\langle \rho \rangle \tilde{W}^2}{r} - \frac{2\mu_e \tilde{V}}{r^2} + S_V$
$\tilde{W}$	$-\frac{\langle \rho \rangle \tilde{V} \tilde{W}}{r} - \frac{\tilde{W}}{r^2} \frac{\partial}{\partial r} (r \mu_e)$
$\tilde{k}$	$G - C_D \langle \rho \rangle \tilde{\varepsilon}$
$\tilde{\varepsilon}$	$\frac{(C_1 \tilde{\varepsilon} G - C_2 \langle \rho \rangle \tilde{\varepsilon}^2)}{k}$

$$S_V = \frac{\partial}{\partial x} \left(\mu_e \frac{\partial \tilde{U}}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \mu_e \frac{\partial \tilde{V}}{\partial r} \right) \quad (4.3)$$

$$G = \mu_e \left[2 \left\{ \left(\frac{\partial \tilde{U}}{\partial x} \right)^2 + \left(\frac{\partial \tilde{V}}{\partial r} \right)^2 + \left(\frac{\tilde{V}}{r} \right)^2 \right\} \right.$$

$$\left. + \left(\frac{\partial \tilde{U}}{\partial r} + \frac{\partial \tilde{V}}{\partial x} \right)^2 + \left\{ r \frac{\partial}{\partial r} \left(\frac{\tilde{W}}{r} \right) \right\}^2 + \left(\frac{\partial \tilde{W}}{\partial x} \right)^2 \right] \quad (4.4)$$

The turbulent coefficients are estimated as,

$$\mu_e = C_\mu \langle \rho \rangle \frac{\tilde{k}^2}{\tilde{\varepsilon}} + \mu_l \quad (4.5)$$

$$\Gamma_\phi = \frac{\mu_e}{\sigma_\phi} \quad (4.6)$$

where μ_e is the effective viscosity and μ_l is the laminar viscosity. The $(k - \varepsilon)$ model is a popular turbulence model in engineering applications and has been studied extensively by many workers. Over the next few paragraphs, we point out some important features of this model.

While an equation for the turbulent kinetic energy transport is derived exactly, this is not the case for the dissipation of turbulence energy. The latter, by definition, is due to viscous action. However, at a high Reynolds number, the turbulent dissipation is a weak function in flow viscosity. Rather, dissipation is determined by the rate at which the energy is transferred to the small scale eddies, that is, by inertial action. In principle, an

Table 4.2: Modified $(k - \varepsilon)$ model constants by Abujelala and Lilley (1984)

Constants	Standard	Modified
C_μ	0.09	0.1250
C_1	1.44	1.4400
C_2	1.92	1.5942
σ_k	1.00	1.0000
σ_ε	1.30	1.1949

equation for ε can be derived from the velocity equation. However, this equation would give no guidance to the modelling since it pertains to the viscous process rather than to the rate-controlling inertial process. Consequently, an equation for ε relies almost entirely on empiricism and physical intuition.

The other feature of the present form of the $(k - \varepsilon)$ model to be pointed out is the implicit assumption of the isotropy of the velocity fluctuations. Specifically, velocity fluctuations are assumed to be directional invariants. This assumption is known to be violated in swirling flow. Departure from isotropy is intensified by increasing the swirl number (Lilley and Chigier, 1971). The non-isotropy of velocity fluctuations can be accounted for using turbulence models, which are based on the formulation of higher order moments such as Reynolds stress models. However, this advantage seems to be lost in practical applications. This is explained by the fact that both experimental data available for verification and ease of solution decrease with increasing levels of closure. Fueyo et al. (2000) pointed out that the comparison between the two models (Reynolds stress and $(k - \varepsilon)$) revealed no serious advantage for one over the other when considering the entire flow field around a bluff body. A similar comment was made by Spalding (1991). Sloan (1985) recommended the $(k - \varepsilon)$ model for its robustness and economy.

The empirical constants in the standard $(k - \varepsilon)$ model were optimized by Abujelala and Lilley (1984) to model swirling flow, as shown in Table 4.2. These modified constants are used in the case of swirling flow in the present work.

For the solution technique, a structured, staggered grid algorithm developed by Lilley and Rhode (1982) was used to solve the Favre-averaged steady state equations of mass, momentum, turbulent kinetic energy and dissipation. The finite volume method was used for solving these non-linear partial differential equations. The SIMPLE algorithm, developed by Patanker (1980), was implemented. The discretized differential equations constitute a set of strongly coupled simultaneous algebraic equations.

Finally, it is pointed out that the original algorithm developed by Lilley and Rhode (1982) was modified in the present work in the following manner:

1. Time averaged quantities were replaced by Favre-averaged quantities.
2. Handling variable density flow instead of being limited to constant density.
3. The original algorithm was developed for a single geometrical configuration of swirling flow in an axi-symmetric duct with expansion angle. It was modified to handle different geometries such as bluff body stabilized flow.
4. The constants of the standard $(k - \varepsilon)$ model used by Lilley and Rhode (1982) were replaced by an optimized set in the case of swirling flow (Table 4.2).

4.2 Lagrangian Monte Carlo Method (Conventional Approach)

In this section, solving the PDF transport Equation 3.40 using a conventional Monte Carlo algorithm is discussed. We start by presenting a rough algorithm with the aim of explaining the general procedures and the spirit of the Monte Carlo method. Then, the basic elements of the Monte Carlo method are discussed in more details.

4.2.1 General Solution Algorithm

In the Lagrangian Monte Carlo method, the transport equation of the PDF is solved by direct simulation. The PDF is represented by an ensemble of N stochastic particles which model fluid particles. Each particle (n) carries attributes of position, $\underline{X}^n(t)$, density, $\rho^n(t)$, mass $m^n(t)$ and scalar, $\Phi_1^n(t), \Phi_2^n(t), \dots, \Phi_{\alpha+1}^n(t) = \Phi^n(t)$, where α is the number of species and $\alpha + 1$ stands for temperature.

The solution algorithm may be broadly outlined as follows:

1. The flow domain is discretized into cells and the mean velocity turbulent flow field is solved for each node using the finite volume method. As a result, turbulent flow parameters (velocity, pressure, turbulent kinetic energy, and dissipation) are known at each node.
2. The particles position, scalar value, and mass are initialized at time zero. Good initial conditions should satisfy the mass continuity and realizability of PDF distribution. (For example, the mass in a cell calculated from the finite volume module should be equal to the total mass of the particles inside this cell calculated from the Monte Carlo module).
3. Flow field parameters (velocity, turbulent kinetic energy, energy dissipation and pressure) are interpolated from the cell nodes to the particle positions.
4. In a time step (Δt), particles are allowed to move in the physical domain according to the stochastic differential equation that governs the Lagrangian particle position as a function of time (Equation 3.73, for example). For marching the stochastic differential equation in time, information from Step (3) is used.
5. During the same time period, Δt , the chemical reaction is advanced for each particle according to its concentration and temperature, $\Phi^n(t)$, at the beginning of the time

- step. Each particle can be thought of as a batch reactor. At the end of this time step, old concentrations and temperatures are updated with the new ones.
6. During the same time step (Δt), some particles leave the physical domain. These particles are removed from the ensemble. Reflection boundary conditions are applied to the particles which hit the solid walls.
 7. During the same time step, Δt , some fresh particles are introduced to the physical domain. The number and mass of these particles should satisfy the mass flow rate constraint. Additionally, the concentration and temperature of these particles are defined according to the combustion condition (for example, in the case of premixed combustion, all the fresh particles should have the same air-to-fuel ratio).
 8. Using the particle search-locate algorithm (to be described later), the cell hosting each particle is determined. By the end of the search-locate process, it is known which particles are hosted in which cells.
 9. Mixing is allowed at the new particle positions. For particle interaction models (Curl model, for example), in each cell, two particles are chosen randomly and allowed to mix. This is repeated with a frequency determined by turbulent flow parameters. In the LMSE mixing model, every particle (not randomly chosen ones) is relaxed towards the field mean value at the particle position. The relaxation rate is determined by turbulence parameters.
 10. The density at each grid point is interpolated from the surrounding particles and then passed to the finite volume algorithm.
 11. Using the new density, the velocity field is calculated.
 12. Steps (3) to (11) are repeated until a steady state solution is obtained.

4.2.2 Particle Representation

In a Monte Carlo simulation, the continuous PDF is replaced with an ensemble of N discrete particles. Each particle is considered as a fine grained PDF (one realization of the ensemble). Therefore we can write,

$$P_N(\Psi, X; t) = \frac{1}{N} \sum_{n=1}^N \delta(\Psi - \Phi^n(t)) \quad (4.7)$$

Equation 4.7 implies the requirement that P_N must converge to the modelled PDF in the limit of very large number of particles. However, this convergence is usually very difficult to test numerically as it requires the testing of all the higher moments statistics. Instead, convergence is determined in the mean square sense. In mathematical literature, this is known as weak convergence. Consequently, for a function Q of the random variable $\Phi(t)$, the mean,

$$\langle Q(\Phi(t)) \rangle = \int Q(\Phi(t)) P(\Psi, X; t) d\Psi \quad (4.8)$$

is estimated using discrete particles as,

$$\langle Q(\Phi(t)) \rangle_N = \frac{1}{N} \sum_{n=1}^N Q(\Phi^n(t)) \quad (4.9)$$

$\langle Q \rangle_N$ is required to converge to the true mean $\langle Q \rangle$ in a mean square sense, i.e.,

$$\lim_{\Delta t \rightarrow 0, N \rightarrow \infty} \langle (\langle Q \rangle_N - \langle Q \rangle)^2 \rangle = 0 \quad (4.10)$$

4.2.3 Stochastic Differential Equations

As explained in Chapter 3, for each modelled (closed) PDF transport equation, there is a corresponding system of stochastic differential equations. The latter have the advantage

of more direct interpretation when dealing with stochastic particles. Consequently, they are preferable in Lagrangian Monte Carlo simulation.

The strategy for deriving the equivalent stochastic differential equations to the modelled PDF transport equation is exactly the same as the one used in Chapter 3. First, the Fokker-Planck equation is derived, then the drift and diffusion coefficients are determined by comparing them to the stochastic differential equation in its standard form.

In a time step Δt , the position and composition of each particle evolve according to the stochastic differential equations,

$$\underline{X}^{(n)}(t + \Delta t) = \underline{X}^{(n)}(t) + \tilde{U}(\underline{X}^{(n)}(t), t)\Delta t + \Delta \underline{X}_{turb}^{(n)} \quad (4.11)$$

$$\begin{aligned} \underline{\Phi}^{(n)}(t + \Delta t) &= \underline{\Phi}^{(n)}(t) + \Delta \underline{\Phi}_{reaction}^{(n)} + \Delta \underline{\Phi}_{mix}^{(n)} \\ &= \underline{\Phi}^{(n)}(t) + \underline{S}^{(n)}(\underline{\Phi}^{(n)}(t))\Delta t + \Delta \underline{\Phi}_{mix}^{(n)} \end{aligned} \quad (4.12)$$

$\underline{S}^{(n)}$ is the chemical production rate for particle (n). This term is calculated according to the assumed reaction mechanism. Equations 4.11 and 4.12 are written in general form. The terms $\Delta \underline{X}_{turb}^{(n)}$ and $\Delta \underline{\Phi}_{mix}^{(n)}$ have to be specified according to the turbulent diffusion and turbulent mixing models. The turbulent diffusion term is modelled as (*cf.* Chapter 3),

$$\Delta \underline{X}_{turb}^{(n)} = \left[\frac{\nabla D_t}{\langle \rho \rangle} \right]_{\underline{X}^{(n)}(t)} \Delta t + \left[\frac{2\Delta t D_t}{\langle \rho \rangle} \right]_{\underline{X}^{(n)}(t)}^{\frac{1}{2}} \underline{\eta} \quad (4.13)$$

where $\underline{\eta}$ is a vector of independent standardized (zero mean and unit variance) Gaussian random variables. The scalar mixing term $\Delta \underline{\Phi}_{mix}^{(n)}$ in Equation 4.12 is modelled using the LMSE model (*cf.* Chapter 3),

$$\Delta\Phi_{mix}^{(n)} = -\frac{1}{2\tau}C_{\Phi}(\Phi^{(n)} - \tilde{\Phi})\Delta t \quad (4.14)$$

where τ is the turbulent fluctuations dissipation time scale.

Equations 4.11-4.14 imply a Favre-averaged transport equation for the corresponding Eulerian PDF $\tilde{P}(\Psi; \mathbf{X}, t)$ of the form,

$$\begin{aligned} \frac{\partial[\langle\rho\rangle\tilde{P}]}{\partial t} + \frac{\partial[\langle\rho\rangle\tilde{U}_i\tilde{P}]}{\partial x_i} + \frac{\partial[\langle\rho\rangle S_{\alpha}\tilde{P}]}{\partial \Psi_{\alpha}} \\ = \frac{\partial}{\partial x_i} \left[D_t \frac{\partial \tilde{P}}{\partial x_i} \right] + \frac{1}{2\tau} C_{\Phi} \frac{\partial}{\partial \Psi_{\alpha}} [\langle\rho\rangle(\Psi_{\alpha} - \tilde{\Phi}_{\alpha})\tilde{P}] \end{aligned} \quad (4.15)$$

where $\alpha = 1, \dots, Ns + 1$ and Ns is the number of species. Clearly, Equation 4.15 is closed.

Equations 4.11-4.14 are applied to each particle (n). Knowing the particle position and composition at time t , Equations (4.11-4.14) can be solved for the particle (n) position and composition at time $t + \Delta t$.

4.2.4 Fractional Time Step Approximation

The modelled PDF transport Equation 4.15 or alternatively the equivalent system of stochastic differential Equations 4.11-4.14, is solved at each time step, Δt . The stochastic differential Equations 4.11-4.14 should be solved simultaneously. Alternatively, considering the modelled PDF Equation 4.15, all the processes (mean and turbulent convection, chemical reaction and turbulent mixing) affect the PDF evolution simultaneously. The application of the Monte Carlo method to simulate the simultaneous effect of these processes encounters considerable difficulties. Therefore, the PDF evolution Equation 4.15 is approximated using fractional time steps (Pope, 1985; Hsu, 1991). The essence is to

convert the parallel and simultaneous processes into sequential processes in a sufficiently small time step, the purpose is to simplify the solution procedures.

We first write the PDF time derivative in Equation 4.15 in finite difference form,

$$\frac{\partial \tilde{P}}{\partial t} = \frac{\tilde{P}(t + \Delta t) - \tilde{P}(t)}{\Delta t} \quad (4.16)$$

The convection, chemical reaction and mixing operators are denoted by $\mathcal{O}_1$, $\mathcal{O}_2$ and $\mathcal{O}_3$, respectively. Then, Equation 4.15 can be written as,

$$\frac{\partial \tilde{P}}{\partial t} = (\mathcal{O}_1 + \mathcal{O}_2 + \mathcal{O}_3) \tilde{P} \quad (4.17)$$

or in finite difference form,

$$\tilde{P}(t + \Delta t) = (1 + (\mathcal{O}_1 + \mathcal{O}_2 + \mathcal{O}_3)\Delta t) \tilde{P}(t) \quad (4.18)$$

where,

$$\mathcal{O}_1 = -\tilde{U}_i \frac{\partial}{\partial X_i} + \frac{1}{\langle \rho \rangle} \frac{\partial}{\partial X_i} D_t \frac{\partial}{\partial X_i} \quad (4.19)$$

$$\mathcal{O}_2 = -\frac{\partial S_\alpha}{\partial \Psi_\alpha} \quad (4.20)$$

$$\mathcal{O}_3 = \frac{1}{2\tau} C_\Phi \frac{\partial}{\partial \Psi_\alpha} (\Psi_\alpha - \tilde{\Phi}_\alpha) \quad (4.21)$$

Now, consider an evolution equation of the form,

$$\tilde{P}(t + \Delta t) = (1 + \Delta t \mathcal{O}_1)(1 + \Delta t \mathcal{O}_2)(1 + \Delta t \mathcal{O}_3) \tilde{P}(t) \quad (4.22)$$

$$\begin{aligned}
\tilde{P}(t + \Delta t) &= [1 + \Delta t(\mathcal{O}_1 + \mathcal{O}_2 + \mathcal{O}_3) + \Delta t^2(\mathcal{O}_3\mathcal{O}_2 \\
&\quad + \mathcal{O}_3\mathcal{O}_1 + \mathcal{O}_2\mathcal{O}_1) + \Delta t^3(\mathcal{O}_1\mathcal{O}_2\mathcal{O}_3)]\tilde{P}(t) \\
&= \tilde{P}(t) + \Delta t(\mathcal{O}_1 + \mathcal{O}_2 + \mathcal{O}_3)\tilde{P}(t) + O^2(\Delta t^2)
\end{aligned} \tag{4.23}$$

A second expression for $\tilde{P}(t + \Delta t)$ is obtained from the Taylor series expansion around t ,

$$\begin{aligned}
\tilde{P}(t + \Delta t) &= \tilde{P}(t) + \frac{\partial \tilde{P}}{\partial t} \Delta t + \frac{\partial^2 \tilde{P}}{\partial t^2} \frac{\Delta t^2}{2!} + \dots \\
&= \tilde{P}(t) + \frac{\partial \tilde{P}}{\partial t} \Delta t + O(\Delta t^2)
\end{aligned} \tag{4.24}$$

Equating the right-hand sides of Equations 4.23 and 4.24 and dividing by Δt , we obtain,

$$\frac{\partial \tilde{P}}{\partial t} = (\mathcal{O}_1 + \mathcal{O}_2 + \mathcal{O}_3)\tilde{P} + O(\Delta t) \tag{4.25}$$

which, except for the first order truncation error, is the same as Equation 4.17. Therefore, Equation 4.22 is first order accurate in time. Note that the additive form of operators in Equation 4.17 implies that the corresponding processes are parallel (simultaneous). On the other hand, the multiplicative form of operators in Equation 4.22 implies that the corresponding processes are in series (sequential).

To summarize, by employing the fractional time step approximation, the stochastic particles evolution can be modelled by three processes in sequence in time step Δt . The first process is the convection by both mean and turbulent velocity. This causes the translation of the particle positions in the physical space according to the operators $(1 + \Delta t\mathcal{O}_1)$. The second process is the chemical reaction, which causes translation of particle

concentration and temperature in the phase space according to the operator $(1 + \Delta t \mathcal{O}_2)$. The third process is mixing, which causes the particle concentration and temperature to evolve in the phase space according to the operator $(1 + \Delta t \mathcal{O}_3)$. The specific forms of $\mathcal{O}_1$, $\mathcal{O}_2$, and $\mathcal{O}_3$ are given by Equations 4.19, 4.20, and 4.21.

4.2.5 Particles Search-Locate Algorithm

Mixing is an interaction process. Ideally, this involves the interaction between a particle and its closest neighbours. In a Lagrangian Monte Carlo simulation, this is modelled as an interaction between a chosen particle and any other particle (or group of particles) inside the same cell. That is to say, for a particle in a defined position, the closest particle could be any particle inside the same cell. Therefore, mixing calculation requires not only the knowledge of the position of the particles but also the cells hosting these particles.

Also, as previously mentioned, the flow density at each node is interpolated from the neighbouring particles. Similarly, the particles mean velocity and turbulent diffusion coefficients are obtained by interpolation from the nodal values of the hosting cells.

Taking account of all of these considerations requires accurate knowledge of the cell that contains each particle at the end of each time step (Δt). This can be acquired using what is called the Search-Locate algorithm.

Particle tracking for three-dimensional complicated geometry, which is usually solved using an unstructured grid, is a non-trivial problem. It requires an efficient algorithm otherwise, the Search-Locate process will be time consuming. This matter is reviewed by Chorda et al. (2002).

In the case of a structured grid, the problem of particle tracking is much simpler. This is the case in the present work. Consider, for example, an axi-symmetric flow. The following simple algorithm was found sufficient for our purpose,

1. The physical domain is divided into a number (ND) of sub-domains, as shown in

Figure 4.2. Each sub-domain, Ω_k , is defined by boundaries and its associated cells.

2. Knowing the particle position, the sub-domain Ω_k hosting the particle is determined.
3. Inside the sub-domain (determined in Step 2), the cell hosting the particle is defined by comparing the particle position (X_p, Y_p) to the cell boundaries. The cell (i, j) hosting the particle at position p satisfies the conditions,

$$x_i < x_p < x_{i+1} \quad (4.26)$$

$$y_i < y_p < y_{i+1} \quad (4.27)$$

4. Once the cell is defined, it is stored such that the particle attributes (such as a scalar Φ) is defined in terms of the particle number (n_p) and the cell label (i, j) .

4.2.6 Particle-Field and Field-Particle Interpolation

Usually, the field means or Favre-averaged quantities within a certain cell are estimated from the properties of the particles hosted by this cell. The calculation domain is covered by a grid system. In most cases, this grid system is chosen to coincide with the finite volume grid. The field mean values at the nodal locations are then calculated by interpolation from the particles in the dependence region. This is clarified in Figure 4.3. There, the field mean values at node (o) are calculated from the particles in the surrounding region, Ω_o . The boundaries of Ω_o are marked by thick lines. The field means (Favre averages) can be calculated as (Li and Modest, 2001),

$$\tilde{\Phi} = \frac{1}{m_o} \sum_{p \in \Omega_o} b_{po} m_p \Phi_p \quad (4.28)$$

Figure 4.2: Particles search-locate algorithm.

where the summation is applied to all the particles that belong to the region Ω_o ($p \in \Omega_o$). Φ_p is the scalar value of the particle at (x_p, y_p) coordinates. m_o is the normalized particle mass and is calculated as,

$$m_o = \sum_{p \in \Omega_o} b_{po} m_p \quad (4.29)$$

b_{po} is a weight factor that expresses the weight of the particle contribution to point (o). One expects that the closer the particle position to the node (o), the larger its contribution to the mean calculation and consequently, the larger value of b_{po}

In the present work, b_{po} is calculated using bilinear interpolation (Li and Modest, 2001; Mobus et al., 2001). Consider a particle, p , in location (x_p, y_p) in a cell, as shown in Figure 4.4. The contribution of the particle at point p to the cell nodes is calculated as (Li and Modest, 2001),

Figure 4.3: The dependence region Ω_o for the field point (o) interpolation from particles.

Figure 4.4: Particle in cell geometry (adopted from Li and Modest (2001)) .

$$b_{p_{i,j}} = fg \quad (4.30)$$

$$b_{p_{i+1,j}} = (1-f)g \quad (4.31)$$

$$b_{p_{i+1,j+1}} = (1-f)(1-g) \quad (4.32)$$

$$b_{p_{i,j+1}} = f(1-g) \quad (4.33)$$

where,

$$f = \frac{x_{i+1} - x_p}{x_{i+1} - x_i}, \quad g = \frac{y_{j+1} - y_p}{y_{j+1} - y_j} \quad (4.34)$$

Not only are nodal mean values interpolated from particles, but it is also necessary to calculate several quantities at each particle position. For example, the coefficients of Equation 4.13 are calculated at each particle position by interpolation from the field values stored at the nodes of the hosting cell. In the present work, the field means at an arbitrary particle position are linearly interpolated from the nodal values of the particle's hosting cell. If q denotes any mean quantities stored at vertices $q_{i,j}$, the values at arbitrary particle position p are calculated as,

$$q_p = q_{i,j}b_{p_{i,j}} + q_{i+1,j}b_{p_{i+1,j}} + q_{i+1,j+1}b_{p_{i+1,j+1}} + q_{i,j+1}b_{p_{i,j+1}} \quad (4.35)$$

where $b_{p_{i,j}}$ are weight factors calculated as previously shown.

4.2.7 Time Step

A time step (Δt) should be chosen properly for solving the stochastic differential equations and, consequently, for advancing the particles. For example, in simulations of complicated geometries, fine grid resolution is usually employed to properly detect the solution details in regions of large gradients. In conventional Monte Carlo algorithms, the time step is chosen on a global basis (Kannenbergh and Boyd, 2000). This means that the particle motion is limited by the residence time in the smallest cell. On the other hand, if a larger time step is chosen, poor results may be encountered as the particles will cross smaller cells without effectively contributing to them.

The time step is limited by the extended Courant number criterion (Xu and Pope, 1999). For example, in an axi-symmetric flow, the time step is chosen such that (Li and Modest, 2001),

$$\Delta t_i = \min \left\{ \left(\frac{k}{\varepsilon} \right)_i, N_{CFL} \frac{\Delta x_i}{|\tilde{U}_i|}, N_{CFL} \frac{\Delta y_i}{|\tilde{V}_i|} \right\} \quad i = 1, 2, \dots, N_c \quad (4.36)$$

N_c is the total number of cells in the computational domain. Δx_i and Δy_i are the dimensions of the cell (i) in x and y directions. $\tilde{U}_i$ and $\tilde{V}_i$ are the maximum velocities in cell (i) in x and y directions, respectively. $(\frac{k}{\varepsilon})$ represents the turbulence time scale in cell (i), and $\frac{\Delta x_i}{|\tilde{U}_i|}$ and $\frac{\Delta y_i}{|\tilde{V}_i|}$ represent the residence time of the particle in cell (i) in the x and y directions, respectively. Finally, N_{CFL} is called the particle *CFL* number (Courant-Fridrichs-Lewy). The N_{CFL} number should be less than 1 and is typically chosen between 0.6 and 0.7 (Mobus et al., 2001). Therefore, the global time step is chosen as the smallest over all the cells covering the flow domain,

$$\Delta t = \min \{ \Delta t_i, i = 1, 2, \dots, N_c \} \quad (4.37)$$

However, this choice of time step suffers from a serious disadvantage. It slows down the rate of convergence as the particles motion in the larger cells are limited by the residence time constraints in the smaller cells. This fact was confirmed by experimental computer runs of a conventional Monte Carlo algorithm as a preparatory work for the present chapter. This may lead to the point where the simulation becomes impractical due to excessive computational requirements such as in the case considered in the present work which seeks to iteratively optimize a gas turbine combustor. In the improved Monte Carlo algorithm, a remedy for this problem will be considered.

4.3 Improved Lagrangian Monte Carlo Algorithm

In this section, an improved scheme is presented. The aim of this algorithm is to improve computational efficiency and reduce numerical error. A local time step, together with variable stochastic fluid particle mass and second order accurate predictor-corrector scheme, is used in the improved scheme.

4.3.1 Local Time Step

It was previously explained that the use of a global constant time leads to inefficient computational scheme and slower convergence rate. Not only convergence requirements but also accuracy of the numerical method implies a smaller time step. A fractional time step approximation is used in the Lagrangian Monte Carlo method mixing process. This approximation leads to an error which is first order in time. Clearly, the smaller the time step, the smaller the error.

If a method could be advocated in such a way that the time step is chosen based on local CFL number criterion, the convergence would be accelerated and simultaneously, the accuracy improved. In other words, for smaller cells or high velocity regions, a small time

step is used and for larger cells or regions of slower flow motion a larger time step is used.

Kannenbergh and Boyd (2000) proposed a varying time step scheme for Monte Carlo calculations of gas molecules in a very low density flow. Mobus et al. (2001) suggested the application of this scheme to the Lagrangian Monte Carlo composition PDF. Shortly thereafter, Li and Modest (2001) applied this scheme to the case of mixing layer flow of hot and cold air. In this scheme, the local time step is chosen based on local CFL number criterion. Let Δt_l be the local time step such that,

$$\Delta t_l = t_{l+1} - t_l \quad (4.38)$$

where t_l is the initial time and t_{l+1} is the time at the end of the local period. For a particle n in a cell i at a local time level t_l , the local time step is chosen as,

$$(\Delta t_l)_i = \min \left\{ \frac{\tilde{k}}{\tilde{\varepsilon}}, N_{CFL} \frac{\Delta x}{|\tilde{U}|}, N_{CFL} \frac{\Delta y}{|\tilde{V}|} \right\}_i \quad (4.39)$$

This way, the local time step will vary from cell to cell depending on the cell geometry and flow parameters.

An adequate procedure, which ensures that all the particles are in the same time level, is to specify a constant global time step. At the end of this global time step, the field mean values are calculated as a weighted summation of the local time steps involved in the reference global time step. The weighting factor is estimated by the ratio of the local to the global time step.

In a local time step scheme, the global time step Δt is chosen to be large enough to exhaust many local steps. If, for example, the particle position is calculated directly in a global time period Δt , it will travel from point A to D , crossing many cells, as shown in Figure 4.5. In the local time step scheme, a different strategy is used. The particle moves from point A to point D in many local sub-moves corresponding to many local time steps;

Figure 4.5: Particle trajectory in a global time step (AD) and local time steps ($ABCD'$), (adopted from Li and Modest (2001))

from point A to B ; from B to C ; and finally, from C to D' . Let us say that the particle experiences n_l sub-moves in global time step Δt , then,

$$\sum_{i=1}^{n_l} (\Delta t_l)_i = \Delta t \quad (4.40)$$

From Equation 4.40 it can be seen that the last local time step must not be chosen based on the local CFL number. Instead, it is chosen such that all the particles are in the same physical time, $t + \Delta t$. The last local period for the last sub-move satisfies the inequality,

$$(\Delta t_l)_{n_l} \leq \min \left\{ \frac{\tilde{k}}{\tilde{\varepsilon}}, N_{CFL} \frac{\Delta x}{|\tilde{U}|}, N_{CFL} \frac{\Delta y}{|\tilde{V}|} \right\}_i \quad (4.41)$$

where i here is the cell hosting the particle at local time t_{nl-1} .

The field mean values are calculated at the end of each global time step such that the contribution of the particle in a local time step is weighted by the ratio of local to the global time step (Kannenbergh and Boyd, 2000). Therefore Equations 4.28 and 4.29 are

replaced by the following equations (Li and Modest, 2001),

$$\tilde{\Phi}_o^{k+1} = \frac{1}{m_o} \sum_{l=1}^S \sum_{p \in \Omega_o} m_p^k b_{po}^{k,t_l} \frac{\Delta t_l}{\Delta t} \Phi_n^{k,t_l} \quad (4.42)$$

$$m_o = \sum_{l=1}^S \sum_{p \in \Omega_o} m_p^k b_{po}^{k,t_l} \frac{\Delta t_l}{\Delta t} \quad (4.43)$$

where S is the number of sub-moves in global time step Δt , Δt_l is the local time step at sub-move l , t_l is the local timer, and k denotes the global time step.

We close the discussion of local time steps scheme with an important note on the mixing model used in such a scheme. As far as the LMSE mixing model is employed, there is no technical problem in combining it with the local time stepping scheme. The LMSE is a deterministic relaxation model. All the particles encounter mixing in each time step. Moreover, the decay of the variance is referenced to the mean values. These mean values can be effectively calculated from the field nodal values. Therefore, the model can naturally be implemented in each local time step.

For their part, particles collision models (such as the Curl model) are stochastic models. Not all the particles will encounter mixing in a certain time step, but only randomly chosen pairs. Also, the mixing mechanism evolves by the interaction of the particles. That is, each mixing event involves two randomly chosen particles. Consequently, the particles encountered in each interaction should be in the same time level. As a result, this mixing model cannot be applied with varying local time steps. Rather, the mixing events have to be introduced at the end of each global time step. This introduces severe constraints on the maximum value of the global time step. These constraints originate from the fractional time steps approximation.

In summary, the use of the LMSE mixing model is straightforward and fits the local

time step scheme. On the other hand, the application of particles collision models with such a scheme involves certain difficulties.

4.3.2 Predictor-Corrector Scheme

In conventional schemes, the stochastic differential Equations 4.11-4.14 are first order accurate in time. A predictor-corrector scheme, which is second order accurate in time, is used in the present work (Pope, 1995). The predictor step is applied to the motion of the particles in physical space (Li and Modest, 2001),

$$\underline{X}_{np}^{k,t_{l+1}} = \underline{X}_n^{k,t_l} + \left[\tilde{U} + \frac{\nabla D_t}{\langle \rho \rangle} \right]_{\underline{X}_n^{k,t_l}} \Delta t_l + \left[2\Delta t_l \frac{D_t}{\langle \rho \rangle} \right]_{\underline{X}_n^{k,t_l}}^{\frac{1}{2}} \eta \quad (4.44)$$

where n refers to the n^{th} particle, p refers to the predictor value, k is the k^{th} global time step and t_l is the local time. All the mean values are determined at the initial position $\underline{X}(t)$.

Next, the corrector step is applied to both the motion of particles in physical space and the evolution of their scalar values (by mixing and reaction) in phase space,

$$\begin{aligned} \underline{X}_{nc}^{k,t_{l+1}} &= \underline{X}_n^{k,t_l} + \frac{1}{2} \left\{ \left[\tilde{U} + \frac{1}{2} \frac{\nabla D_t}{\langle \rho \rangle} \right]_{\underline{X}_n^{k,t_l}} + \left[\tilde{U} + \frac{1}{2} \frac{\nabla D_t}{\langle \rho \rangle} \right]_{\underline{X}_{np}^{k,t_{l+1}}} \right\} \Delta t_l \\ &\quad + \frac{1}{\sqrt{2}} \left\{ \left[\Delta t_l \frac{\nabla D_t}{\langle \rho \rangle} \right]_{\underline{X}_n^{k,t_l}}^{\frac{1}{2}} + \left[\Delta t_l \frac{\nabla D_t}{\langle \rho \rangle} \right]_{\underline{X}_{np}^{k,t_{l+1}}}^{\frac{1}{2}} \right\} \eta \end{aligned} \quad (4.45)$$

while the scalar value is calculated as,

$$\begin{aligned}
\Phi_{nc}^{k,t_{l+1}} &= \Phi_n^{k,t_l} + \underline{S}^{k,t_l} \Delta t_l \\
&- \left(\Phi^{k,t_l} - \frac{(\tilde{\Phi})_{X_n^{k,t_l}} + (\tilde{\Phi})_{X_{np}^{k,t_{l+1}}}}{2} \right) \frac{C_\Phi \Delta t_l}{(\tau)_{X_n^{k,t_l}} + (\tau)_{X_{np}^{k,t_{l+1}}}}
\end{aligned} \tag{4.46}$$

Here the subscript c denotes the corrector value, $\tilde{\Phi}$ is the mean field value either at the initial particle position X_n^{k,t_l} or at the predictor particle position $X_{np}^{k,t_{l+1}}$, and τ is the turbulence time scale.

The fractional time step approximation explained earlier is more realistic when used with the predictor-corrector scheme. That is, the coefficients required for calculating the evolution equation are determined at the beginning and the end of the time period, rather than at the beginning of the time period exclusively.

4.3.3 Variable Particle Mass

The mass of the flow contained in each cell of the grid covering the flow domain varies due to either variation in cell size or variation in density. For a group of particles in a cell, the total mass of these particles should be equal to the mass of the flow inside this cell in order to ensure the mass conservation. Consequently, cells containing small amount of mass (cells of small size or cells containing low density flow) will encounter few particles. On the other hand, cells containing large amount of mass (cells of large size or cells containing high density flow) will encounter large number of particles. In both cases, the number of particles deviates considerably from the average. This leads to a large statistical error because of the cells containing few particles and a waste of computer time because of cells containing too many particles. Optimum simulation conditions are

attained by having a uniform distribution of the number of particles in all the cells covering the solution domain (Kannenberg and Boyd, 2000).

Particles mass in a certain cell may be initialized by dividing the mass of the flow in the cell volume by the number of particles it hosts. This satisfies the consistency requirements between the particles and the flow field at the initial time. Pope (1985) concluded that, if the spatial mass distribution of the particles is consistent with the flow field at the initial time, and if the mean velocity field satisfies the continuity equation, then the spatial mass distribution of the particles will be consistent with the mass distribution of the flow field all the time, as long as the particles velocity are interpolated from such a velocity field.

Consider, for example, an axi-symmetric flow. The volume of a cell must be calculated from the appropriate annulus. The volumes of cells located at large distances from the axis of symmetry are therefore larger in comparison to those cells of similar cross sectional area near the axis. Consider a cell k , with volume $\forall_k$, area in the plane containing the axis of symmetry A_k , and radial location of the centroid r_k , then,

$$\forall_k = 2\pi r_k A_k \quad (4.47)$$

Let the number of particles in the cell k be N_{pk} , each with mass Δm_p , then,

$$\Delta m_p N_{pk} = \forall_k \langle \rho_k \rangle \quad (4.48)$$

Therefore,

$$\frac{N_{pk}}{A_k} = \frac{2\pi}{\Delta m_p} r_k \langle \rho_k \rangle \quad (4.49)$$

$\frac{N_{pk}}{A_k}$ is defined as particle number density. It can be observed from Equation 4.49 that, when $\forall_k$ is small (i.e., for cells closer to the axis of symmetry), the particle number density is small. If adjustable particle weight factor w^n is introduced for the n^{th} particle, such

that particle (n) carries mass $w^n \Delta m_p$, then Equation 4.49 will be modified to (Pope, 1985),

$$\frac{N_{pk}}{A_k} = \frac{2\pi}{\Delta m_p} r_k \frac{\langle \rho_k \rangle}{\langle w_k \rangle} \quad (4.50)$$

where $\langle w_k \rangle$ is the average weight factor of particles in k^{th} cell. Therefore, the particle number density can be made uniform by controlling the weight factor. Each stochastic fluid particle represents a certain mass of the flow. As long as the spatial distribution of the particles mass does not violate the consistency condition, there is no reason why the mass represented by the particles should be the same in all parts of the flow field. This principle allows us to use the weighting factors. The weighting factors w^n are mainly used to compensate for large disparities in cell volume or density distribution (Haworth and Eltahry, 1991).

Therefore, the particle variable mass can be modified in several ways to maintain a uniform distribution of particle number in each cell “particle number density”. For example, consider once again the case of axi-symmetric flow. Let us assume for simplicity a constant density flow and constant plane area of each cell. Therefore, the cells volume will vary only by varying the radial position of the cell centroid. When a particle moves from a cell of lower radial dimension to a higher one, its mass will increase linearly with the radial coordinate to compensate for the mass increment in each cell. Vice versa, when a particle moves in the opposite direction its mass will decrease. In a series of successive moves, the mass of the particle may increase or decrease more or less than a specified limit (Lapenta and Brackbill, 1994).

If the particle mass increases more than a specified limit, it can be split into two particles. If the particle mass is smaller than a specified limit, the particle can be removed from the population as this particle does not carry much information and tracking it lead to waste of computer time.

Alternatively, if the number of particles in a certain cell increases more than the average number of particle per cell, then some of the particles can be combined with one another to reduce the total number of particles in this cell. On the other hand, if the number of particles in a cell decreases to a level well below the average, the particles that carry larger mass can be split, thus increasing the total number of particles in this cell.

The only constraint imposed on this practice (particle mass control) is that the weighted averages of a group of particles in a cell should be left unaltered (Lapenta and Brackbill, 1994). In the present work, particle mass control is used in a way that it complies with this rule. For example, particle-splitting procedures are implemented in the present work as follows: the high mass particles are split into two particles each, carrying half the mass and the same scalar value and both particles will occupy the same position. These procedures keep the weighted mean unchanged in a cell.

In the case of particle recombination, the procedures is slightly more complicated. Consider, for example, two particles with masses m_1 and m_2 , scalar values Φ_1 and Φ_2 and positions X_1 and X_2 . The question is how to calculate the new particle properties in a way that the mean remains unchanged. A simple procedure involves locating the new particle at a weighted average position (Li and Boyd, 2001). The mass of the new particle is the sum of the two masses. The scalar value of the new particle takes the value Φ_1 , with probability $\frac{m_1}{m_1+m_2}$, and takes the value Φ_2 with probability $\frac{m_2}{m_1+m_2}$. This is applied in our code using acceptance-rejection procedures, as follows: the total probability is $\left(\frac{m_1}{m_1+m_2} + \frac{m_2}{m_1+m_2}\right)$ and equal to one. A random number is generated between zero and one. If the value of the generated random number is less than $\frac{m_1}{m_1+m_2}$, then Φ_{new} takes the value Φ_1 . If the value of the generated random number is greater than $\frac{m_1}{m_1+m_2}$, then Φ_{new} takes the value Φ_2 .

4.3.4 Improved Solution Algorithm

A relatively detailed algorithm is presented in this section. This algorithm incorporates ideas previously discussed, as follows:

1. Specify a global time step.
2. Initialize particles distribution over the flow domain. A number of particles N_{pc} is distributed randomly inside each cell. The mass of the particles is chosen in order to ensure continuity inside each cell,

$$\sum_{p=1}^{N_{pc}} \Delta m_p = m_{cell}$$

3. Assign an initial concentration and temperature to each particle. The initial conditions must verify the realizability of the PDF distribution (for example, chemical equilibrium conditions).
4. Solve the flow field using the finite volume method.
5. Introduce inlet fluid particles according to the specified inlet mass flow rate together with the global time step.
6. Interpolate particle velocity, pressure and turbulence parameters from nodal values resulting from Step 4.
7. Calculate the local time step using Equation 4.39.
8. Move the particles according to the predictor Equation 4.44 using the time step calculated in Step 7. The mean values used in calculating the coefficients in Equation 4.44 are calculated at the initial time.

9. Determine the new cells containing the particles after the motion resulting from Step 8. This is done using the search-locate algorithm.
10. Interpolate the flow field variables at the particles new position calculated in Step 8 using the nodal values of host cells determined at Step 9.
11. Calculate the corrected position of the particles using Equation 4.45.
12. Calculate chemical kinetics for each particle (each particle acts as an independent batch reactor).
13. Apply Equation 4.46 for calculating scalar values of particles after mixing using LMSE model.
14. Determine the new cells hosting the particles after the position correction calculated in Step 11.
15. If the particle is out of the domain, remove the particle from the ensemble.
16. If the particle crosses the solid walls or symmetry lines, apply reflection boundary conditions.
17. Modify the particle mass if they changed the initial cell that hosted the particle.
18. Store the local time step, the particle scalar values, densities and masses in a matrix defined by particles labels.
19. Repeat Steps 6 to 17 until the sum of the local time steps for each particle is equal to the global time step specified in Step 1.
20. Using the coefficients in the matrix calculated in Step 18, interpolate the field nodal values (density, scalar) using Equations 4.42 and 4.43.

21. Apply particle mass control procedures to obtain uniform distribution of particles in cells.
22. Using the new nodal density values, calculate the flow field.
23. The field nodal values are averaged over a specific number of global iterations. These procedures are found effective at removing the fluctuations in the solution variables. Also, it helps to accelerate the convergence as the number of particles can be considered virtually as the sum of the particles in each of the iterations over which the average is taken.
24. Repeat (5) to (23) until a steady state solution is obtained. The steady state solution is considered in terms of the variable that has the slowest rate of convergence.

4.3.5 Performance Comparison of Conventional versus Improved Algorithm

4.3.5a Computational Work Comparison

In this section, we roughly estimate the number of calculations required for the improved algorithm as opposed to the conventional algorithm. This amount of work can be measured by the number of calculations required for each scheme (Li and Modest, 2001). The relative computational efficiency of the two schemes can be measured by the ratios of the amount of work of each, $\frac{W_{imp}}{W_{conv}}$.

Let N be the total number of particles. W_P is the computational work per particle per time step. I is the number of time steps to obtain the final convergence. Therefore,

$$W_{conv} \propto I_{conv} N W_P \quad (4.51)$$

To insert the time step into this expression, I_{conv} can be estimated as,

$$I_{conv} = \frac{t}{\Delta t_{conv}} \quad (4.52)$$

where t is the total time required for convergence, Δt_{conv} is the time step employed in the conventional scheme. Then,

$$W_{conv} \propto \frac{t}{\Delta t_{conv}} N W_P \quad (4.53)$$

For the improved scheme, two factors are considered in calculating the amount of work. First, an extra work is done due to particles splitting and it is denoted by W_a . Second, in time step Δt_{imp} , the particle encounter l sub-moves on average. Therefore,

$$W_{imp} \propto N I_{imp} (l W_P + W_a) \quad (4.54)$$

Substituting for the number of time steps for obtaining the convergence in the improved scheme,

$$W_{imp} \propto N \frac{t}{\Delta t_{imp}} (l W_P + W_a) \quad (4.55)$$

Using Equations 4.53 and 4.55, the ratio of the amount of computational work of the two schemes is estimated as,

$$\frac{W_{imp}}{W_{conv}} = \left(l + \frac{W_a}{W_P} \right) \frac{\Delta t_{conv}}{\Delta t_{imp}} \quad (4.56)$$

Increasing Δt_{imp} has two opposite effects on the amount of computational work given by Equation 4.56. The ratio decreases as a direct result of increasing Δt_{imp} and decreases in an indirect way due to the effect of Δt_{imp} on increasing l (the number of sub-moves in one global time step Δt_{imp} .) However the rate of increment l is much slower than the increment Δt_{imp} and the ratio $\frac{W_{imp}}{W_{conv}}$ tends to be less than unity.

4.3.5b Statistical Error Comparison

Another issue for performance analysis is the numerical error. Error analysis in Monte Carlo method is usually more difficult to evaluate than in the finite difference method. Here, we only consider the statistical error as it is the dominant source of error in Monte Carlo methods. The statistical error arises from the use of finite sample size in calculating the field means (this definition corresponds to the case of weak convergence). It is measured by the standard deviation and is found to be inversely proportional to the reciprocal of the square root of the number of particles in a cell (N_{pc}),

$$Error_{st} \propto \frac{1}{\sqrt{N_{pc}}} \quad (4.57)$$

This relation indicates an unpleasant behaviour of the Monte Carlo methods. The statistical error decreases slowly with increasing N_{pc} .

Assume the average number of particles in a cell is N_{pav} . Using particle number density controlling techniques, the number of particles per cell $(N_p)_{imp}$ is very close to N_{pav} in the improved scheme. In the conventional scheme, small volume cells contain a number of particles $(N_p)_{conv}$ which is much smaller than N_{pav} . Therefore,

$$(Error_{st})_{imp} \propto \frac{1}{\sqrt{(N_p)_{imp}}} \quad (4.58)$$

$$(Error_{st})_{conv} \propto \frac{1}{\sqrt{(N_p)_{conv}}} \quad (4.59)$$

but,

$$(N_p)_{imp} \approx N_{pav} \quad (4.60)$$

and,

$$(N_p)_{conv} < N_{pav} \quad (4.61)$$

or alternatively,

$$(N_p)_{conv} = factor \times N_{pav} \quad (4.62)$$

where, $factor < 1$, then,

$$(Error_{st})_{conv} \propto \frac{1}{\sqrt{factor \times N_{pav}}} \quad (4.63)$$

Then, the ratio between the statistical error generated from the two algorithms can be estimated as,

$$\frac{(Error_{st})_{imp}}{(Error_{st})_{conv}} = \sqrt{factor} < 1 \quad (4.64)$$

4.3.6 Notes on the Monte Carlo Coding

4.3.6a Gaussian Random Number Generator

Let $A = (A_1, A_2)$ be a random vector with uniform distribution in the unit circle $\Omega' = \{(A_1, A_2) | 0 < A_1^2 + A_2^2 < 1\}$. It can be proven (Ottinger, 1996),

$$B_j = g_j(A_1, A_2) = \sqrt{\frac{-2\ln(A_1^2 + A_2^2)}{A_1^2 + A_2^2}} A_j \quad j = 1, 2 \quad (4.65)$$

is a Gaussian random variable. Therefore, this result can be used as a basis for generating a Gaussian random variable. The following algorithm is used,

1. Generate uniformly distributed random variable A_1 , between zero and one.
2. Generate another uniformly distributed random variable A_2 , between zero and one.

3. Transform both A_1 and A_2 from $[0,1]$ to $[-1,1]$ using,

$$A_1 = 2 \times A_1 - 1$$

$$A_2 = 2 \times A_2 - 1.$$

4. Calculate $A_{circ} = \sqrt{A_1^2 + A_2^2}$.
5. If A_{circ} is outside a unit circle, go to Step 1.
6. Use Equation 4.65 to generate the Gaussian random variable.
7. End.

4.3.6b Particles Indexing

Assume a configuration of 2 cells and 10 particles. Each particle is identified by a label. Assume that at time zero, 6 particles labelled from 1 to 6 are in cell 1, while 4 particles labelled from 7 to 10 are in cell 2. In time period Δt , some particles are moved randomly from cell 1 to cell 2 and vice versa. A possible arrangement is for cell 1 to contain 5 particles labelled 1, 5, 6, 8, and 9 while for cell 2 to contain the remaining particles labelled 2, 3, 4, 7, and 10. This simple example simulates particle motion in PDF solution algorithm.

In implementing particle number density control, it would be much simpler if the particles inside each cell are reindexed after each global time step Δt . Using particles indexing after time step Δt in the above example, the particles in cell 1 would be labelled from 1 to 5, while the particles in cell 2 would be labelled from 6 to 10. This enables direct access to the particles, a procedure which simplifies other submodules in the solution algorithm. Moreover, particles indexing is indispensable in mixing models that employ particles collision such as the Curl model. This technique is used in the solution algorithm and its procedures are best explained by the Fortran subroutine listed in Figure 4.6.

```

**particle indexing subroutine
*****
subroutine pindex(npartot)
  *nmax----->is the max number of cell in x direction
  *jmaxn(i)---->is the maximum number of cell in vertical direction
  *indx(1,i,j)-->the total number particles in cell i,j
  *indx(2,i,j)-->is the starting label of particles in cell i,j
  *npartot----->is the total number of particles in domain
  *part(1,n)---->particle n position coordinate in x direction
  *part(2,n)---->particle n position coordinate in y direction
  *lookcel----->search locate subroutine, given the particle x,y
  *              position, it determine the host cell i,j
  *lcr(k)-----> is the new temporary index
  do 20 i=1,nmax
    do 20 j=1,jmaxn(i)
      indx(1,i,j)=0
      indx(2,i,j)=0
20  continue
    do 40 n=1,npartot
      call lookcel(part(1,n),part(2,n),i,j)
      indx(1,i,j)=indx(1,i,j)+1
40  continue
    m=0
    do 60 i=1,ni
      do 60 j=1,jmaxn(i)
        indx(2,i,j)=m
        m=m+indx(1,i,j)
        indx(1,i,j)=0
60  continue
    do 80 n=1,npartot
      call lookcel(part(8,n),part(9,n),i,j)
      indx(1,i,j)=indx(1,i,j)+1
      k=indx(2,i,j)+indx(1,i,j)
      lcr(k)=n
80  continue
  return
end

```

Figure 4.6: Fortran subroutine for particle reindexing.

4.4 Chemical Kinetics

Chemical kinetics have a major impact on the accuracy of predictions of turbulent combustion models. Detailed reaction mechanisms are essential for emissions or stability (ignition and blowout) calculations.

As previously discussed, some of the theories of turbulent combustion employ the infinite chemistry assumption. This leads to a considerable simplification of chemistry to the level of one global reaction that produces global effects such as burning velocity, flammability limits and adiabatic flame temperature (Westbrook and Dryer, 1981). However, the new restrictive limits on emissions led to more attention to be given to chemical kinetics. Consider the predictions of NO_x emissions in gas turbine combustors as an example. The concentration of NO_x is one to two orders of magnitude lower than in equilibrium concentration (Kuznetsov and Sabel'nikov, 1990). A typical example will be shown in the next section as the bluff body stabilized flame measurements reported by Nandula et al. (1996) are compared with predictions. While the reported NO concentrations measured in the former reference ranges from 3 to 10 *ppm*, the equilibrium value is estimated to be 1442 *ppm* in the same reference. Furthermore, NO_x emissions are strongly dependent on the temperature. Thus, any deviation from equilibrium conditions would greatly affect the NO_x emissions predictions.

4.4.1 Stiffness of the Chemical Kinetics Equations

Consider the equation,

$$y' = \lambda y \tag{4.66}$$

A solution to the ordinary differential Equation 4.66 has the form,

$$y = ce^{\lambda t} \quad (4.67)$$

For a negative λ , then y decays by a factor e^{-1} in a time period of $\frac{-1}{\lambda}$. The latter is the time scale (Gear, 1971).

Consider a system of two decoupled differential equations (Gear, 1971),

$$y' = -y, \quad y(0) = 1 \quad (4.68)$$

$$z' = -1000z, \quad z(0) = 1 \quad (4.69)$$

The solution to these equations takes the form of,

$$y = C_y e^{-t} \quad (4.70)$$

$$z = C_z e^{-1000t} \quad (4.71)$$

That is, z decays rapidly and becomes negligible compared to y , which decays slowly.

The fast varying variable z will control the stability of the problem and, therefore, the bounds on the time step. Usually z is an intermediate species which decays to an insignificant level, so that the truncation error is determined by the slow component y . If conventional numerical methods are used for solving the system of Equations 4.68 and 4.69, time steps not greater than the time scale of z should be used. This is known as the problem of stiffness.

The chemical kinetics encountered in combustion lead to a system of ordinary differential equations in which the independent variable is the time and the dependent variables are the species concentrations. The time derivatives of the dependent variables are the reaction rates. The reaction rates in combustion chemistry span many orders of magnitudes. In other words, the chemical kinetics time scales cover a wide band from very fast reactive species (radicals) to very slow ones. For this reason, the common methods of integrating

ordinary differential equations are not suitable for the chemical kinetics.

The time step for advancing solution of the chemical kinetics is limited by the fast rates. Simultaneously, the total time required to complete the integration is limited by the slowest reaction. The difference between the slowest and fastest reaction is several orders of magnitude. This imposes extraordinary requirements on the computer time for the integration of chemical kinetics.

4.4.2 Reaction Mechanisms

Combustion reaction mechanisms are chain mechanisms. The basic idea of chain mechanisms is that the products of one step may serve as reactants of one or more subsequent steps. The chain nature of combustion is particularly significant in developing new mechanisms or in reducing detailed ones. Often, reactive chain centers or active species are single atoms called free radicals. As hydrocarbon species proceed in reaction chains, each intermediate species is produced and consumed by a few major reactions. This may allow for the derivation of algebraic expressions for these species from their steady state relations. Different types of reaction mechanisms are briefly discussed below.

- (i) **Detailed Mechanisms:** A typical example of detailed mechanism is the GRI-Mech 3.0 (Bowman et al., 2002). This is a list of 325 elementary chemical reactions and associated rate coefficient expressions. Thermochemical parameters for 53 species are involved in these reactions. In practice, detailed mechanisms are not readily used in turbulent combustion models. However, they serve as a starting point for deriving reduced mechanisms or as a reference for testing the performance of reduced mechanisms (Nicol et al., 1999).
- (ii) **Reduced Mechanisms:** Reduced mechanisms are developed to simulate the most important features of a chemical reaction. Therefore, few species and chemical re-

actions are involved. These simplified mechanisms are more tractable for practical applications.

Starting with detailed mechanisms, reduced reaction mechanisms can be derived. Basically, there are two distinctive ways of deriving reduced mechanisms: the first, by employing assumptions of steady states and partial equilibrium and the second, by systematic reduction based on sensitivity analysis. The first relies on physical assumptions while the second relies on extensive calculations. Reduced mechanisms are useful in practical applications of turbulent combustion models as the computational efforts are reduced by replacing some of the ordinary differential equations with algebraic ones. Also, reduced mechanisms allow for the application of the asymptotic method for flame analysis.

- (iii) **Global Reactions Mechanisms:** A global reaction is a reaction for which the reaction rate does not follow stoichiometry rules as opposed to an elementary reaction. The overall reaction rate equation is expressed as a combination of an overall Arrhenius expression and dependency on the fuel and oxidant concentrations (e.g., Table 4.3). The quantitative expressions for global reactions are commonly derived from the temperature and concentration dependencies of reaction rate data in a stirred reactor or a shock tube. However, the conditions of the validity of these reactions are of major concern. These conditions are usually defined by range of inlet temperature, equivalence ratio, and pressure.

4.4.3 Candidate Reaction Mechanism

The reaction mechanisms used in practical applications are either the reduced mechanisms or the global ones. Integration of the reduced mechanisms is much more time consuming than integration of the global mechanisms. This is because the stiffness of the

Table 4.3: Five-step global kinetic mechanism for Methane oxidation and NO formation. Units are Kmoles, cubic meters, seconds and Kelvin. (Nicol et al. 1999).

$CH_4 + \frac{3}{2}O_2 \Rightarrow CO + 2H_2O$	$R_1 = 10^{15.220}[CH_4]^{1.460}[O_2]^{0.5217} \exp\left(\frac{-20643}{T}\right)$
$CO + \frac{1}{2}O_2 \Rightarrow CO_2$	$R_2 = 10^{14.902}[CO]^{1.6904}[O_2]^{1.570} \exp\left(\frac{-11613}{T}\right)$
$CO_2 \Rightarrow CO + \frac{1}{2}O_2$	$R_3 = 10^{14.349}[CO_2]^{1.0} \exp\left(\frac{-62281}{T}\right)$
$N_2 + O_2 \Rightarrow 2NO$	$R_4 = 10^{23.946}[CO]^{0.7211}[O_2]^{4.0111} \exp\left(\frac{-53369}{T}\right)$
$N_2 + O_2 \Rightarrow 2NO$	$R_5 = 10^{14.967}T^{-0.5}[N_2][O_2]^{0.5} \exp\left(\frac{-68899}{T}\right)$

reduced mechanisms is more significant than that of the global ones. Also, because integration of the reaction rates in the reduced mechanisms requires the calculation of steady state species concentrations, which is time consuming itself (Fueyo et al., 2000).

Consequently, the global reaction mechanisms, developed by Nicol and co-workers (Nicol et al., 1995; Nicol et al., 1999), is used for the chemical kinetics calculations in the present work. This is a five-step mechanism for Methane oxidation and NO formation, as shown in Table 4.3. The net production or destruction rate for each species is given as (Nicol et al., 1999),

$$\frac{d[CH_4]}{dt} = -R_1 \quad (4.72)$$

$$\frac{d[CO_2]}{dt} = R_2 - R_3 \quad (4.73)$$

$$\frac{d[CO]}{dt} = R_1 + R_3 - R_2 \quad (4.74)$$

$$\frac{d[NO]}{dt} = 2R_4 + 2R_5 \quad (4.75)$$

The last two steps in the reaction mechanism are for *NO* calculations. The first of these is for calculating non-thermally formed *NO* such as prompt *NO*. The second is for calculating thermally-formed *NO*. The thermally-formed *NO* depends mainly on temperature, as can be seen in the expression of the reaction rate R_5 . The non-thermally formed *NO* depends on free radicals. Nicol et al. (1999) pointed out that *CO* is indicative of the free radicals and, consequently, the reaction rate R_4 depends on the *CO* concentration.

The five-step global mechanism was developed for modelling lean premixed gas turbine combustors. The reaction was developed at conditions of 650 *K* for the inlet temperature while the equivalence ratio ranges from 0.45 to 0.75. Beyond these conditions, the mechanism has not been validated.

Finally, it is noted that the exponents of the reaction rates (Table 4.3) are all non-negative numbers. This is an advantageous property from a computational point of view. It was noted by Coffee (1985) that negative exponents in a global reaction rate affect both the convergence and the accuracy of calculations. An example of a global reaction rate with negative exponents is the two-step mechanism by Westbrook and Dryer (1982). In fact, the author's experience with this two-step reaction mechanism confirms Coffee's warning about negative exponents in global reaction rates.

4.4.4 Solution of Chemical Kinetics Equations

DVODE, a package of subroutines for the numerical solution of a stiff or non-stiff system of ordinary differential equations with variable coefficients, is used for solving the

chemical kinetics equations. In principle, the chemical kinetics rate reactions can be cast in the form,

$$\frac{d\phi(i)}{dt} = f(i, t, \phi(1), \phi(2), \dots, \phi(Ns)) \quad i = 1, \dots, Ns \quad (4.76)$$

with the initial conditions specified at t_o . Given the initial values of $\phi(i)$, we want to integrate the system of Equation 4.76 to determine $\phi(i)$ at later times. Equations of the form 4.76, together with the Jacobian matrix are supplied to the DVODE algorithm (Brown et al., 1989). The solver employs the method of backward differentiation formulas to solve the stiff differential equations. This method is common for solving systems of stiff equations and it is described in detail by Gear (1971).

The coefficients of the system of Equations 4.76 are calculated for each particle at each time step. Starting with these coefficients together with the particle initial composition, the system of differential equations is integrated in time using the DVODE algorithm.

4.5 Model Evaluation: Bluff Body Stabilized Combustor

A model evaluation that compares predictions with measured data provides confidence and certainty in the modelling assumptions. Nandula et al. (1996) obtained measurements in a bluff body stabilized combustor at lean premixed conditions. These Laser-Doppler Anemometry (LDA) measurements of velocity and a combination of Rayleigh scattering, spontaneous Raman scattering and laser induced fluorescence (LIF) measurements of chemical species and temperature were obtained to provide a source of information against which models can be evaluated.

The combustion chamber shown in Figure 4.7 was configured by mounting a stainless

Table 4.4: Uncertainty in chemical species and temperature measurements (Nandula et al., 1996)

Scalar	%Error
CH_4	3.3
H_2O	5.1
CO_2	5.1
NO	7.6
CO	17.6
Temperature	1.0

steel conical bluff body coaxially at the center of the combustor to serve as a flame holder. The uncertainty involved in the chemical species and temperature measurements (Nandula et al., 1996), based on a single-shot uncertainty analysis, is reported in Table 4.4.

The boundary conditions and numerical parameters used to model the bluff body stabilized combustor will be presented. Measured and predicted profiles of the axial velocity, temperature, and concentrations of CH_4 , H_2O , CO_2 , CO , and NO at various locations in the combustor will be compared and discussed.

4.5.1 Boundary Conditions

The mass flow rate for the bluff body combustor was reported as 3960 SLPM for the air and 244 SLPM (standard liters per minute) for the CH_4 fuel. This corresponds to an equivalence ratio of 0.586. A turbulence grid was placed at the entrance of the combustor section, upstream from the bluff body. The corresponding free stream turbulence at the inlet of the combustor (just downstream from the turbulence grid) was 24%. The inlet flow temperature was 300 K and the inlet pressure was 1 atm. A combustor wall temperature of 500 K was kept constant during the experiment. Zero radial velocity was specified at the inlet. At the line of symmetry, a zero gradient with respect to the radial direction were assumed for the axial velocity while the radial velocity component was assumed to

Figure 4.7: Schematic and turbulent flame structure of bluff body stabilized lean premixed combustor (from Nandula et al. (1996)).

be zero. Outflow boundary conditions were specified by zero gradients of the velocity components with respect to the axial direction. Boundary conditions were also specified for the stochastic particles in the Monte Carlo method. Stochastic particles attempting to leave the domain at the wall or line of symmetry are reflected back into the domain (reflection boundary conditions). Convective heat loss was calculated for each cell adjacent to the wall (wall cells) based on the law of the wall for heat transfer (Launder and Spalding, 1974). This heat flux was subtracted from the particles residing in the near-wall cells.

4.5.2 Particle Number Independence

Simulations were performed using particle number densities of 15, 25 and 50 particles per cell, respectively. A structured grid resolution of 35×27 was used for solving the turbulent flow (as recommended by Lilley and Rhode (1982)). Figure 4.8 shows predictions of temperature profiles in the radial direction using the three different particle number densities at four different axial locations: $\frac{x}{d} = 0.1, 0.3, 0.6$, and 1.0 , where d is the bluff body diameter. The simulation conditions were similar to the experimental conditions used by Nandula et al. (1996). The results from the three particle number densities match one another almost everywhere in the four axial locations. Therefore, 15 particles per cell were used in the other simulations of the bluff body stabilized combustor presented in this chapter. The same number of particles per cell is also used for the swirl stabilized combustor calculations presented in the next section.

The particle number independence test presented in Figure 4.8 shows the superiority of the improved algorithm over the conventional algorithms. A rough figure for the number of particles per cell used in conventional schemes was given in Table 2.1 (Chapter 2). It is found there that the number of particles per cell of the order of 100 is usually used in similar calculations.

Figure 4.8: Particle number independence test of the improved algorithm of the composition PDF model (experimental data from Nandula et al. (1996)).

4.5.3 Results and Comparisons

Calculations were implemented using a Pentium 4, Intel 2800 MHZ processor. A structured grid resolution of 35×27 was used for solving the turbulent flow and 15 particles per cell were used for the Monte Carlo simulation. The steady state solution in terms of the NO concentrations were obtained in 1100 global iterations and a global time step of 0.002 second with corresponding computational time of about 51 minutes.

4.5.3a Velocity

The predicted radial profiles of mean axial velocity are compared to the measured velocity field at four different axial locations, as shown in Figure 4.9. These locations are specified at axial distances $\frac{x}{d} = 0.1, 0.3, 0.6$, and 1.0 , respectively. It is shown that the predicted axial profiles are in good agreement with the measurements. Two gross features of the velocity field are captured by the numerical simulation: the recirculation zone and the shear layer.

The recirculation zone along the center line is indicated by the negative axial velocity. This zone is also obvious from the directions of the arrows in Figure 4.10. This recirculation zone is responsible for keeping continuous combustion by back-mixing the hot products with the incoming cold reactants. The shear layer is also well predicted and indicated by the region of large velocity gradient in Figure 4.9.

4.5.3b Temperature

The predicted radial profile of the temperature distribution is compared to the measured temperature at the same specified four axial planes, as shown in Figure 4.11. In general, the predicted temperature profiles compare reasonably well with the measured temperature. The temperature profiles reveal the location of cold reactants and hot products within the combustion chamber. Also, the location of the region where cold and hot

Figure 4.9: Measurements and predictions, using the improved algorithm of the composition PDF model, of mean axial velocity profiles in the bluff body stabilized combustor (experimental data from Nandula et al. (1996)).

Figure 4.10: Bluff body velocity field, in the case of combustion, using the improved algorithm of the PDF composition model.

flow are mixed is indicated by the steep temperature gradients. It should be noted that the temperature in the shear layer is generally under-estimated. possible explanation for the under-estimation of the temperature distribution is the excessive mixing between cold and hot products. This excessive mixing indicates high mixing rate which is directly linked to the turbulence parameters (turbulent kinetic energy and dissipation rate).

4.5.3c Major Species

Figures 4.12, 4.13, and 4.14 represent the radial profiles of three major species CH_4 , H_2O , and CO_2 at four different axial locations. Overall, the major species are well predicted.

The comparison of the predicted CH_4 mole fraction showed good agreement with the measurements, as shown in Figure 4.12. The recirculation region where CH_4 is consumed is indicated by the very small amount of CH_4 mole fraction. It is also of interest to note

Figure 4.11: Measurements and predictions, using the improved algorithm of the composition PDF model, of mean temperature profiles in the bluff body stabilized combustor (experimental data from Nandula et al. (1996)).

Figure 4.12: Measurements and predictions, using the improved algorithm of the composition PDF model, of mean CH_4 mole fraction profiles in the bluff body stabilized combustor (experimental data from Nandula et al. (1996)).

Figure 4.13: Measurements and predictions, using the improved algorithm of the composition PDF model, of mean H_2O mole fraction profiles in the bluff body stabilized combustor (experimental data from Nandula et al. (1996)).

Figure 4.14: Measurements and predictions, using the improved algorithm of the composition PDF model, of mean CO_2 mole fraction profiles in the bluff body stabilized combustor (experimental data from Nandula et al. (1996)).

from the measurements that the gradients of CH_4 in the shear layer are less steep as one moves downstream. This feature is well captured by the predictions as it appears from the profile at $\frac{x}{d} = 0.1$, which encounters sharp gradients in the shear layer while in the case of $\frac{x}{d} = 1.0$, the gradients are less steep and the shear layer is wider.

Another interesting observation can be made by comparing CH_4 mole fraction profiles (Figure 4.12) to the temperature profiles (Figure 4.11). It is found that the regions where the temperature is under-estimated are in spatial correspondence to the regions where the fuel mole fractions are over-estimated. This indicates that the temperature predictions are to a great extent influenced by the CH_4 oxidation reaction. A direct implication of this observation is that a one- or two-step global reaction mechanism may be sufficient for obtaining good temperature distribution inside the combustor assuming that the CH_4 oxidation is well represented by this mechanism.

Comparisons of the predicted H_2O mole fraction with the measured values are shown in Figure 4.13. It is found that the predicted H_2O mole fractions are in very good agreement with the measurements. This is likely because the reaction rate of H_2O represented by the present reaction mechanism being sufficiently fast so as to not be influenced by the mixing process.

The predicted CO_2 mole fraction are shown in Figure 4.14. The radial profiles match well the measurements, specifically, the predictions in the shear layer region. Also, the expansion of the shear layer width while moving downstream is well predicted. Under-estimated values of CO_2 are observed in the shear layer side closer to the recirculation zone. These under-estimated values of the CO_2 mole fraction are probably due to over-estimated values of the fuel at this region, which means less CO production.

4.5.3d Minor Species

The predictions of the minor species, CO and NO , were compared against the experimental values at four different axial locations, as shown in Figures 4.15 and 4.16. In general, accurate predictions of minor species is extremely difficult and strongly dependent on the reaction mechanism.

In all profiles of the CO mole fraction, the peak values were under-estimated. However, moving downstream, the predicted peak values approach the measured ones. Despite the discrepancies between the measured and predicted peak values, the position of the peaks were accurately predicted.

The values of the CO mole fraction in the recirculation zone are under-estimated at $\frac{x}{d} = 0.1$ and 0.3 . However, it is in good agreement with the measurements at $\frac{x}{d} = 0.6$ and 1.0 . Also, the quenching due to the shear layer mixing is indicated by large CO mole fraction in this region. This is explained by the fact that quenching prevents further oxidation of CO into CO_2 , a reaction which is promoted by a higher temperature level.

NO predicted mole fractions are compared to the measured values, as shown in Figure 4.16. Clearly, the values of NO mole fraction are greatly under-estimated over the entire flow domain. It is believed that the explanation for this is two-folds. The first is violating the range of valid conditions for the application of the global reaction mechanism (Nicol et al., 1999). These conditions are 650 K for the inlet temperature and an equivalence ratio between 0.45 and 0.75 . The second reason is believed to be also connected with the ability of the mechanism to predict NO production at very lean conditions. Similar trends in NO predictions at similar conditions was reported by Hamer and Roby (1997). In their simulation of premixed mixture in an axi-symmetric combustor, the predicted average value of NO mole fraction at the exit was 1 ppm , corresponding to average exit temperature of 1563 K and an equivalence ratio of 0.51 .

To investigate the effects of violating the valid range of conditions for the global mech-

Figure 4.15: Measurements and predictions, using the improved algorithm of the composition PDF model, of mean CO mole fraction (ppm) profiles in the bluff body stabilized combustor (experimental data from Nandula et al. (1996)).

Figure 4.16: Measurements and predictions, using the improved algorithm of the composition PDF model, of mean *NO* mole fraction (*ppm*) profiles in the bluff body stabilized combustor (experimental data from Nandula et al. (1996)).

anism on *NO* predictions, calculations were performed at an inlet temperature of 650 *K*. This is the inlet temperature at which the mechanism was derived. The results of temperature and *NO* mole fraction predictions at $\frac{x}{d} = 0.1$ are shown in Figures 4.17 and 4.18, respectively. It is shown that the predicted levels of *NO* mole fraction at 650 *K* are higher than the *NO* mole fraction predictions at 300 *K* by nearly an order of magnitude.

Figure 4.17:
Temperature profiles for
inlet temperatures of
650 *K* and 300 *K*.

Figure 4.18: *NO* mole
fraction (*ppm*) profiles for
inlet temperatures of
650 *K* and 300 *K*.

4.6 Model Evaluation: Swirl Stabilized Combustor

Here, the improved composition PDF algorithm is evaluated against measurements in a swirl stabilized combustor operating under lean premixed conditions. Temperature and species concentrations measurements in an axi-symmetric combustor were reported by Flores and Hedman (1996). Later, velocity measurements for the same geometry and flow condition were reported by Hedman et al. (2002). However, species concentrations measurements are not used in the model evaluation due to problems encountered in matching

equilibrium concentrations as reported by Cannon et al. (1997). Therefore, the predictions will only be compared with the velocity and temperature measurements.

Coherent Anti-Stokes Raman Spectroscopy (CARS) was used to measure gas temperature and species concentrations, while Laser Doppler Anemometry (LDA) was used for velocity measurements. The experimental setup is shown in Figure 4.19. The swirler geometry is shown in Figure 4.20, while the premixed injector is shown in Figure 4.21. The combustor was equipped with a quartz window to enable optical access. A schematic drawing of the combustor geometry, including the locations at which the CARS data were collected, is shown in Figure 4.22. It illustrates that data collection was extended from 5 to 150 *mm* along the axial direction and from 0 to 30 *mm* in the radial direction. The same radial range was specified for velocity measurements. The maximum error in the LDA measurements was estimated to be $\pm 10\%$.

4.6.1 Boundary Conditions

The inlet mass flow rate was kept constant at 500 SLPM, with an equivalence ratio of 0.8. The combustor was operated at atmospheric pressure and the inlet temperature was 298 *K*. The combustor wall was isothermal, with a constant temperature of 1000 *K*.

In general, the inlet velocity boundary conditions were poorly described. No measurements were available for the velocity profile at the immediate inlet of the combustor. Therefore, the assumed axial velocity distribution at the combustor inlet (marked in Figure 4.21) was obtained by interpolating from the closest plane at which measurements were specified. This plane is 5 *mm* downstream from the combustor inlet (Figure 4.22). Moreover, a sensitivity analysis was performed by slightly altering the interpolated axial velocity distribution until the best match with the measurements was obtained. In all cases, the inlet radial velocity was assumed to be zero. The inlet tangential velocity profile was calculated from both the swirl number and the axial velocity profile, assuming

Figure 4.19: Experimental setup (from Flores et al., 1996).

solid body rotation (Hedman et al., 2002). The swirl number was 0.74 and a turbulence intensity of 40% was used at the inlet.

At the line of symmetry, zero gradients with respect to the radial direction was assumed for the axial and the tangential velocity while the radial velocity component was assumed to be zero. Outflow boundary conditions were specified by zero gradients of the velocity components with respect to the axial direction. Boundary conditions were also specified for the stochastic particles in the Monte Carlo method. Stochastic particles attempting to leave the domain at the wall or line of symmetry are reflected back into the domain (reflection boundary conditions). Convective heat loss was also calculated for each cell adjacent to the wall (wall cells) based on the law of the wall for heat transfer (Launder and Spalding, 1974). This heat flux was subtracted from the particles residing in the near-wall cells.

Figure 4.20: Swirler geometry (adapted from Flores et al., 1996).

Figure 4.21: Premixed injector (adapted from Flores et al., 1996).

Figure 4.22: Sampling locations for CARS measurements (from Flores et al., 1996).

Figure 4.23: The measured iso-contours for mean axial velocity field in the swirl stabilized combustor (adapted from Hedman et al. (2002)).

4.6.2 Results and Comparisons

Calculations were implemented using a Pentium 4, Intel 2800 MHZ processor. A structured grid resolution of 35×27 was used to solve the turbulent flow and 15 particles per cell were used for the Monte Carlo simulation. The steady state solution in terms of the NO concentrations was obtained in 1200 global iterations and a global time step of 0.002 second, with corresponding computational time around 62 minutes.

4.6.2a Velocity

Instantaneous measurements were used to obtain mean velocities. Interpolation of the mean values allowed for the creation of iso-contour plots (Hedman et al., 2002). Recirculation zones can be identified by the examination of the zero axial velocity contours. Recirculation regions obtained from measurements are shown in Figure 4.23. The corresponding predicted recirculation regions are shown in Figure 4.24. Two recirculation zones can be identified: a central recirculation zone and a side recirculation zone. Depending on the swirl number and the inlet velocity, either of the two recirculation zones acts as a flame stabilizer by back-mixing of hot gases into cold fresh gases (containing fuel).

A rough picture of the effect of the heat released by combustion on the flow field can be obtained by comparing the velocity distribution in the case of cold flow conditions (shown

Figure 4.24: The predicted iso-contours for mean axial velocity field in the swirl stabilized combustor.

Figure 4.25: The predicted velocity field and recirculation zones in the case of cold flow.

in Figure 4.25) to the case of hot flow conditions (shown in Figure 4.24). The effect of heat released on the flow field is manifested by the distinctive character of the recirculation zones in the case of cold flow in comparison to the case of combustion. For example, the central recirculation zone forward boundary is located closer to the inlet in the case of combustion. Also, the location of the maximum recirculation zone width for the case of combustion is shifted further downstream than for the case with cold flow conditions. These results match the observations previously made in Chapter 2 (Figure 2.3).

The predictions of the mean axial velocity profiles are compared to the experimental values at four axial locations of 10, 20, 40, and 175 *mm*, as shown in Figure 4.26. The

Figure 4.26: Measurements and predictions, using the improved algorithm of the composition PDF model, of mean axial velocity profiles in the swirl stabilized combustor (experimental data from Hedman et al. (2002)).

predictions compare reasonably well with the measurements of the mean axial velocity. The magnitude and locations of the maximum velocities are well represented almost everywhere. The size and the shape of the velocity jet is represented by the positive part of the velocity profile and it is well captured by the predictions. The negative centerline velocities (back-flow) were under-estimated at the first three axial locations.

The mean radial velocity profile predictions are compared to the measurements at axial positions of 10, 20, 40, 175 *mm*, as shown in Figure 4.27. The radial velocity profiles are well represented at the axial locations of 40 and 175 *mm*. Near the combustor inlet, at axial locations of 10 and 20 *mm*, the magnitude of the positive and negative radial velocities were under-estimated. The flow entrainment is indicated by the negative velocities on the combustor side, far from the centerline. These negative velocities are generally well predicted.

4.6.2b Temperature

The comparisons between the predicted and the measured temperature profiles at four axial locations of 20, 30, 40 and 100 *mm* are shown in Figure 4.28. Two factors may be emphasized in comparing the predicted temperature profiles to the measurements. The first is that the radiation heat transfer has not been accounted for in the present calculations. This led to an over-estimation of the magnitude of the maximum calculated temperature. This is clearly identified in the temperature profile at the axial location of 100 *mm*. The second factor is that the equivalence ratio for both predictions and calculations (0.8) is outside the valid range for the chemical kinetics mechanism (0.4 to 0.75) used in the present calculations. In that sense, these comparisons can be considered to be of a more qualitative rather than quantitative nature. In general, the values of the minimum temperature is reasonably well predicted. The location of the minimum temperature is shifted to the left at the first three axial locations. The predicted radial spread of the

Figure 4.27: Measurements and predictions, using the improved algorithm of the composition PDF model, of mean radial velocity profiles in the swirl stabilized combustor (experimental data from Hedman et al. (2002)).

mean temperature profile was under-estimated almost everywhere. Since the radial spread of the mean velocity components is generally well predicted, the under-estimation of the radial spread of the mean temperature profiles may be attributed to over-estimation of the turbulent mixing rate in the shear layer.

4.6.2c Species Concentrations

The predicted O_2 concentrations profiles at four axial locations are shown in Figure 4.29 as an example of major species predictions. The regions of high O_2 concentrations reveal the existence of unburnt gases and consequently lower temperature. A comparison between the O_2 profiles (Figure 4.29) and the temperature profiles (Figure 4.28) shows a correspondence between the regions of low values of O_2 on one hand and regions of high temperature on the other. Near equilibrium values of O_2 mole fractions (0.03869) are reached close to the wall at the first three axial locations and everywhere at the last axial location where the fuel is burned completely.

The predicted NO concentrations profiles at four axial locations are shown in Figure 4.30 as an example of minor species calculations. The maximum predicted value of NO concentration is almost 4.5 *ppm*. Likely this value is under-estimated as it was the case in the bluff body predictions. The NO concentrations predicted here, as well as in the bluff body case, strongly suggest that NO predictions are the species most influenced by the violation of the valid inlet temperature range at which the global mechanism was derived.

Nevertheless, the predicted NO concentration profiles in Figure 4.30 show an expected and correct physical behaviour. The minimum values of NO concentration corresponds to the minimum values of temperature and increase as the temperature rises. Also, when moving downstream, a slight increment in maximum value of the predicted NO concentrations is observed. In other words, the production of NO is not significantly affected by

Figure 4.28: Measurements and predictions, using the improved algorithm of the composition PDF model, of mean temperature profiles in the swirl stabilized combustor (experimental data from Flores and Hedman (1996)).

Figure 4.29: Predictions, using the improved algorithm of the composition PDF model, of mean O_2 mole fraction profiles in the swirl stabilized combustor.

post-flame process. *NO* formation is mostly a monotonically increasing function of axial location, but it nevertheless, shows a weak dependence on residence time.

4.7 Summary

An improved Lagrangian Monte Carlo composition PDF algorithm was developed in the present chapter. A hybrid method was employed in this algorithm. This hybrid method consisted of the finite volume method for solving the inert flow equations and the Monte Carlo method for solving the composition PDF transport equation. The LMSE mixing model was used for modelling the turbulent mixing process. Chemical kinetics was modelled using a five-step, seven-specie global reaction mechanism. It was solved using the DVODE algorithm; an algorithm for solving a system of stiff ordinary differential equations with variable coefficients. Improvements over the conventional Lagrangian composition PDF models performance and computational efficiency were achieved through the implementation of time splitting, variable stochastic fluid particle mass control, and a second order time accurate (predictor-corrector) scheme used for solving the stochastic differential equations governing the evolution of the particles. The algorithm of the improved model was discussed in detail as opposed to a generic algorithm for the conventional models. The particle independence test showed that a considerable reduction in the number of particles and the total time for convergence was obtained, in contrast to conventional schemes.

The model predictions were evaluated by comparing them to published experimental data of two combustor configurations: bluff body and swirl stabilized combustors, in the case of lean premixed turbulent flames. The velocity field, temperature and major species concentrations were well predicted. Trends and gross features of *CO* concentrations were also reasonably well predicted. Some discrepancies were found in the predictions of *NO*

Figure 4.30: Predictions, using the improved algorithm of the composition PDF model, of mean *NO* mole fraction (*ppm*) profiles in the swirl stabilized combustor.

concentrations. Analysis and computational evidence suggested that these discrepancies were mainly due to violating the valid range of inlet conditions necessary for the application of the chemical kinetics mechanism (inlet temperature range), and to the capability of the chemical kinetics mechanism.

Chapter 5

Numerical Modelling and Evaluation: Generalized Stochastic Reactor Model

5.1 Historical Background

5.1.1 Classical Theory of Chemical Reactors

Historically, the development of turbulent combustion models advanced in two main streams. One stream was adapted by mechanical engineers and the other by chemical engineers. The former relies on simplifying assumptions concerning chemical kinetics specifically, infinitely fast chemistry, while the latter relies on simplifying assumptions concerning the mixing process and is called the chemical reactors theory (Essenhigh, 1971).

It is useful, for the advancement of this discussion, to classify the mixing processes. In practical combustion systems, the mixing process may be classified as macro-mixing

Figure 5.1: Schematic drawing of flow within a modern gas turbine combustor (from Tonouchi et al., 1997).

and micro-mixing processes. According to Tonouchi et al. (1997): “macro-mixing is the gross convective recirculation or back-mixing that brings thermally hot fluid particles into physical proximity to cold particles”. In other words, macro-mixing is an integral scale mixing which is characterized by the general flow motion.

Micro-mixing is mixing at the molecular level. When two fluid particles are brought together by the macro-mixing process, the molecular diffusion of heat and mass between the two particles is defined in terms of the micro-mixing process. Therefore, as stated by Tonouchi et al. (1997): “micro-mixing allows the hot particles to ignite the cold particles through the diffusion of heat and mass”.

Figure 5.1 shows the general flow characteristic in a modern gas turbine combustor. Two regions can be identified: the back-mixing region or primary zone, and plug flow region or dilution zone. The function of the primary zone is to anchor the flame and to provide combustion of the fuel, while the function of the dilution zone is to achieve complete combustion and to control the mean temperature and temperature profile acceptable to the turbine inlet. The division of the gas turbine combustor into regions of distinct mixing

Figure 5.2: Reactors network modelling of a gas turbine combustor.

character is the basic idea underlying the representation of the combustor by a network of chemical reactors. Figure 5.2 shows a typical reactors network corresponding to the combustor shown in Figure 5.1. The combustor is represented by two reactors in series: a perfect or well stirred reactor (WSR), followed by a plug flow reactor (PFR). The well stirred reactor represents a control volume with an inlet and outlet mass flow rate, as shown in Figure 5.3. The reactants are assumed to be perfectly mixed at both macro- and micro-mixing levels immediately after they are introduced to the reactor volume. Subsequently, the combustion process in a well stirred reactor is assumed to be controlled by chemical kinetics. The advancement of chemical kinetics depends on the residence time for the gases in the reactor. The average residence time inside the reactor is defined as,

$$\tau_r = \frac{\rho \mathcal{V}}{\dot{m}} \quad (5.1)$$

where $\mathcal{V}$ is the reactor volume and $\dot{m}$ is the mass flow rate. The residence time distribution of the gases inside the reactor can be used to quantify the macro-mixing process. Let $f(t)$ be the residence time distribution function such that $f(t)dt$ represents the fraction of mass which exits the reactor during a residence time interval of t to $t + dt$. In a well stirred reactor, the residence time distribution is found to be exponentially decaying (Levenspiel, 1972),

Figure 5.3: Schematic of well stirred reactor (adapted from Turns (2000)).

$$f(t)_{WSR} = \frac{1}{t_r} \exp\left(-\frac{t}{t_r}\right) \quad (5.2)$$

Consequently, deviation from perfect macro-mixing (back-mixing) can be roughly quantified by the deviation of the residence time distribution function of a real reactor from the distribution assumed by Equation 5.2.

The plug flow reactor shown in Figure 5.4 represents another idealization extreme. No mixing is allowed in the axial direction (no back-mixing), while uniform properties are assumed to be in the direction perpendicular to the flow. In other words, it represents parallel one-dimensional flow. In plug flow reactors, the residence time distribution function is represented by a Dirac delta function,

$$f(t)_{PFR} = \delta(t - \tau_r) \quad (5.3)$$

Figures 5.5 and 5.6 show another example of representing a double annular combustor by a network of reactors.

Figure 5.4: Schematic of plug flow reactor (adapted from Turns (2000)).

Figure 5.5: Double annular gas turbine combustor (from Correa and Overton, 1988).

Figure 5.6: Reactors layout of the double annular combustor.

5.1.2 The Theory of Stochastic Reactors

Both the well stirred reactors and the plug flow reactors represent idealizations of the mixing process found in real combustion systems. In principle, it is possible to account for imperfect back-mixing by introducing a residence distribution which deviates from the well stirred reactor residence time distribution given by Equation 5.2. Also, in real combustion systems, a considerable deviation from infinite micro-mixing is found. An important step towards the relaxation of the assumption of infinite micro-mixing was the introduction of the stochastic reactors or the partially stirred reactors model. This model was first introduced by Curl (1963) to describe the concentration probability distribution function of liquid droplets mixing. Curl derived a governing equation for the concentration probability density function,

$$\begin{aligned}
& \frac{\partial}{\partial t} P(\Psi; t) + \frac{1}{\tau_r} [P(\Psi; t) - P_o(\Psi; t)] + \frac{\partial}{\partial \Psi} [\dot{W} P(\Psi; t)] \\
& = 2\omega_{\Phi} \int \int P(\Psi_p; t) P(\Psi_q; t) \delta(\Psi - \frac{1}{2}(\Psi_p + \Psi_q)) d\Psi_p d\Psi_q - 2\omega_{\Phi} P(\Psi; t) \quad (5.4)
\end{aligned}$$

where ω_{Φ} is the mixing frequency defined by Equation 3.88 and $P_o(\Psi; t)$ is the probability density function for the feed to the reactor. Spielman and Levenspiel (1965) first applied the Monte Carlo method to the solution of Equation 5.4. In a Monte Carlo simulation, the mass flow rate of fresh reactants is assumed constant and is represented by a discrete number flow rate of equal mass particles given by,

$$\dot{N}_r = \frac{\dot{m} N_r}{\rho \forall} \quad (5.5)$$

where N_r is the number of particles, $\forall$ is the reactor volume, $\dot{m}$ is the mass flow rate into the reactor and ρ is the average density inside the reactor. During their transit through the reactor volume, the particles undergo continuous adiabatic chemical reaction and mix according to the Curl model. Particle pairs are selected to mix at a specified time interval at a rate determined by the turbulence frequency. The first particle is selected at random from the particles population inside the reactor, and the second particle is also randomly selected from the particles population inside the reactor. It is important to note that the particles are selected without reference to their position. That is, any two particles inside the reactor are assumed to be close to each other. Implicitly, this implies an infinite macro-mixing. This is obvious by noting the absence of the spatial argument in Equation 5.4. In conclusion, the stochastic reactor model accounts for finite macro-mixing. However, it assumes infinite macro or back-mixing.

Many workers have implemented the stochastic reactor model for solving combustion

systems. This model is particularly suitable for studying pollutant formation in combustion devices (Flagan and Appleton, 1974). Butler and Pratt (1986) used the model for studying Methane combustion in a jet stirred reactor. Radhakrishnan and Pratt (1986) used the stochastic reactor model to study turbulent flames stability limits. For example, in studying the ignition limits, the particles inside the reactor are assumed to be in an unburned condition. The temperature of the inlet particles is raised gradually until the reaction spreads inside the reactor. This defines the temperature for ignition at a certain equivalence ratio. Opposite procedures are employed for the analysis of blow-out limits.

Correa (1995) used the stochastic reactor model for a detailed comparison of the Curl and LMSE mixing models. Tonouchi and Pratt (1995) modified the stochastic reactor model to account for finite macro-mixing. The idea is to estimate the residence time distribution; then, mixing is allowed only for particle pairs which spent a similar amount of time inside the reactor. Later, this model was used by Tonouchi et al. (1997) for modelling different configurations of gas turbine combustors operating under premixed and partially premixed conditions.

5.2 Generalized Stochastic Reactor Model

5.2.1 Model Development

The classical stochastic reactors are attractive models from the point of view of simplicity and computational cost. Simplicity arises from the assumption of infinite macro-mixing, which removes the need for stochastic particle tracking. Economy of computation can be seen by comparing the number of particles needed for modelling a combustor in cases of the stochastic reactor model and the composition PDF model (assuming both models produce the same statistical error). Let us assume that the reactor volume is composed of N_c cells. The number of particles per cell is N_{pc} . Then the statistical error in the stochastic

reactor model (Equation 4.57) can be estimated as the statistical error encountered in the composition PDF model multiplied by factor $\frac{1}{\sqrt{N_c}} \ll 1$, assuming that both models (stochastic reactor and composition PDF) use the same number of particles over the whole reactor volume. Vice versa, if both models are assumed to encounter the same statistical error, then a smaller number of particles will be used for the stochastic reactor model.

On the other hand, the stochastic reactor model suffers from some non-physical behaviour. That is, the flow inside the reactor is assumed to be infinitely macro-mixed. Limiting our discussion to the Curl mixing model without losing generality, this is manifested by:

1. The stochastic particle pairs are selected for mixing with equal probability and without reference to their spatial location. For example, the model does not differentiate between two configurations with the same average mixing frequency, (ω_Φ) even if they encounter different gross flow features (back-mixing).
2. The stochastic particles are chosen to exit the reactor with equal probability, i.e., without age distribution bias. For example, a particle which has just entered the reactor may be selected to exit immediately.

Here, we propose a new model which may be considered a compromise between the composition PDF model and the stochastic reactor model. This model will be called the generalized stochastic reactor model (GSR). As the name implies, this model can be considered as a generalization of the classical stochastic reactor model in the sense that a Lagrangian particle tracking is applied to the stochastic particles. This allows for a more realistic mixing process; a particle randomly selected will be allowed to mix only with one of the particles in its neighborhood.

The basic output of this model is a PDF distribution which is averaged over the reactor volume. In that sense, the generalized stochastic reactor model can be considered to be a

degenerate from the composition PDF model. In other words, employing volume averaging procedures, the GSR model can be derived from the composition PDF model.

The fact that the GSR model deals with volume-averaged statistics, rather than spatially distributed ones, should not cause an under-estimation of its usefulness in practical applications. In many cases of practical interest, one is interested in the global performance parameters of the combustor rather than the spatially distributed ones. Consider pollutant emissions as an example. It is sufficient, by all practical considerations, to know the rate of emissions production at the outlet of the combustor. Similar considerations apply to the combustor stability, efficiency, the average temperature at the outlet and the rate of power generation. This does not apply to the pattern factor (although, it will be shown later that spatial details can be extracted from the GSR model enabling a reasonable estimation of the quality of the pattern factor).

Next, the basic elements of the GSR model are considered. The starting point is the diagnosis of the combustor into regions of homogeneous turbulence fluctuations. This is done using a turbulence model, for example, the $(k - \varepsilon)$ model. The turbulence kinetic energy (k) and the turbulence energy rate of dissipation (ε) are used to calculate the turbulence fluctuation dissipation time scale, $(\frac{k}{\varepsilon})$, over the entire flow domain. The combustor is then divided into regions of almost constant fluctuations dissipation time scale (or turbulence frequency), as shown in Figure 5.7. Each of these regions defines a generalized stochastic reactor boundary.

It may be noted that the generalized stochastic reactors are characterized solely by turbulence frequency. This implies that the generalized stochastic reactor is equivalently characterized by homogeneous scalar fluctuations dissipation time scale (mixing frequency), as given by Equation 3.84. Unlike the classical stochastic reactors, no requirements are imposed on the uniformity of the mean flow.

In order to derive a governing equation for the volume-averaged PDF over the gener-

Figure 5.7: Descritization of a combustor into GSR volumes.

alized stochastic reactor volume, we start with the transport equation for the composition PDF (Equation 3.35). For convenience, it will be written for the case of a single scalar,

$$\frac{\partial P(\Psi; \underline{X}, t)}{\partial t} + \frac{\partial}{\partial \Psi} (P(\Psi; \underline{X}, t) \dot{W}) = -\frac{\partial}{\partial x_j} \langle U_j \wp \rangle + D \frac{\partial^2 P(\Psi; \underline{X}, t)}{\partial x_j \partial x_j} - D \frac{\partial^2}{\partial \Psi^2} \left\langle \left(\frac{\partial \Phi}{\partial x_j} \right)^2 \wp \right\rangle \quad (5.6)$$

Neglecting the molecular diffusion term and employing volume averaging over the reactor volume $\forall$,

$$\begin{aligned} \frac{1}{\forall} \int_{\forall} \frac{\partial P(\Psi; \underline{X}, t)}{\partial t} d\forall + \frac{1}{\forall} \int_{\forall} \frac{\partial}{\partial \Psi} (P(\Psi; \underline{X}, t) \dot{W}) d\forall \\ = -\frac{1}{\forall} \int_{\forall} \frac{\partial}{\partial x_j} \langle U_j \wp \rangle d\forall - \frac{1}{\forall} \int_{\forall} D \frac{\partial^2}{\partial \Psi^2} \left\langle \left(\frac{\partial \Phi}{\partial x_j} \right)^2 \wp \right\rangle d\forall \end{aligned} \quad (5.7)$$

Substituting the unclosed mixing term by the Curl approximation,

$$\frac{1}{\forall} \int_{\forall} \frac{\partial P(\Psi; \underline{X}, t)}{\partial t} d\forall + \frac{1}{\forall} \int_{\forall} \frac{\partial}{\partial \Psi} (P(\Psi; \underline{X}, t) \dot{W}) d\forall$$

$$\begin{aligned}
&= -\frac{1}{\mathcal{V}} \int \frac{\partial}{\partial x_j} \langle U_j \wp \rangle d\mathcal{V} + \frac{2}{\mathcal{V}} \int \omega_{\Phi} \int \int P(\Psi_p; \underline{X}, t) P(\Psi_q; \underline{X}, t) \delta(\Psi - \frac{1}{2}(\Psi_p + \Psi_q)) d\Psi_p d\Psi_q d\mathcal{V} \\
&\quad - \frac{2}{\mathcal{V}} \int \omega_{\Phi} P(\Psi; \underline{X}, t) d\mathcal{V}
\end{aligned} \tag{5.8}$$

Noting that,

$$P(\Psi; t) = \frac{1}{\mathcal{V}} \int P(\Psi; \underline{X}, t) d\mathcal{V} \tag{5.9}$$

Assuming ω_{Φ} is homogeneous over the reactor volume, then,

$$\begin{aligned}
&\frac{\partial P(\Psi; t)}{\partial t} + \frac{\partial}{\partial \Psi} (P(\Psi; t) \dot{W}) \\
&= -\frac{1}{\mathcal{V}} \int \frac{\partial}{\partial x_j} \langle U_j \wp \rangle d\mathcal{V} + \frac{2\omega_{\Phi}}{\mathcal{V}} \int \int \int P(\Psi_p; \underline{X}, t) P(\Psi_q; \underline{X}, t) \delta(\Psi - \frac{1}{2}(\Psi_p + \Psi_q)) d\Psi_p d\Psi_q d\mathcal{V} \\
&\quad - 2\omega_{\Phi} P(\Psi; t)
\end{aligned} \tag{5.10}$$

It may be noted that the extraction of the homogeneous mixing frequency outside the volume integral has a non-trivial implication. The mixing frequency is to be interpreted such that it is applied to the whole reactor volume rather than being localized in space. It may be also noted that the spatial argument has disappeared from all the terms in Equation 5.10, except for the turbulent diffusion and collision operator terms. This is also a non-trivial observation which clarifies an essential feature of the GSR model. For example, the existence of a spatial argument in the collision operator indicates that particle pairs are selected for mixing based on their spatial locations. A particle interacts with its

closest neighbour in the physical space. Information on the location of the particles is provided and updated in each time step by Lagrangian particle tracking. The latter is calculated from the mean motion and turbulent diffusion terms.

Despite the fact that Equation 5.10 represents a volume-averaged composition PDF transport equation, it entails (conceptually) two types of volume averaging. That is, the volume averaging of the first and the second term on the left-hand side and the last term on the right-hand side differs in nature from the volume averaging of the turbulent diffusion and collision operator terms. In the former terms, the volume averaging is of intrinsic or direct nature. This means that one calculates volume-averaged quantities directly without going into more fine detail. In the latter terms, the volume averaging is indirect. This is indicated by the existence of the integral operator and the spatial argument. It means that one has to calculate fine details first (spatially-distributed quantities), which are then used for calculating the averages.

5.2.2 An Illustrative Example

Consider the planar flow over a backward-facing step, for which the schematic is shown in Figure 5.8. This flow was investigated experimentally by Pronchich and Kline (1986). A recirculation zone occurs just behind this step. The distance of the reattachment point from the step is X_R . Figure 5.9 shows the stream-wise velocity variance ($\langle u'^2 \rangle$) profiles normalized by U_{ref}^2 . Experimental data are unavailable for the kinetic energy or turbulence dissipation. However, assuming isotropic turbulence, $\langle u'^2 \rangle$ can be used as an estimation of the turbulence kinetic energy.

In considering Figure 5.9, two levels of turbulent kinetic energy can be distinguished: a higher kinetic energy level in the recirculation zone and a lower kinetic energy level in the jet flow zone. It may also be noted that the turbulent kinetic energy decays as one moves upstream. The turbulence dissipation time scale can be estimated as,

Figure 5.8: Schematic of the backward-facing step (from Pronchik and Kline, 1986).

Figure 5.9: Profiles of $\frac{\langle u'^2 \rangle}{U_{ref}^2}$ (from Pronchik and Kline, 1986).

$$\tau = \frac{k}{\epsilon} \quad (5.11)$$

where,

$$k \approx \frac{3}{2} \langle u'^2 \rangle \quad (5.12)$$

and,

$$\epsilon \approx \frac{\langle u'^2 \rangle^{\frac{3}{2}}}{l} \quad (5.13)$$

where l is the characteristic length scale. Using the last three equations, the turbulence dissipation time scale can be estimated as,

$$\tau \approx c \frac{l}{\sqrt{\langle u'^2 \rangle}} \quad (5.14)$$

where c is a proportionality constant. In terms of turbulent kinetic energy, the dissipation time scale can be estimated as,

$$\tau \approx c_k \frac{l}{\sqrt{k}} \quad (5.15)$$

where c_k is another constant. l can be taken as H for the recirculation region and as W_1 for the jet flow region (Figure 5.8). The turbulence frequency ($\frac{1}{\tau}$) can be considered as a measure of the turbulent mixing activity. The higher the turbulence frequency, the higher the mixing rate. From Equation 5.15, two levels of turbulence mixing can be distinguished in the back-step flow configuration: a higher turbulent mixing level in the recirculation region and a lower turbulent mixing level in the jet flow region.

A possible layout of the GSR based on the mixing frequency distribution is shown in Figure 5.10. In fact, this layout shows clearly the weak point of the GSR model. When comparing Figures 5.8 and 5.10, it can be seen that the mixing frequency is not exactly

Figure 5.10: Reactors layout of the backward-facing step configuration .

uniform, at least in the reactors representing the recirculating flow region. The greater the non-uniformity of the mixing frequency distribution, the further the GSR model departs from the real case. In principle, it is possible to obtain a more realistic representation by increasing the number of reactors in the transverse direction. However, this would lead to more computational time as the number of particles increases. A remedy for this weakness will be considered in Subsection 5.2.4.

5.2.3 Number of Particles

Assuming uniform distribution of mixing frequency over the reactor volume, it will be shown that the GSR model possesses two main advantages over the conventional PDF models. The first can be seen by considering the statistical error, while the second (which is specific to the Curl mixing model) can be seen from the consideration of what we will call “cut-off number of particles”.

Consider the statistical error of the field means, averaged over the reactor volume. The issue of particle number for the GSR model is evaluated by comparing it to the conventional composition PDF models. Assume a reactor with volume V_r , over which the mixing frequency $(\omega_\Phi)_r$ is uniform. The reactor is composed of N_c equal volume cells, each with a volume V_i , as shown in Figure 5.11. The mixing frequency in each cell is uniform

Figure 5.11: Distribution of turbulence mixing frequency ω_Φ over the reactor volume.

and equal to $(\omega_\Phi)_i$. The average number of particles per cell is N_{pav} . Then,

$$V_r = N_c V_i \quad (5.16)$$

and,

$$(\omega_\Phi)_r = (\omega_\Phi)_i \quad (5.17)$$

Now, the volume-averaged mean field statistical error may be estimated for both the composition PDF and GSR models for the sake of comparison. In the PDF composition model, one calculates the mean of the random variable and any other statistical quantity, locally in space. Next, one uses these local averages (say average over a cell) in order to calculate the volume-averaged statistics. Consequently, the statistical error is estimated locally, i.e., based on the number of particles per cell, as,

$$(Error_{st})_{PDF} \propto \frac{1}{\sqrt{N_{pav}}} \quad (5.18)$$

In the GSR model, the volume average of the mean field values is considered directly

over the reactor volume. Therefore, the statistical error is estimated by the total number of particles inside the reactor volume ($N_c N_{pav}$),

$$(Error_{st})_{r-GSR} \propto \frac{1}{\sqrt{N_c N_{pav}}} \quad (5.19)$$

Therefore,

$$\frac{(Error_{st})_{r-GSR}}{(Error_{st})_{PDF}} = \frac{1}{\sqrt{N_c}} \ll 1 \quad (5.20)$$

It is emphasized that the comparison of statistical error considered here is concerned with the mean field values averaged over the reactor volume. Also, it was assumed that the mixing frequency is uniform over the reactor volume.

Another important advantage of the GSR model, from the point of view of the number of particles, arises with the use of the Curl mixing model. Again, this issue is considered in terms of the comparison between the composition PDF and the GSR models. Consider first, the composition PDF model; the number of mixing events in cell i during time period Δt is estimated as,

$$N_{mix} = (\omega_\Phi)_i N_{pc} \Delta t \quad (5.21)$$

We define the number of particles required for the occurrence of at least one mixing event at a certain turbulent mixing frequency $(\omega_\Phi)_i$, and a time period Δt , as the cut-off number of particles (N_{pcof}), where,

$$2(\omega_\Phi)_i N_{pcof} \Delta t = 1 \quad (5.22)$$

Subsequently,

$$N_{pcof} = \frac{0.5}{(\omega_{\Phi})_i \Delta t} \quad (5.23)$$

In fact, this cut-off number of particles can be the actual practical limit on the minimum number of particles used in mixing pairs models. In regions of intensive turbulence, such as the primary zone, the mixing frequency is high while N_{pcof} is relatively low. In low intensity turbulence regions, such as the dilution zone, the mixing frequency is low and N_{pcof} is relatively high. If the number of particles per cell (N_{pc}) is lower than N_{pcof} , no mixing events will occur in regions of low turbulence intensity.

When the GSR model is applied to a reactor r , which is composed of N_c cells, then,

$$(N_{pcof})_r = \frac{0.5}{N_c (\omega_{\Phi})_r \Delta t} \quad (5.24)$$

where $(N_{pcof})_r$ is the cut-off number of particles in the reactor. In comparing $(N_{pcof})_r$ to N_{pcof} , it can be seen that the former is smaller than the latter by a factor of $\frac{1}{N_c}$. For a reactor composed of 5 cells, if N_{pcof} is 100, then $(N_{pcof})_r$ is 20.

5.2.4 Improved Generalized Stochastic Reactor Algorithm (Turbulent Mixing Frequency Bias)

In the present subsection, a further improvement to the GSR model is considered. Referring to Equation 5.10, it can be shown that the composition PDF and the GSR models are equivalent to one another if the mixing frequency ω_{Φ} is uniform within the reactor volume. In reality that is not the case. Nonetheless, this equivalence can be approached by increasing the number of reactors. However, this may lead to a corresponding increment in computational time. Moreover, the strict requirements of uniform mixing rate over the reactor volume cause a difficulty in selecting the layout of the reactors.

The improvement proposed here aims to increase the accuracy of the GSR even with

a rough selection of reactors volumes. Consider a reactor volume where the turbulence frequency is non-uniformly distributed, as shown in Figure 5.11. The reactor volume is divided into N_c cells such that the turbulence frequency levels $(\omega_\Phi)_1, (\omega_\Phi)_2, \dots, (\omega_\Phi)_{N_c}$ are uniform over each cell.

As the rate of mixing is proportional to the turbulence frequency, particles hosted by cells with a higher turbulence frequency level would encounter more mixing events than particles hosted by cells of a lower turbulence frequency level. This is equivalent to saying that the particles hosted by cells of a higher turbulence frequency level have a higher probability of being selected for mixing than particles hosted by cells of lower mixing frequency level.

To account for the fact that the mixing frequency is not accurately uniform over the reactor volume, a modified Curl mixing model in which the selection of particle pairs for mixing is biased by the turbulence frequency distribution is proposed. The mixing mechanism is modified such that the particles in cells with a higher turbulence frequency level have a higher probability of being selected for mixing. With this modification, the GSR model is less sensitive to the arbitrariness involved in selecting the volumes of the reactors. Of equal importance, is that the model allows for a correct iteration between the finite volume method and the Monte Carlo method in the hybrid solution algorithm.

A simple way of implementing this modification is to introduce a weight factor for each particle which is proportional to the turbulence frequency (mixing rate) at the location of the particle. This weight amounts to modifying the probability of choosing a particle for mixing as previously explained. In terms of the Monte Carlo simulation, the implementation of this algorithm is similar to the algorithm for the mixing of particles of unequal mass, as explained in the following subsection.

5.2.5 Curl Mixing Model for Particles of Unequal Mass

The original coalescence dispersion models are applied to particles of equal mass. Two particles p and q are selected from the ensemble with a certain probability p_{mix} , in a time step Δt , such that the number of particle pairs chosen for mixing is,

$$N_{mix} = (\omega_{\Phi})_r N_{pr} \Delta t \quad (5.25)$$

where N_{pr} is the total number of particles in the reactor. This equation can be derived (*cf.* Chapter 4) by requiring that the proposed mixing model produce the correct decay of scalar variance. After mixing, each particle has a new scalar value equal to the mean of the two particle scalar before mixing.

Now, we consider the more general case where two particles of an unequal mass are chosen as a mixing pair. Intuitively, the scalar values of the particles with a greater mass should dominate the mixing process. If the mass of a particle “(i)” is denoted by m_i , then in order to match this criterion, scalar values after mixing are calculated as,

$$\Phi_p(t + \Delta t) = \Phi_q(t + \Delta t) = \frac{1}{m_p + m_q} (m_p \Phi_p(t) + m_q \Phi_q(t)) \quad (5.26)$$

However, this modification alone is not sufficient for deriving the correct exponential decay of the scalar variance (Nooren et al., 1997). This is explained by the fact that we modified the mechanism by which the particles exchange quantities, yet the probability of selecting certain particles for mixing is still the same, i.e., all the particles in the ensemble may be chosen with equal probability aside from the difference in their masses. Clearly, this should not be the case; particles with a greater mass should have a higher probability of being selected. In other words, the probability of selecting a particle should be biased by its mass. It was shown by Nooren et al. (1997) that the probability of choosing a particle pairs may be estimated as,

$$P_{mix} = \frac{N_{pr}}{\sum_{i=1}^{N_{pr}} m_i} \frac{1}{2} (m_p + m_q) (\omega_\Phi)_r \Delta t \quad (5.27)$$

in order to produce the correct decay of scalar variance.

Here, we propose a simple algorithm for the implementation of the unequal particle mass-Curl mixing model. For the group of particles inside the reactor volume, an array of particle normalized mass is constructed. These particles mass are normalized such that their total sum is unity. Next, a transformation rule is applied to all particles in the reactor. For example, the first particle normalized mass, $(m_1)_n$, where (n) denotes normalized mass, ranges from zero to $(m_1)_n$. The second particle normalized mass ranges from $(m_1)_n$ to $(m_1)_n + (m_2)_n$. The third particle normalized mass ranges from $(m_1)_n + (m_2)_n$ to $(m_1)_n + (m_2)_n + (m_3)_n$ and so on. A random number is then generated between 0 and 1. This random number corresponds to a certain particle, as shown in Figure 5.12. The larger the particle mass, the higher the probability of being selected. After selecting particle pairs for mixing, their scalar values evolve according to Equation 5.26.

Let us explain this algorithm with a simple example. Assume 3 particles in a reactor with mass m_1 , m_2 , and m_3 , respectively. Assume the particle mass are such that $m_1 = 3m$, $m_2 = 5m$, and $m_3 = 2m$. According to the former suggestion, the particles mass are first normalized such that their sum is equal to unity. Applying this rule to the three particles, then, $(m_1)_n = \frac{3m}{10m} = 0.3$, $(m_2)_n = 0.5$, and $(m_3)_n = 0.2$. A transformation is applied such that the mass of the first particle ranges from 0 to 0.3, the second from 0.3 to 0.8 and the third from 0.8 to 1. A random number is generated between 0 and 1; say 0.6. This means that the second particle has been chosen for mixing.

The reason for considering this algorithm in detail is that it can be used as a basis for different sorts of bias in selecting the particle pairs for mixing (for example, age bias or mixing frequency bias). It may be noted that the present algorithm corresponds to

Figure 5.12: Transformation of particle mass.

uniform probability distribution and appropriate changes should be granted for other forms of probability distributions.

5.2.6 Notes on the Solution Algorithm

Many of the solution procedures for the GSR model are similar to the procedures considered for the Lagrangian composition PDF model in Chapter 4 and, therefore, will not be repeated. Here, we consider instead the distinctive features of the GSR model in the solution algorithm:

- Based on the cold flow solution, the combustor is discretized into volumes. Each volume represents a reactor. A reactor comprises a group of cells. The choice of reactor volume is based on the criterion of the uniformity of turbulence frequency.
- The mixing process is applied to each reactor in a global time step as follows:

1. A stochastic particle is selected at random inside the reactor. This random selection is biased by the particle mass and the turbulence frequency distribution inside the reactor.
2. The cell (labelled i, j, k) hosting the selected particle is defined using the search locate algorithm.
3. A second particle is selected for mixing with the particle selected in Step 1. This particle must be selected from the cell hosting the first particle (labelled i, j, k).
4. The two particles are allowed to mix according to Equation 5.26.
5. These procedures continue in each reactor such that the number of particle pairs selected for mixing are, $N_{mix} = (\omega_\Phi)_r N_{pr} \Delta t$ where N_{pr} is the number of particles in the reactor and $(\omega_\Phi)_r$ is the mixing frequency averaged over the reactor volume,

$$(\omega_\Phi)_r = \frac{1}{V_r} \sum_{i=1}^{N_c} (\omega_\phi)_i V_i \quad (5.28)$$

where N_c is the number of cells in the reactor, V_r is the reactor volume, V_i is the cell (i) volume and $(\omega_\phi)_i$ is the mixing frequency in cell (i).

- The solution is terminated when the steady state solution is reached. Steady state solution is considered in terms of the average concentrations over the reactor volume.

5.3 Model Evaluation: Bluff Body Stabilized Combustor

The GSR model is evaluated first by comparison against experimental data in a bluff body stabilized combustor obtained by Nandula et al. (1996). The combustor geometry

Figure 5.13: Reactors layout of the bluff body stabilized combustor.

and experiment conditions are the same as previously described in Chapter 4. The chemical kinetics mechanism is also the same as the one discussed in Chapter 4. A structured grid resolution of 35×27 was used for solving the turbulent flow and 25 particles per cell were used for the Monte Carlo simulation. The reactors layout of the combustor is shown in Figure 5.13, where the transverse direction is covered by two reactors: one for the jet flow region characterized by low mixing activities and the other for the recirculating flow region characterized by a high level of mixing activities. The width of each reactor is chosen to be the width of the associated cells.

5.3.1 Particle Number Independence

Simulations were performed using particle number densities of 15, 25, and 50 particles per cell, respectively. Figure 5.14 shows the predictions of the temperature profiles in the radial direction using the three different particle number densities at four different axial locations, $\frac{x}{d} = 0.1, 0.3, 0.6$, and 1.0 , where d is the bluff body diameter. Except for a slight discrepancy in the 15 particles per cell predictions of the temperature profile in the recirculating flow region at $\frac{x}{d} = 0.1$, the predictions from the 15, 25, and 50 particles per cell are nearly matched everywhere.

Compared with the particles independence test for the Lagrangian PDF model (Figure 4.8), it is found that the GSR model is more sensitive to the change in the number of

Figure 5.14: Particle number independence test of the GSR model (experimental data from Nandula et al. (1996)).

particles. This may be attributed to the nature of the mixing mechanisms used in each of the two models (GSR and Lagrangian PDF). The Curl mixing model, which is a stochastic model, is used with the GSR calculations, while the LMSE mixing model, which is a deterministic model, is used in the Lagrangian PDF calculations. The stochastic models are more sensitive to the number of particles than are the deterministic models. This is explained by the fact that in the LMSE model, mixing is obtained by enforcing the instantaneous particle scalar value to decay towards the mean. This mean is actually a field parameter (calculated with reference to the field rather than the particles). This reference to the field values implies less dependence on the number of particles.

5.3.2 Results and Comparisons

Calculations were implemented using a Pentium 4, Intel 2800 MHZ processor. The steady state solution in terms of the *NO* concentrations was obtained in 4000 global iterations with corresponding computational time around 125 minutes.

5.3.2a Temperature

The predicted radial profiles of the mean axial temperature are compared to the measured temperature field at four different axial locations, as shown in Figure 5.15. In general, the predicted temperature profiles compare well with the measured temperature. The location of the cold reactants and hot products within the combustion chamber is indicated by the low and high temperature levels, respectively. The location of the shear layer is indicated by the steep temperature gradient.

Further conclusions can be made by comparing the predicted temperature profiles with the results obtained from the Lagrangian composition PDF model (Figure 4.11). The quality of the predictions is almost the same in the two models. Specifically, the two models predict almost the same results near the line of symmetry where the flow is

Figure 5.15: Measurements and predictions, using the GSR model, of the mean temperature profiles in the bluff body stabilized combustor (experimental data from Nandula et al. (1996)).

the back-flow characterized by a large average residence time. This large value of the residence time implies chemical equilibrium conditions. In other words, the development of the chemical reaction and consequently, the heat released is independent of the mixing mechanism and the turbulence level. A slight discrepancy in the predictions of the two models may be noticed in the shear layer region. Since the two algorithms employ the same turbulence model, this discrepancy may be attributed to the use of different mixing mechanisms (LMSE and Curl mixing model). However, both algorithms agree in under-estimating the predicted temperature in the shear layer region. This common feature points to a common source and supports what has been suggested in Chapter 4; that the excessive mixing due to over-estimation of turbulence production is likely the cause of this under-estimation in the shear layer region.

5.3.2b Major Species

The comparison of the predicted mean CH_4 mole fraction with the measured values is shown in Figure 5.16. It is shown that the predicted CH_4 concentrations are in good agreement with the measured data. Some gross features of the predictions of CH_4 mole fraction profiles may be observed in Figure 5.16. The fuel is totally consumed in the recirculation zone near the line of symmetry. This is an expected result as the flow in this region is characterized by a large value of residence time which allows for the consumption of fuel in lean mixture conditions. The profile of CH_4 is well predicted in the shear layer region, specifically at $\frac{x}{d} = 0.6$ and 1.0. Moreover, the gradient of the shear layer is less steep as one moves downstream, which is also confirmed by measurements.

The comparison of the predicted H_2O mole fraction with the measured values is shown in Figure 5.17. The predicted H_2O mole fractions are in very good agreement with the measurements as was the case in the Lagrangian PDF model. In fact, this agreement between the two models (GSR and Lagrangian PDF) in achieving very good results for

Figure 5.16: Measurements and predictions, using the GSR model, of mean CH_4 mole fraction profiles in the bluff body stabilized combustor (experimental data from Nandula et al. (1996)).

H_2O concentrations profiles, despite using two different mixing mechanisms, confirms the previous suggestion that the time scale of H_2O formation reaction is small compared to the mixing time scale. This difference in time scales implies that the H_2O rate of formation is independent from the mixing process.

The predicted mean CO_2 mole fraction profiles together with the measurements are shown in Figure 5.18. The radial profiles are in good agreement with the measured data. The CO_2 mole fraction level is well predicted in the recirculated flow region, close to the line of symmetry where chemical equilibrium is developed. The shear layer region boundary is also well predicted. However, the gradients in the predicted shear layer are less steep than the measured ones, except at $\frac{x}{d} = 1.0$.

5.3.2c Minor Species

The predictions of the minor species, average CO and NO mole fractions are compared against measurements in four different positions, as shown in Figures 5.19 and 5.20. In general, the gross features of the CO mole fraction distribution are well predicted. The trends and directions of increment and decrement are well captured. The positions of peak values are in good agreement with the measurements. However, the value of the peak is under-estimated at the first two planes: $\frac{x}{d} = 0.1$ and 0.3 . Moving downstream, predictions approach quantitatively the measured data.

As was the case in the Monte Carlo Lagrangian model (Chapter 4), NO concentrations are greatly under-estimated compared to the measurements. However, this result is not totally unexpected. The two different models with two different mixing mechanisms, both, under-estimate NO concentrations. This strongly suggests that the causes for this under-estimation are independent from the model. Rather, it confirms the conclusion previously drawn which suggests that the violation of the valid range of inlet temperature and the predicting capability of the kinetics mechanism are the main reasons for the discrepancy.

Figure 5.17: Measurements and predictions, using the GSR model, of mean H_2O mole fraction profiles in the bluff body stabilized combustor (experimental data from Nandula et al. (1996)).

Figure 5.18: Measurements and predictions, using the GSR model, of mean CO_2 mole fraction profiles in the bluff body stabilized combustor (experimental data from Nandula et al. (1996)).

Figure 5.19: Measurements and predictions, using the GSR model, of mean CO mole fraction (ppm) profiles in the bluff body stabilized combustor (experimental data from Nandula et al. (1996)).

Figure 5.20: Measurements and predictions, using the GSR model, of mean *NO* mole fraction (*ppm*) profiles in the bluff body stabilized combustor (experimental data from Nandula et al. (1996)).

5.4 Model Evaluation: Swirl Stabilized Combustor

Here, the GSR model is evaluated against measurements in a swirl stabilized combustor operating under lean premixed conditions. Velocity, temperature, and species concentrations measurements in an axi-symmetric combustor were reported by Flores and Hedman (1996) and Hedman et al. (2002). The combustor geometry and experiment conditions are the same as previously described in Chapter 4. The chemical kinetics mechanism is also the same as in Chapter 4. A structured grid resolution of 35×27 was used for solving the turbulent flow and 25 particles per cell were used for the Monte Carlo simulation.

5.4.1 Results and Comparisons

Calculations were implemented using a Pentium 4, Intel 2800 MHZ. The steady state solution in terms of the average *NO* concentrations were obtained in 6000 global iterations, with corresponding computational time around 205 minutes.

5.4.1a Temperature

The comparisons of the predicted and the measured temperature profiles at four different axial locations of 20, 30, 40, and 100 *mm* are shown in Figure 5.21. The mean temperature profiles are in good agreement with the measurements at axial locations of 20 and 30 *mm*. At an axial location of 40 *mm*, the minimum predicted temperature is over-estimated in comparison to the measured data. Far from the combustor inlet, at axial location of 100 *mm*, the predicted mean temperature profile is over-estimated in comparison to the measurements. This over-estimation is attributed to neglecting the heat transferred by radiation in the present calculations.

It is instructive to compare the predictions of the mean temperature profiles using the GSR model (Figure 5.21) to the predictions produced by the lagrangian PDF model

Figure 5.21: Measurements and predictions, using the GSR model, of mean temperature profiles in the swirl stabilized combustor (experimental data from Flores and Hedman (1996)).

(Figure 4.28). As observed in the two figures, the main difference is manifested in the spread of the radial profile. It is emphasized that the main factor that may cause the difference in the predictions lies in using two different mixing mechanisms (LMSE and the modified Curl mixing model). This conclusion is strengthened by the calculations done by Correa (1995), who used simple classical stochastic reactor model that provides an ideal platform for comparing the two mixing mechanisms.

5.4.1b Major Species

The predicted mean O_2 mole fraction profiles at four different axial locations are shown in Figure 5.22 as an example of a major species calculations. It may be observed that the mean O_2 mole fraction profiles are in logical correspondence to the mean temperature profiles shown in Figure 5.21. For example, the regions of high O_2 concentrations, which indicate the existence of unburned gases, correspond to regions of a lower temperature. This is particularly the case in the jet flow region, near the combustor inlet, where the fresh mixture did not mix with the back-flow hot products. Compared to species concentrations profiles predicted by the Lagrangian composition PDF model, it is found that the profiles predicted by the GSR model are more fluctuating in space. These fluctuations may be attributed to the use of the stochastic mixing model in the latter. In addition, a lower level of O_2 concentrations is observed in the GSR predictions near the line of symmetry when compared to the predictions made by the Lagrangian composition PDF model. This explains the higher level of temperature found in the same region (Figure 5.21) relative to the Lagrangian PDF calculations (Figure 4.28).

5.4.1c Minor Species

The predicted mean NO mole fraction profiles at four different axial locations are shown in Figure 5.23 as an example of a minor species calculation. As shown in the figure,

Figure 5.22: Predictions, using the GSR model, of mean O_2 mole fraction profiles in the swirl stabilized combustor.

Figure 5.23: Predictions, using the GSR model, of mean *NO* mole fraction (*ppm*) profiles in the swirl stabilized combustor.

under-estimation of the *NO* concentrations profiles provides another evidence supporting the suggestion that predictions of *NO* concentrations are most affected by the violation of the inlet temperature conditions at which the reaction mechanism was derived. Nevertheless, *NO* concentrations predicted by the GSR algorithm reveal a correct physical behaviour when compared with predictions made by the Lagrangian composition PDF model (Figure 4.30). The average value of the *NO* mole fraction predicted by the former is lower than the one predicted by the latter. This is explained by the fact that the average temperature predicted by the GSR is lower than the value predicted by the Lagrangian composition PDF. A higher temperature level means a higher level of thermal *NO* concentrations is attained.

5.5 Summary

To sum up, the GSR is a newly developed model which relies on the generalization of the concept of the classical stochastic reactor to account for both finite micro-mixing and finite macro-mixing processes. The premises of the model are to reduce computational efforts while maintaining considerations of accuracy. The finite macro-mixing is achieved by Lagrangian particle tracking, while the finite micro-mixing is related to turbulence characteristics. The model is essentially a PDF formulation, governed by the transport equation of a volume-averaged PDF over the reactor volume. An important improvement to the performance of the model was achieved with the introduction of turbulence mixing rate bias (turbulence frequency bias) in selecting particle pairs to mix in the modified Curl mixing mechanism. This modification leads to more realistic calculations and also causes the model to be less sensitive to the choice of the reactors network.

The model was evaluated by comparison against published experimental data for bluff body and swirl stabilized axi-symmetric combustors, and promising results were obtained.

Average temperature, major species and *CO* concentrations were well presented. Some discrepancies were found in average *NO* concentrations predictions. However, analysis indicates that it was mainly attributed to the violation of the valid inlet temperature range for the application of the chemical reaction mechanism.

Compared to the improved Monte Carlo Lagrangian composition PDF algorithm (Chapter 4), the GSR model shows that neither model is superior to the other from the point of view of calculation accuracy. However, the improved Lagrangian composition PDF algorithm is found to be advantageous from the point of view of computational time.

Chapter 6

Design Optimization Applications

6.1 Overview and Motivation

Three components are required to allow for a good design optimization scheme of gas turbine combustors:

1. An efficient and robust turbulent combustion model.
2. An efficient optimum search algorithm.
3. A well-posed optimization problem formulation.

Up to this point, efforts in the present research have been directed towards the development of the first component. That is, two turbulent combustion models have been developed and evaluated for the purpose of integration in an optimization scheme. From the point of view of design optimization, each of these two combustion models may be used as an evaluator in an optimization scheme. The role of the evaluator is merely to provide a measure of the quality of the objective one would like to find in the final design. It also provides criteria for checking for any violations of the constraints imposed on the design variables. This information is then supplied by the evaluator to the optimum search algorithm as

a database for a decision-making process aimed at improving the design further. These steps are repeated until a termination criterion, such as a certain number of designs without further improvement or the attainment of a pre-defined objective value, is met.

It is the intent of this chapter to consider the last two components (optimization method and problem formulation) among the three basic components of the optimization scheme. First, the basics of optimization are considered briefly with the aim of selecting an optimization method. The genetic algorithms (GA) method is selected as the candidate optimum search algorithm. The rationale and criteria for this selection are discussed. Then, the fundamental issues related the design of gas turbine combustors are briefly reviewed. Design requirements and parameters are re-cast in terms of design optimization terminology (objectives, constraints, and design variables). Finally, optimization examples are presented for simplified combustor geometry, which demonstrate the effectiveness of the optimization scheme in finding a credible optimum.

The effectiveness of the optimization scheme is demonstrated in terms of the robustness, practicality and validity of the scheme. Robustness is manifested by the capability of the combustion model (evaluator) to converge under randomly and drastically varying initial conditions specified by the optimizer in each iteration. Practicality is expressed in terms of the computational time and the specifications of the computational facility. The validity of optimization results are the most difficult to verify. This can be attributed to the scarceness of combustion experiments which consider the effect of the variation of combustor geometry and parametric analysis. However, some procedures are followed in the present research which demonstrate a reasonable level of confidence in the optimization results. In principle, combustion models were evaluated and tested against experimental measurements for two different configurations (bluff body and swirl stabilized combustors). Also, applications of the optimization scheme are presented for relatively simple combustor geometry, while keeping the main features of a real gas turbine combustor. This allows

for the analysis of trends in the optimization results. In addition, parametric analysis of the objectives against selected design variables, which help to test the final optimization results, is presented.

6.2 Optimum Search Algorithm (Genetic Algorithms)

6.2.1 Background

Referring to the optimization problem formulation represented in Equation 1.1, the objective function may be thought of as a multi-dimensional surface in the design variables space. In other words, every point on this surface is defined by coordinates which represent the values of the corresponding design variables. The boundaries of this multi-dimensional surface are defined by the constraints imposed on the design variables.

These constraints may be introduced in explicit or implicit form. The explicit form of constraints means that the range in which the design variables are allowed to vary in the context of the optimization process is directly specified. For example, if the length of the combustor is chosen as a design variable, then explicit constraints may be applied by specifying the minimum and maximum length. An implicit form of constraints may be introduced by specifying boundaries on the range of variations of a physical function, a range which may be expressed implicitly in terms of a subset of the design variables. For example, constraints may be imposed on the range of variations of the pattern factor at the combustor outlet. These constraints will be transferred indirectly to constraints on the combustor length and dilution zone geometry.

In that sense, an optimum design is defined as a feasible design which acquires an extremum for the specified objective. A feasible design is a design which does not violate any of the imposed constraints. Consequently, from the point of view of an optimum search algorithm, two designs are identical if their objectives and design variables are also

Figure 6.1: Schematic diagram for classifications of an optimization scheme .

identical.

Optimization schemes may be classified from different points of view, as shown in Figure 6.1. From the point of view of problem formulation, it may be classified as either unconstrained or constrained optimization. In the case of unconstrained optimization, the extremum (minimum or maximum) will occur most likely in the interior of the feasible domain at a peak or in a valley. There may be multiple places where a peak or a valley exists. The optimum search algorithm seeks to find the global optimum as opposed to the local optimum. In the case of constrained optimization, the optimum solution will most likely lie on a line or a surface defined by one or more constraints. There are different methods for handling the constraints in an optimization algorithm. As an example, the rejection method, which rejects any design configuration that violates the specified constraints. Another example is the penalty method, where the objective function is penalized when it violates the constraints. The penalty is imposed on the objective function value such that it is proportional to the degree of violation of the constraints (meaning it increases by increasing a certain measure of the violation).

From the point of view of design variables, the optimization scheme may be classified as a scheme with either continuous or discrete design variables. Continuous design variables may assume any real number in a certain range. Examples of continuous design variables are the length, volume, and cross section area of a combustor. Discrete design variables assume only the value of an integer number in a certain range. Examples of discrete design variables are the number of primary or secondary zone holes, the number of cooling holes, and the number of swirler blades. For example, the number of primary zone holes may be five or six or seven in the context of an optimization process. Generally speaking, the handling of discrete variables is more complicated than continuous ones and is usually referred to as combinatorial optimization. Hybrid algorithms are used for handling designs involving both continuous and discrete variables.

For its part, the objective function, may be classified as a single or a multi-objective optimization problem. The latter is sometimes referred to as Pareto optimal formulation. Algorithms employed for a single objective cannot be applied directly to a multi-objective formulation. Moreover, the extension of the former to the latter is far from straightforward. The simplest way to handle a multi-objective optimization is to transform the problem into a single objective problem. This single objective function takes the form of a linear combination of several objectives, each scaled by a weight factor according to its importance in the final design.

Finally, from the point of view of the optimum search algorithm, it may be broadly categorized as gradient or non-gradient-based optimization algorithms. Gradient-based algorithms make use of the gradients to guide the direction of the search towards extremum. This implies the use of well-behaved functions. Sometimes, this may be a stringent restriction on the performance of gradient-based algorithms. Examples of such methods are the steepest descent and Newtons methods. Examples of non-gradient-based methods are simulated annealing and genetic algorithms. Each of them can be considered as a random

search method.

6.2.2 Genetic Algorithms

Genetic algorithms are selected as the optimum search algorithm in the present work. The reason for this selection will be discussed in the next subsection. In the present subsection, basics of the method are introduced.

Genetic algorithms are stochastic, non-linear optimization routines loosely based on theories of biological evolution (Goldberg, 1989). In contrast to more traditional optimization methods which use gradient information to move between successively better points in the solution space, GA operate on populations of solutions using models of natural selection, reproduction, and mutation. The starting point is to arrange the initial values of design variables in groups. Each group of values of the design variables is a member of what is termed a population. Each member of the population (group of design variables) is decoded into a binary string (zeros or ones) referred to as a gene. Each bit of this binary string is called a chromosome.

The goal of the GA is to continually develop its population in the direction of the improvement of the design from the point of view of the objective criterion. Natural selection or survival of the fittest is simulated by assigning a higher probability of breeding to those members of the population who more closely resemble the assumed optimum.

GA incorporate these features of natural evolution in a computer algorithm. Members of the population (genes or groups of design variables) are used to evaluate an objective function, yielding what is called fitness. The members of the population that possess good fitness obtain a better chance of survival by being assigned greater preference of breeding. GA select parents (pairs of population members) according to the corresponding values of the objective function (fitness). New groups of design variables (children) are reproduced by recombining parts of the selected parents. The children are then evaluated for

Figure 6.2: Flow diagram for typical genetic algorithm.

fitness and inserted back into the population. These steps are repeated until a termination criterion is met.

A flow diagram showing the general procedures for typical GA is shown in Figure 6.2. In this diagram, two processes need explanation: crossover and mutation. Crossover is by far the most common mechanism for mixing parents to produce children (Goldberg, 1989). The simplest form of crossover involves the production of two children from two parents using what is called a single point crossover.

Mutation aims to simulate the jumps that occur in species evolution (for example, the creation of the eyes for the first time in a blind creature). These jumps may be thought of

as a random distortion of the genetic structure. It leads to the maintenance of some level of diversity in the population (Goldberg, 1989). This is done by randomly choosing one of the bits that form the string representing a group of design variables and flipping it over (for example, from one to zero). As it is the case in nature, mutation is implemented with very low probability.

The following is a detailed algorithm that describes the procedures for implementing a GA (Goldberg, 1989):

1. Create a random choice of design parameters, called the parameter set, to be put into an objective function. Calculate how well the parameter set fits and assign it a number. This is called the fitness of the parameter set.
2. Convert the parameter set from floating point numbers to binary strings. Each binary string is called a gene and each bit of the string is called a chromosome. The collection consisting of the parameter set, the binary strings, and the fitness, is called a citizen.
3. Repeat Steps (1) and (2) a number of times, each time saving the citizen in an array. This collection of citizens is called the population. The initial set of citizens is called the parents.
4. Select two good parents, meaning parents with good fitness. The selection process should take into consideration the fitness of the parents and ensure that parents with good fitness have the opportunity to breed, and parents with bad fitness do not.
5. Allow the two parents chosen in Step (4) to mate by taking some chromosomes from each parent to create a new, complete binary string. Call this a child. Once the child is created, turn the binary string back into floating point numbers. After the floating point numbers are calculated from the binary strings, calculate the fitness

of the set.

6. Repeat Steps (4) and (5) until there are as many children as there are parents.
7. Expose the children to a low mutation rate, by flipping or switching a few bits randomly.
8. Transfer the children array to the parent array. This is the new generation.
9. Repeat Steps (4) through (8) until the population converges.

6.2.3 Why Genetic Algorithms

It is emphasized that the performance of a certain search algorithm is problem dependent. No algorithm will absolutely outperform the others.

In searching an unexplored solution space, a trade-off must be established between two conflicting goals: exploiting the information contained in the best-known solutions and exploring new regions. Pure exploitation makes exclusive use of existing solutions, while at the same time, it abandons all known solutions that may exist elsewhere. Gradient-based methods are good examples of exploitative methods where the best known solution is always used as a starting point for improvement. Such techniques take a very narrow view of where opportunities for improvement lie. They are extremely dependent on their starting location and are vulnerable to becoming trapped in a local optimum. At the other extreme, totally random search (stochastic) methods provide excellent exploration but make no use whatsoever of acquired knowledge. Therefore, these methods may be time-consuming when the search space is large.

A properly implemented GA strikes a balance between these two extremes by simultaneously processing information obtained from potential solutions scattered throughout the solution space. Indeed, the distinguishing characteristics of GA are their adaptability and

robustness, which means that they are not hindered by the nature of the objective function. GA are capable of optimizing discontinuous, disjoint, and other poorly-behaved functions and they are one of the few available alternatives in the absence of a priori information regarding the form of the solution space (in experimental optimization, for example). In fact, this is the case in the problem of optimization of gas turbine combustors. Other factors that favor the implementation of GA are outlined here:

1. The GA method may be extended to include a multi-objective optimization process. This is an important property for optimizing complicated systems such as gas turbine combustors. One may try to avoid the multi-objective optimization by keeping only one objective and changing the others into implicit constraints. However, the introduction of constraints requires extremely accurate knowledge of the influence of changing the design variables on the objectives. In many situations, this is not the case so the multi-objective optimization may be the best approach.
2. The GA can deal with either continuous or discrete design variables, or a combination of both. This is also an important characteristic for the optimization of gas turbine combustors as the design variables could be continuous (length, volume, cross-section area, and swirl number) or discrete (the number of primary or secondary zones holes, the number of cooling holes and the number of swirler blades).

Finally, the main disadvantage to using GA is that the rate of convergence of solution towards an optimum becomes increasingly slow as it approaches the global optimum value. To overcome this problem a hybrid optimum search algorithm is usually employed. At the early stages of optimization, GA is used, while a conventional method (gradient-based method) is used at the final stage. This hybrid algorithm combines the advantages of avoiding local optima at the early stages and avoiding slow convergence at the final stage.

6.3 Overview of Gas Turbine Combustors Design

6.3.1 Objectives and Design Variables

The problem of gas turbine combustor design may be summarized in terms of both the requirements imposed on a successful design and the design configuration that enables the achievement of these requirements. Once the requirements are defined, the evaluation of a certain design may be thought of as equivalent to answering the question: how close are the performance parameters of the combustor to the specified target. This implies the necessity of the existence of certain global parameters that measure combustor performance.

Considering the formulation of a design optimization problem, objectives and physical constraints may be considered as a subset of the group of parameters that measure the combustor performance in addition to weight and size. Also, design variables may be considered as a subset of the group of independent parameters that uniquely define the combustor configuration. The general requirements imposed on the performance parameters (objectives and constraints) of gas turbine combustors may be summarized as follows (Lefebvre, 1987; Mellor, 1990):

1. Combustion efficiency: defined as the percentage of available chemical energy in the fuel which is converted to heat. Any loss of combustion efficiency represents wasted fuel. The requirements to meet *CO* and unburned hydrocarbon emissions regulations for gas turbines dictate that high levels of combustion efficiency, about 99.9 percent, over most of the operating range be attained.
2. Pressure loss: pressure loss is undesirable because it detracts from gas turbine thermal efficiency and power. However, a minimum pressure drop must be accepted to promote rapid fuel-air mixing within the combustor and effective cooling of the combustor walls.

3. Range of stability: The range here is understood in reference to equivalence ratio, inlet temperature and pressure under which the combustor is able to operate successfully. Table 6.1 includes data of a typical aircraft combustor range of operating conditions. It shows the severity of the conditions under which the combustor must be able to maintain its operability.
4. Exit temperature distribution: this distribution is measured in terms of pattern factor, $(\frac{T_{loc}-T_{av}}{T_{loc}-T_3})$, where T_3 is the combustor inlet temperature, T_{av} is the average temperature at the combustor exit and T_{loc} is the local temperature. Typical exit temperature distribution is shown in Figure 6.3 indicating that lower temperatures are desirable both at the root of the turbine blade, where the mechanical stresses are maximum and at the tip, where cooling is more difficult.
5. Emissions: this includes smoke, carbon monoxide (CO), oxides of nitrogen (NO_x) and unburned hydrocarbons. Lower pollutant emissions are recent driving forces for advanced engine design.
6. Weight and size: short combustion systems are required in modern aircrafts engines for reducing the engine weight.
7. Durability: measured in terms of operating hours or flight cycles, the durability requirements may affect the design in several ways. For example, cooling air flow distribution may be used to reduce the thermal stresses. Also, structural members used for stiffening the combustors in highly loaded regions must be considered.

In reference to Figure 6.4, which shows a cross-section of a conventional diffusion flame turbine combustor, design variables may be summarized as:

1. Size of the primary, secondary and dilution zones.

Table 6.1: Aircraft combustor operating conditions (from Mellor, 1990).

Typical combustor operating condition	Inlet Temperature (K)	Inlet Pressure (atm)	Fuel/air ratio
Ground start	220 - 320	0.8 - 1.4	0.020
Idle	400 - 475	2 - 3	0.010 - 0.015
Cruise	700	10	0.015 - 0.025
Takeoff	800	30	0.020 - 0.030
Altitude ignition	220 - 340	0.3 - 1	0.010 - 0.030

Figure 6.3: Typical exit temperature distribution at combustor outlet (adapted from Mellor, 1990).

Figure 6.4: Conventional combustor cross-section (from Mellor, 1990).

2. Number, size, location and shape of the holes of the primary and dilution zones.
3. Size, shape, location and number of cooling slots.
4. The shape and the length of the diffuser.
5. The swirl number and the swirler type.
6. The relative size of the outer casing and liner.

6.3.2 A Discussion on the Optimization Problem Formulation

Generally, formulating the problem of design optimization of a gas turbine combustor may be classified into two main types: the first is the formulation of the optimization problem for a newly developed combustor, and the second is the improvement of an existing design. For the second type, a lower degree of freedom is available in the problem formulation as the outer shape and the inlet flow conditions of the combustion chamber must be kept fixed. One may also try to keep some previously known good characteristics in the older design by carefully omitting certain design variables that are thought to control

these good characteristics as well as by limiting the range of change to the selected design variables to be narrow.

As a suggested example for newly developed combustors, one may ask for an optimized design which meets a given targeted value of combustion efficiency at a given outlet temperature and size (length and volume). Constraints may be introduced to the emissions, stability limits and pattern factor. Specifically, constraints on the stability limits may be applied using acceptance-rejection criterion by which the optimized design would be accepted only if it complies with the specified stability limits.

Finally, it may also be noted that not only global performance variables but local variables may be used as an objective function, as well. However, it is likely that the optimization problem in the case of local variables will be formulated as a minimum-maximum (min-max) problem. For example, the temperature distribution at the combustor outlet may be treated locally, as the hot streaks at certain points may affect the life of the turbine nozzle guide vanes. In this case, one may wish to minimize the maximum temperature wherever it appears. The targeted point (point of maximum temperature) may not be fixed and the optimization algorithm should trace its position in each new iteration.

6.4 Optimization Applications

6.4.1 Problem Considered

Parametric analysis and design optimization examples are demonstrated with respect to the simplified hypothetical combustor geometry shown in Figure 6.5. The combustor is axi-symmetric with a flat swirler and a side-wall expansion angle (θ). It operates at lean, fully premixed conditions. The combustor length is 278 mm, its radius is 62.50 mm, and the inlet flow area is $3E3mm^2$. The inlet axial flow velocity is 30 m/sec and the inlet radial velocity is zero. The equivalence ratio is set to 0.6, and the inlet temperature is

Figure 6.5: Axi-symmetric combustor geometry.

set to 600 K , so as to simulate a realistic compressor outlet. Constant temperature of 1000 K is specified for the combustor wall. Symmetry and outlet boundary conditions are as specified in Chapter 4. The improved Monte Carlo Lagrangian composition PDF algorithm is used for solving the turbulent combustion. A grid resolution of 28×22 is used for solving the turbulent flow and 15 particles per cell are used for the Monte Carlo simulation.

6.4.2 Parametric Analysis

The inclusion of all the design variables in the optimization problem formulation allows for a better chance of finding the overall best design. However, the addition of more design variables space dimensions complicates the shape of the objective function and the search for an optimum solution. In this case, the reduction of dimensions of the design variables space is necessary. However, the selection of the design variables to be removed is not arbitrary. It may be done heuristically by choosing what are thought to be the most effective variables that control a certain objective function.

A more systematic way of reducing the number of design variables is to employ parametric analysis. Parametric analysis not only aims at specifying the effectiveness of changing the design variables on the objective function, but it also helps to define the feasible de-

Figure 6.6: The effect of changing the swirl vane angle on the outlet average temperature , CO , and NO mole fraction (expansion angle is 31.54 degrees).

sign space. A feasible design space represents the envelope of all possible combinations of design variables that do not violate the imposed constraints and consequently, it diagnoses a well-posed optimization problem. Here, two geometric design variables are chosen for both the parametric analysis and optimization applications: the swirl vane angle and the combustor side wall expansion angle. Average emissions concentrations (NO and CO) and the temperature at the combustor outlet are calculated in the course of changing the selected design variables.

The effects of changing the swirl vane angle (and consequently the associated swirl number) on the average NO and CO concentrations and on the temperature at the combustor outlet are shown in Figures 6.6 and 6.7, respectively. The swirl vane angle is allowed to vary in the range of 65 to 74.5 degrees, with step resolution of 0.5 degree. Two cases are considered with two different constant expansion angles of 31.54 and 39.19 degrees, respectively.

The effect of the change in the swirl number on the recirculation zones in a free jet

Figure 6.7: The effect of changing the swirl vane angle on the outlet average temperature, CO , and NO mole fraction (expansion angle is 39.19 degrees).

has been studied experimentally (Lilley, 1985). Experimental measurements show that as the swirl number increases, the recirculation zone becomes longer, reaching a maximum length at a certain swirl number and subsequently becomes shorter and wider at a higher swirl number. The effect of changing the swirl number in the case of confined flow is more complicated. The precise effect of the swirl number on the flow field is found to depend on other geometrical factors such as the degree of confinement. Therefore, studies concerning the effect of the swirl number on pollutant emissions are strongly configuration-dependent and do not provide general quantitative correlations with other geometrical or performance parameters.

In Figures 6.6 and 6.7, it is shown that as the vane angle (swirl number) increases, both the average exit temperature and NO concentrations decrease, while CO concentrations increase. This is a logical physical behaviour; the increment of CO concentrations indicates less heat released because the oxidation of the CO to CO_2 (an exothermal reaction) does not occur. Therefore, one expects the average temperature and consequently, the formed

thermal NO , to decrease.

The global influence of changing the swirl number may be considered as the resultant of more elementary processes that have conflicting effects on the flow field. By increasing the swirl number, the entrainment of cooled combustion reactants increases, thereby leading to CO quenching (an increment in the formed CO concentrations). This also leads to a reduced average temperature and lower thermal NO production. On the other hand, increasing the swirl number enhances turbulent mixing as well as the availability of oxygen, all of which lead to a better opportunity for the oxidation of CO to CO_2 and consequently, an improvement in the combustion efficiency. In turn, the average temperature rises and subsequently, thermal NO concentrations increases. Referring to Figures 6.6 and 6.7, it can be seen that the entrainment of the cooled flow has a dominant effect. However, the competition among different processes explains the existence of non-linearity and local minima in the behaviour of the curves.

The effect of changing the side wall expansion angle in the range of 31 to 47.5 degrees, with step resolution of 0.5, at two different constant vane angles of 66 and 70 degrees, is shown in Figures 6.8 and 6.9, respectively. Despite the high degree of non-linearity observed in the behaviour of the average outlet NO and CO concentrations and temperature, no conclusion can be drawn about global trends in the behaviour of these quantities as a function in the side wall expansion angle. This is consistent with experimental measurements which showed that the gradual change in the expansion angle has a minimal effect on the flow field (Lilley, 1985), an observation which is also confirmed by the parametric analysis shown in Figures 6.8 and 6.9.

In conclusion, as far as the two design variables are concerned, the swirl number has a profound effect on flow characteristics and emissions. The side wall expansion angle has a limited effect on emissions in the case considered. From the point of view of optimization of emissions, this means that the original problem with the two design variables (swirl

Figure 6.8: The effect of changing the side wall expansion angle on the outlet average temperature , CO , and NO mole fraction (vane angle is 66 degrees).

Figure 6.9: The effect of changing the side wall expansion angle on the outlet average temperature , CO , and NO mole fraction (vane angle is 70 degrees).

vane angle and expansion angle) may be reduced to one design variable - the swirl vane angle - without greatly affecting the objective (minimum combustion emissions).

6.4.3 Example I: Minimization of *NO* Emissions

Pollution considerations represent the most severe requirements on combustor design, so that the sizing of the combustor may now be determined by pollution considerations rather than relighting requirements (Lefebvre, 1987). In designing gas turbine combustors, an optimization problem formulation should include this objective. As an example, the optimization problem may be stated as: given the combustor geometry and boundary conditions in the problem considered (Subsection 6.4.1), the objective is the unconstrained minimization of average *NO* concentrations at the combustor outlet in terms of changing the swirl vane angle (in the range of 65 to 75 degrees) and the side wall expansion angle (in the range of 31.5 to 47.5 degrees).

To carry out this task, the GA (optimum design search algorithm) was integrated with the Monte Carlo Lagrangian composition model (objective function evaluator). Starting with an initial combustor geometry, the goal of the GA is to continually develop the design parameters (swirl vane angle and side wall expansion angle) in the direction of the improvement of the objective function (minimum *NO* emissions). The improvement is measured by the fittest member in a certain generation. This cycle continues until a termination criterion is met. The termination criterion, in our case, is met when there are 10 successive generations without further improvement in the objective function.

An example of the optimization algorithm output is shown in Figure 6.11. It lists results of the first five generations. Each generation includes four iterations (populations). In Figure 6.11, the fitness of the fittest member (minimum *NO* concentrations) is plotted against the generation number. A converged solution is obtained in 32 generations. Generation zero represents the initial configuration before optimization. The calculation time

on a Pentium 4, Intel, 2800 MHZ processor was of nearly four days. The evolution of the corresponding design variables (swirl vane angle and side wall expansion angle) is shown in Figures 6.12 and 6.13, respectively. These results show that average *NO* concentrations at the combustor outlet are decreasing when increasing the swirl vane angle (swirl number). No definite conclusion can be drawn concerning the effect of changing the expansion angle. These results match conclusions drawn from the parametric analysis previously described.

It is particularly interesting to observe the variation of the average *CO* concentrations at the combustor outlet in the context of optimization of *NO* emissions. As shown in Figure 6.14, average *CO* concentrations moves in the opposite direction of *NO* variation. This is an expected result which highlights a warning that constraints must be imposed on the maximum *CO* emissions for an efficient optimization practice.

6.4.4 Example II: Minimization of *NO* Emissions Using a Reduced Group of Design Variables

By making use of the parametric analysis results, the optimization problem formulated in the previous subsection may be further reduced in terms of the number of design variables space dimensions. An experimental run was attempted using the swirl vane angle as the sole design variable (ranging from 65 to 75 degrees), while the expansion angle was dropped from the group of design space variables. An arbitrary value of the expansion angle was chosen as 39.17 degrees and kept constant throughout the optimization iterations. The results of the evolution of the objective function (average *NO* concentrations) and the corresponding swirl vane angle against the generation number are shown in Figures 6.15 and 6.16, respectively. It is found that average *NO* concentrations are decreasing in the direction of increment of the swirl vane angle. Compared to the best value obtained in Example I ($0.26866E - 05$) after 32 generations, the objective (average *NO* concentrations) converged solution was obtained in 27 generations and the best value of the objective

Generation 1			
Iter	Vane angle	Expansion angle	Fitness(NO mole fraction)
1	70.6185	3.357E+01	-0.000004862
2	65.9818	4.174E+01	-0.000008286
3	72.9180	4.519E+01	-0.000004468
4	68.2633	4.552E+01	-0.000006431
Maximum Fitness		= -0.000004468	
Generation 2			
Iter	Vane angle	Expansion angle	Fitness(NO mole fraction)
1	72.9623	4.300E+01	-0.000003972
2	70.4616	3.821E+01	-0.000005392
3	72.9180	4.519E+01	-0.000004468
4	68.5392	4.526E+01	-0.000006367
Maximum Fitness		= -0.000003972	
Generation 3			
Iter	Vane angle	Expansion angle	Fitness(NO mole fraction)
1	72.9623	3.437E+01	-0.000004074
2	72.9623	4.300E+01	-0.000004122
3	72.9617	3.477E+01	-0.000004053
4	72.9617	3.430E+01	-0.000003987
Maximum Fitness		= -0.000003987	
Generation 4			
Iter	Vane angle	Expansion angle	Fitness(NO mole fraction)
1	72.9617	3.430E+01	-0.000003987
2	68.1034	3.992E+01	-0.000006729
3	66.1393	4.536E+01	-0.000009032
4	65.4251	4.186E+01	-0.000008778
Maximum Fitness		= -0.000003987	
Generation 5			
Iter	Vane angle	Expansion angle	Fitness(NO mole fraction)
1	72.9669	3.444E+01	-0.000003929
2	70.4277	4.127E+01	-0.000005301
3	72.9617	3.483E+01	-0.000003987
4	67.9618	3.442E+01	-0.000006340
Maximum Fitness		= -0.000003929	

Figure 6.10: An example of the optimization algorithm output.

Figure 6.11: Optimization of average *NO* emissions at combustor outlet.

Figure 6.12: Variation of the swirl vane angle with the generation number.

Figure 6.13: Variation of the expansion angle with the generation number.

Figure 6.14: Variation of the CO mole fraction with the generation number.

Figure 6.15: Optimization of average *NO* emissions at combustor outlet using a reduced group of design variables.

function (average *NO* concentrations) was $0.30419E - 05$. This is an important result, as it establishes proof of the importance of the fidelity-cost compromise of the optimization algorithms - a basic theme of the design optimization of systems that are characterized by a large number of variables and encounter complicated phenomena such the one found in gas turbine combustors.

6.4.5 Example III: Minimization of *CO* Emissions

The same problem formulation solved in Example I is repeated here with the objective changed to be the minimum average *CO* emissions at the combustor outlet. This example is considered with the intent of attaining more confidence in the optimization algorithm. It was previously shown that the swirl vane angle (swirl number) is an effective parameter considering *NO* emissions as an objective function. One may expect that the trends in

Figure 6.16: Variation of the swirl vane angle with the generation number using a reduced group of design variables.

variation of the swirl vane angle, in the case of *CO* emissions minimization, is likely to move the opposite direction to the case of *NO* emissions minimization. This is actually the case as shown in Figures 6.17 and 6.18, which show the variation of *CO* concentrations and the swirl vane angle against the generation number, respectively. It is found that the *CO* concentrations increase by increasing the swirl vane angle. The variation of the side wall expansion angle is shown in Figure 6.19. Also, as was the case in *NO* concentrations minimization, there is no a priori trend that can be anticipated regarding the effect of variation of the side wall expansion angle on the *CO* emissions.

6.5 Summary

Elements and applications of the integrated design optimization algorithm for gas turbine combustors were presented. The genetic algorithms were chosen as the design search

Figure 6.17: Optimization of average *CO* emissions at combustor outlet .

Figure 6.18: Variation of the swirl vane angle with the generation number.

Figure 6.19: Variation of the expansion angle with the generation number.

algorithm. Applications of the optimization algorithm were considered in terms of minimization of axi-symmetric combustor emissions (NO and CO concentrations). The optimization of the objective function was obtained in the course of changing the swirl vane angle and the side wall expansion angle as design variables. Parametric analysis and optimization examples demonstrated the effectiveness and practicality of the optimization algorithm in finding credible optimal geometry within a reasonable amount of time using modest computational facility.

Chapter 7

Conclusions and Recommendations

7.1 Conclusions

The objective of this work was to suggest, construct and implement an efficient algorithm for the design optimization of gas turbine combustors in its general form. The purpose was to explore the possibilities and chances of using optimization techniques as an alternative, practical tool for the design of gas turbine combustors. For a well posed optimization problem formulation, two components are required to allow for a successful optimization algorithm: an efficient and accurate turbulent combustion model, and an efficient optimum search algorithm. These components are discussed in the following subsections.

7.1.1 Turbulent Combustion Models

The objective function and physical constraints are determined using turbulent combustion models. Robust and affordable models with high fidelity are essential tools for achieving an efficient optimization algorithm. In the present study, two models were developed and evaluated as alternatives to the existing low fidelity or high cost turbulent

combustion models. These two models are the improved Monte Carlo Lagrangian composition PDF and the generalized stochastic reactor models.

7.1.1a The Lagrangian Composition PDF Model

A hybrid method was employed to develop an efficient Lagrangian composition PDF algorithm. This hybrid method consisted of the finite volume method for solving the inert flow equations and the Monte Carlo method for solving the composition PDF transport equation. Chemical kinetics was modelled using a five-step, seven-specie global reaction mechanism. It was solved using the DVODE algorithm. The latter is an efficient and robust algorithm for solving a stiff system of ordinary differential equations with variable coefficients. The LSME mixing model was used for modelling the turbulent mixing process. The improvement in the model performance was mainly achieved through the implementation of time splitting, variable stochastic fluid particle mass control and second order time accurate (predictor-corrector) scheme for solving the stochastic differential equations governing the particles evolution. These procedures allowed for a considerable reduction in the number of particles and the total time required for convergence in comparison to conventional schemes. The model predictions were evaluated by comparing them to published experimental data of two different combustor configurations: bluff body and swirl stabilized combustors, in the case of lean premixed turbulent flames. The velocity field, temperature and major species concentrations were well presented. Trends and gross features of CO concentrations were also reasonably well presented. Some discrepancies were found in the predictions of NO concentrations. Analysis and computational evidence strongly suggest that these discrepancies are mainly due to the violation of the valid range of inlet conditions necessary for the application of the chemical kinetics mechanism (inlet temperature range).

7.1.1b The Generalized Stochastic Reactor Model

The generalized stochastic reactor model is a newly developed model which relies on the generalization of the concept of classical stochastic reactor in the sense that it accounts for both finite micro- and macro-mixing processes. The macro-mixing process was accounted for by the introduction of the Lagrangian particle tracking, while the micro-mixing process was related to turbulence characteristics. The model is based on a volume-averaged PDF formulation. This formulation was made possible by assuming uniform turbulent mixing rate over the reactor volume. The Curl mixing model was used for modelling the turbulent mixing process. A further improvement in the model performance was achieved by proposing a turbulence frequency bias in selecting particle pairs for mixing. This modification led to a relaxation of the stringent assumption of uniform mixing frequency over the reactor volume. Also, it led to a reduction in the model sensitivity to the selection of the reactors network and volumes. These procedures allowed for a reduction in the computational time by way of an effective reduction in the number of particles used in the simulation compared to the conventional PDF models.

The model predictions were evaluated by comparing them against the experimental data of two combustor configurations: bluff body and swirl stabilized combustors, in the case of lean premixed turbulent flames. Temperature, major species and *CO* concentrations were well predicted. As was the case in the Lagrangian composition PDF model, some discrepancies were found in the predictions of *NO* concentrations. In fact, this confirmed the previous suggestion that these discrepancies resulted mainly from a violation of the valid range of conditions for the application of the chemical kinetics mechanism. Compared to the Lagrangian composition PDF model, none of the two models was found superior to the other from the point of view of predictions accuracy. The difference of predictions in the two models was found to match the published simulation results showing the difference between the two mixing models predictions in the case of the classical

stochastic reactor model (i.e., independent of any other modelling assumption). However, the improved Lagrangian composition PDF model was found advantageous from the point of view of the computational time.

7.1.2 Design Optimization Algorithm

The optimization algorithm was constructed by integrating the Lagrangian composition PDF model, with the GA as an optimum search algorithm. Applications of the optimization algorithm were considered in terms of the minimization of emissions. Parametric analysis and optimization examples were presented. Both average *NO* and *CO* concentrations at the combustor exit were chosen as an objective function in a constraint-free optimization problem formulation. Each of these objectives was minimized in terms of the variations of the swirl vane angle and the side wall expansion angle in an axi-symmetric combustor. Parametric analysis revealed the possibility for the reduction of the two design variables problem formulation (swirl vane angle and side wall expansion angle) into one design variable problem formulation (swirl vane angle). This reduction was applied to the case of minimization of *NO* emissions, and the results confirmed the conclusions drawn from the parametric analysis.

Results obtained from the parametric analysis and the optimization examples are supported by experimental data in the literature concerning the effect of the variation of the swirl number and side-wall expansion angle on the combustor flow field and emissions. Applications considered demonstrated the effectiveness, robustness and practicality of the optimization algorithm in finding credible optimum geometry within a reasonable computational time and using modest computational facility. Results of optimization examples promise good potential for the application of the optimization techniques as an efficient and practical tools for the design of gas turbine combustors .

7.2 Contributions

Contributions arising from the present work can be summarized as:

1. The construction, implementation and analysis of a generic algorithm for the optimization of gas turbine combustors.
2. The development and evaluation of an improved Lagrangian Monte Carlo composition PDF algorithm for solving the turbulent combustion.
3. The introduction, development and evaluation of the novel generalized stochastic reactor model for solving the turbulent combustion.
4. Establishment of a link between the well developed stochastic methods in statistical mechanics and the corresponding models in the stochastic modelling of turbulent combustion, with a focus on the limits of extension and possibilities for improvement.

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