CFD modelling of turbulent non-premixed combustion

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Abstract

The thesis comprises of a thorough assessment of turbulent non-premixed combustion modelling techniques, emphasising the fundamental issue of turbulence-chemistry interaction. The combustion models studied are the flame-sheet, equilibrium, eddy break-up and laminar flamelet models. An in-house CFD code is developed and all the combustion models are implemented. Fundamental numerical issues involving the discretisation schemes are addressed by employing three discretisation schemes namely, hybrid, power law and TVD.

The combustion models are evaluated for a number of fuels ranging from simple H₂/CO and CO/H₂/N₂ to more complex CH₄/H₂ burning in bluff body stabilised burners at different inlet fuel velocities. The bluff body burner with its complex recirculation zone provides a suitable model problem for industrial flows. The initial and boundary conditions are simple and well-defined. The bluff body burner also provides a controlled environment for the study of turbulence-chemistry interaction at the neck zone.

The high quality experimental database available from the University of Sydney and other reported measurements are used for the validation and evaluation of combustion models. The present calculations show that all the combustion models provide good predictions for near equilibrium flames for temperature and major species. Although the equilibrium chemistry model is capable of predicting minor species, the predictive accuracy is found to be inadequate when compared to the experimental data. The laminar flamelet model is the only model which has yielded good predictions for the minor species. For flames at higher velocities, the laminar flamelet model again has provided better predictions compared to predictions of other models considered. With different fuels, the laminar flamelet model predictions for CO/H₂/N₂ fuel are better than those for CH₄/H₂ fuel. The reasons for this discrepancy are discussed in detail.
The effects of differential diffusion are studied in the laminar flamelet modelling strategy. The flamelet with unity Lewis number is found to give a better representation of the transport of species. The laminar flamelet model has yielded reasonably good predictions for NO mass fraction. The predictions of NO mass fraction are found to be very sensitive to differential diffusion effects. This study has also considered the issue of inclusion of radiative heat transfer in the laminar flamelet model. The radiation effects are found to be important only where the temperature is very high.

The study undertaken and reported in this thesis shows that the presently available laminar flamelet modelling concepts are capable of predicting species concentrations and temperature fields with an adequate degree of accuracy. The flamelet model is also well suited for the prediction of NO emissions. The inclusion of radiation heat transfer has enhanced the predictive capability of the laminar flamelet model.
The author wishes to express his deep gratitude and indebtedness to his supervisor Dr. W. Malalasekera for his supervision, guidance, invaluable suggestions and constructive criticism throughout this investigation. The author would like to thank Mr. Henk Versteeg and Dr. Colin Garner for their interest and encouragement in the research work.

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The author wishes to acknowledge the friendly help extended by his colleagues, Aruna Palipana, John Jones, John Henson and Richard Carroni.

The author would like to thank Professor B. Rogg and Dr. W. Wang for kindly providing the code RUN-IDL with which some of the laminar flamelet calculations were performed.

Finally the author expresses gratitude to his wife, Farzana, for her patience, understanding and support and willingly sharing every experience to make success more enjoyable and disappointments more bearable.
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Appendix A  
Appendix B
References
Roman letters

\( a \)
\begin{align*}
\text{strain rate} & \ [	ext{s}] \\
\text{exponent in beta pdf, Eq. (3.9)} \\
\text{temperature exponent in forward and backward reaction rate, Eq. (2.10)}
\end{align*}

\( a_p, a_E, a_W, a_N, a_s \)
\begin{align*}
\text{coefficients of discretised equation, Eq. (3.2)}
\end{align*}

\( A \)
\begin{align*}
\text{area} & \ [\text{m}^2] \\
\text{model constant in Magnussen’s EBU model, Eq. (2.53)}
\end{align*}

\( b \)
\begin{align*}
\text{exponent in beta pdf, Eq. (3.9)}
\end{align*}

\( B \)
\begin{align*}
\text{model constant in Magnussen’s EBU model, Eq. (2.53)}
\end{align*}

\( B_p \)
\begin{align*}
\text{pre-exponential factor, Eq. (2.10)}
\end{align*}

\( C_{EBU} \)
\begin{align*}
\text{model constant in EBU model, Eq. (2.52)}
\end{align*}

\( C_{\epsilon 1}, C_{\epsilon 2} \)
\begin{align*}
\text{turbulence model constant in the } \epsilon \text{-equation, Eq. (2.19)}
\end{align*}

\( C_\mu \)
\begin{align*}
\text{model constant in the definition of turbulent viscosity, Eq. (2.17)}
\end{align*}

\( C_{g1}, C_{g2} \)
\begin{align*}
\text{constants in transport equation of mixture fraction variance, Eq. (2.33)}
\end{align*}

\( C_P \)
\begin{align*}
\text{specific heat} & \ [\text{J/kg K}] \\
\text{proportionality constant, Eq. (2.48)}
\end{align*}

\( d \)
\begin{align*}
\text{diameter of inlet pipe} & \ [\text{m}] \\
\text{diameter of bluff body} & \ [\text{m}]
\end{align*}

\( D_\alpha \)
\begin{align*}
\text{diffusion coefficient of species } \alpha & \ [\text{m}^2/\text{s}] \\
\text{diffusion coefficient of species } \alpha & \ [\text{m}^2/\text{s}]
\end{align*}
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<th>Description</th>
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<tr>
<td>$E$</td>
<td>constant in log-law wall function, Eq. (3.8)</td>
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<tr>
<td>$E_\beta$</td>
<td>activation energy, Eq. (2.10) [J/mol]</td>
</tr>
<tr>
<td>$E_g$</td>
<td>black body emissive power [W/m²]</td>
</tr>
<tr>
<td>$f'$</td>
<td>dimensionless velocity, Eq. (2.36)</td>
</tr>
<tr>
<td>$g_{1}$</td>
<td>gravitational acceleration vector</td>
</tr>
<tr>
<td>$G$</td>
<td>production rate of kinetic energy, Eq. (2.20) [W]</td>
</tr>
<tr>
<td>$h$</td>
<td>enthalpy of mixture [J/kg]</td>
</tr>
<tr>
<td>$H_{fu}$</td>
<td>heating value of fuel [J/kg]</td>
</tr>
<tr>
<td>$i$</td>
<td>turbulence intensity</td>
</tr>
<tr>
<td>$I$</td>
<td>radiation intensity [W/m² sr]</td>
</tr>
<tr>
<td>$J_{i,\alpha}$</td>
<td>mass molecular flux of species $\alpha$, [kg/m² s]</td>
</tr>
<tr>
<td>$k$</td>
<td>turbulence kinetic energy [m²/s²]</td>
</tr>
<tr>
<td>$k_{f\beta}$</td>
<td>Arrhenius rate coefficient of forward reaction, Eq. (2.9) [/s]</td>
</tr>
<tr>
<td>$k_{b\beta}$</td>
<td>Arrhenius rate coefficient of backward reaction, Eq. (2.9) [/s]</td>
</tr>
<tr>
<td>$k_g$</td>
<td>gas absorption coefficient</td>
</tr>
<tr>
<td>$L$</td>
<td>radiation path length, [m]</td>
</tr>
<tr>
<td>$l_m$</td>
<td>turbulent mixing length, Eq. (3.7)</td>
</tr>
<tr>
<td>$l_p$</td>
<td>order of backward reactions, Eq. (2.9)</td>
</tr>
<tr>
<td>$m_p$</td>
<td>order of forward reactions, Eq. (2.9)</td>
</tr>
<tr>
<td>$M_\alpha$</td>
<td>chemical symbol of species $\alpha$, Eq. (2.7)</td>
</tr>
<tr>
<td>$M_m$</td>
<td>mass flow rate at inlet [kg/s]</td>
</tr>
<tr>
<td>$M_{out}$</td>
<td>mass flow rate at outlet [kg/s]</td>
</tr>
<tr>
<td>$p, P$</td>
<td>pressure [N/m²]</td>
</tr>
<tr>
<td>$P()$</td>
<td>probability density function</td>
</tr>
<tr>
<td>$P_e$</td>
<td>critical probability of extinction</td>
</tr>
<tr>
<td>$P_{ext}$</td>
<td>probability of extinction</td>
</tr>
<tr>
<td>$Pe$</td>
<td>Peclet number</td>
</tr>
<tr>
<td>$q_w$</td>
<td>wall heat flux due to radiation [W/m²]</td>
</tr>
<tr>
<td>$r$</td>
<td>radius of inlet pipe [m]</td>
</tr>
<tr>
<td>$R$</td>
<td>Universal gas constant=8.3143 [J/mol]</td>
</tr>
<tr>
<td>$R$</td>
<td>radius of bluff body [m]</td>
</tr>
<tr>
<td>$Re_t$</td>
<td>turbulence Reynolds number</td>
</tr>
<tr>
<td>$s$</td>
<td>stoichiometric mass of oxygen [kg]</td>
</tr>
</tbody>
</table>
Nomenclature

$S_h$ radiation source term, Eq. (8.12) [W/m$^3$]

$S_\Phi$ general source term in transport equations, Eq. (3.1)

$S_C, S_P$ general source term in discretised equation, Eq. (3.3)

$Sc$ Schmidt number

$t$ time [s]

$\tau_k$ Kolmogorov time [s]

$\tau_c$ chemical time [s]

$T$ temperature [K]

$T_g$ gas temperature [K]

$u, U$ axial velocity [m/s]

$u_i$ Cartesian velocity components

$v, V$ radial velocity [m/s]

$V$ volume of computational cell [m$^3$]

$V$ dimensionless velocity, Eq. (2.37)

$W_\alpha$ molecular weight of species $\alpha$ [kg/mol]

$x$ axial distance [m]

$x_i$ Cartesian coordinates

$y$ radial distance [m]

$Y_\alpha$ mass fraction of species $\alpha$

$Z$ mixture fraction

$Z_m$ mass fraction of element $m$

$Z_{sf}$ stoichiometric mixture fraction

$Z'^2$ mixture fraction variance

Greek letters

$\Gamma$ diffusive transport coefficient

$\Gamma()$ Gamma function

$\delta()$ delta function

$\delta_{ij}$ Kronecker delta

$\Delta Z$ reaction zone thickness in mixture fraction space

$\varepsilon$ rate of turbulent kinetic energy dissipation [m$^2$/s$^3$]

$\varepsilon_g$ emissivity of gas
Nomenclature

\( \zeta \) enthalpy defect, Eq. (8.1) [W/kg]
\( \eta \) non dimensional distance, Eq. (2.38)
\( \kappa \) von Karman constant in log-law wall function, Eq. (3.8)
\( \lambda \) factor for turbulent length scale, Eq. (5.2)
\( \mu \) molecular viscosity of mixture [kg/m s]
\( \mu \) mean value of log-normal pdf, Eq. (3.19)
\( \mu_t \) turbulent viscosity [kg/m s]

\( v^\prime \alpha, v^\prime \beta \) stoichiometric coefficients of species \( \alpha \) in reaction step \( \beta \), Eq. (2.7)
\( \rho \) density [kg/m³]
\( \sigma \) Prandtl number
\( \sigma \) standard deviation of log-normal pdf, Eq. (3.19)
\( \sigma_t \) turbulent Prandtl number
\( \sigma_k \) Prandtl number governing diffusion of turbulent kinetic energy, \( k \)
\( \sigma_{\epsilon} \) Prandtl number governing diffusion of turbulent energy dissipation rate, \( \epsilon \)
\( \sigma \) Stefan-Boltzmann constant = 5.6696 \times 10^{-8} \text{ W/m}^2 \text{ K}^4
\( \tau_{ij} \) viscous stress tensor, Eq. (2.3) [N/m²]
\( \tau_w \) wall shear stress [N/m²]
\( \phi \) scalar variable
\( \chi \) scalar dissipation rate [/s]
\( \chi_d \) scalar dissipation rate at the extinction limit [/s]
\( \Psi \) limiter in TVD scheme, Table (3.1)
\( \Omega \) solid angle [sr]
\( \omega_{\alpha} \) net rate of formation of species \( \alpha \) [mol/m³ s]

Subscripts and superscripts

\( \alpha \) species
\( \Lambda \) air
\( b \) black body
\( C \) carbon
Nomenclature

\( DC \) deferred correction
\( eq \) equilibrium
\( F, f, fu \) fuel
\( g \) gas
\( H \) hydrogen
\( in \) inlet
\( NO \) nitric oxide
\( ox \) oxygen
\( out \) outlet
\( O \) oxygen
\( pr \) product
\( st \) stoichiometric

Diacritical marks

\( \bar{\phi} \) time-averaged mean quantity of \( \phi \)
\( \tilde{\phi} \) Favre-averaged mean quantity of \( \phi \)
\( \phi' \) turbulent fluctuation of \( \phi \) after time-averaging
\( \phi'' \) turbulent fluctuation of \( \phi \) after Favre-averaging

Abbreviations

CDS central differencing scheme
CFD computational fluid dynamics
CMC conditional moment closure
cpu central processing unity
DNS direct numerical simulation
DTM discrete transfer method
EBU eddy break-up
EDC eddy dissipation concept
IEM interaction by exchange with the mean
ILDM intrinsic low-dimensional manifold
LIF laser induced fluorescence
<table>
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<tr>
<td>pdf</td>
<td>probability density function</td>
</tr>
<tr>
<td>QUICK</td>
<td>quadratic upstream interpolation for convection kinematics</td>
</tr>
<tr>
<td>rms</td>
<td>root mean square</td>
</tr>
<tr>
<td>RSM</td>
<td>reynolds stress model</td>
</tr>
<tr>
<td>SIMPLE</td>
<td>semi-implicit method for pressure linked equations</td>
</tr>
<tr>
<td>TDMA</td>
<td>tri-diagonal matrix algorithm</td>
</tr>
<tr>
<td>TNF</td>
<td>turbulent non-premixed flame</td>
</tr>
<tr>
<td>UMIST</td>
<td>upstream monotonic interpolation for scalar transport</td>
</tr>
<tr>
<td>TVD</td>
<td>total variation diminishing</td>
</tr>
<tr>
<td>WSGG</td>
<td>weighted-sum-of-gray-gases</td>
</tr>
</tbody>
</table>
CHAPTER 1

Introduction

1.1 General introduction

There is a continuing demand for increased efficiency for gas turbines, furnaces, aero engines and other combustors and a conflicting concern over the problems related to environment pollution and noise. All these have, in the past few decades, resulted in a tremendous burst of interest and research activities in the field of combustion. The simultaneous occurrence of chemical reaction and transport of mass, momentum and energy makes analysis of these problems extremely difficult. Moreover, practical flames are mostly turbulent because of the requirement to produce a high volumetric rate of energy for efficiency and compactness. This complicates the combustion research further even if one addresses the problem at a simplified level in which practical difficulties might be neglected.

A major part of the energy consumed in domestic and industrial applications are produced from the turbulent combustion of gaseous fuel. One of the advantages of using gaseous fuel over the other fossil fuels, for example coal and oil, is that it burns relatively cleanly. Moreover, many countries have large reserves of natural gas. Because of these two factors, gaseous fuel has gained popularity as a source of energy in large scale thermal power plants. However, it is well understood that the reserves of natural gas are limited and it is also well recognised that some of the products of combustion have a negative impact on the environment. CO₂ is recognised as one of the contributors to the green house effects and NOₓ is one of the precursors of the acid rain. Detailed knowledge and a better understanding of different processes involved in the turbulent combustion are therefore essential for the dual purpose of increasing combustion efficiency and reducing pollutant emissions.
Recent advances in measurement techniques and the application of laser diagnostics systems (Dibble et al. 1987) to carefully conceived turbulent flames have greatly advanced the understanding of the finite rate chemistry effects in turbulent flames. Detailed measurements of turbulent flames have been reported, including the scatter plots of major and minor species for a number of fuels and burner configurations (Masri et al. 1990; Masri et al. 1988; Masri et al. 1994; Masri et al. 1996). Masri et al. (1994), Dally et al. (1996) and Dally et al. (1998) have provided extensive single point measurements of reactive and conserved scalars in a range of bluff body stabilised turbulent non-premixed flames. These measurements have revealed extensive and novel information about local structures of turbulent flames. Local extinction and bimodality of measured probability density functions of some reactive scalars are observed leading to blow-off of the flames (Masri et al. 1996). Masri et al. (1994) have shown that the finite rate chemistry effects are not important inside the recirculation zone even when the flame exhibit local extinction at the neck zone of the bluff body flame. Masri et al. (1996) have also shown that the flames are not strictly at equilibrium conditions even when the flame is far away from blow-off. The hydroxyl radical exists in super-equilibrium quantity and the temperature and mass fraction of major species also deviate, though slightly, from the equilibrium condition even at longer residence time. The presence of instantaneous concentrations of some species in excess of the steady laminar flamelet limits have also been reported (Masri et al. 1996). These findings have encouraged researchers to revisit such flows with both experimental and numerical investigations.

Research in the field of turbulent combustion is also driven by the demand for the development of adequate predictive tools for the design and analysis of practical combustion situations which are encountered in industrial applications. In the development of the modelling process, a number of simplifying assumptions are made in the representation of the physical and chemical processes. An essential part of the development of models is the validation of these assumptions. The validation is generally done by comparing the model calculations against the detailed experimental data. From the practical point of view, the experimental configuration used for validation purposes should be simple and well defined, so that the boundary conditions can be set without any ambiguity in the computation. The experimental configuration should also allow the use of the modern non-intrusive laser diagnostic techniques. These requirements make industrial combustors unsuitable for detailed validation studies. Simple jet flames, piloted jet flames and bluff body stabilised flames are generally used as benchmark cases for the
comparison of model predictions. One of the objectives of these validation studies is not only to identify the model that best matches the experimental data, since a model can give a right result for wrong reasons, but also to distinguish the differences in model calculations that result from applying different submodels (TNF 1996).

1.2 Modelling of turbulent combustion

The quantitative treatment of the turbulent combustion phenomenon, at first sight, seems to be straightforward. The governing transport equations are the well-known conservation equations of mass, momentum, energy, and species concentrations. The transport mechanism and the thermodynamic properties of the species involved in a typical combustion situation are well established. Furthermore, the detailed reaction mechanisms of the gaseous fuels involved in practical applications are proven to be reliable and accurate. Despite all these, the crucial problem lies in the solution of governing equations for the turbulent combustion under investigation. The physical processes of convection, diffusion, and reaction in turbulent flames involve a wide range of length and time scales. The computational efforts needed to resolve the length and time scales by the direct numerical solution method exceed, by a large margin, the capacity of present day computers for virtually all turbulent combustion situations of practical interest. The complete deterministic treatment of the governing equations for the practical combustion situation is not possible in the foreseeable future. However, this has been a major driving force behind many research efforts for the development of simplified yet physically realistic descriptions of turbulent combustion.

The present study focuses on the modelling of turbulent non-premixed combustion. In non-premixed combustion, the fuel and air are fed separately into the combustor where chemical reaction takes place. This is in contrast to the premixed flame, where fuel and air mix before reaching the combustion chamber. For safety reasons, combustion in most of the industrial furnaces and gas turbines are of the non-premixed type.

There are currently four main methods of turbulent combustion modelling approaches available for incorporation into CFD: (a) conserved scalar, (b) eddy break-up, (c) laminar flamelet (d) pdf transport/Monte-Carlo method. The last method is theoretically the most accurate and is capable of handling the reaction rate terms without any modelling assumptions. However, the pdf transport/Monte-Carlo model is very resource-intensive and the application of the model for the industrial calculations is
still not wide spread. The remaining three models are viable options for industrial applications. Other combustion modelling approaches available to the user include the conditional moment closure (CMC) and interaction by exchange with the mean (IEM) model, which are, however, not widely used in the practical situations.

The conserved scalar method is the simplest of all models and was first devised in the early 70's. The central assumption of the model is that, whenever fuel and oxygen exist at a point the chemical reaction will instantaneously proceed to completion in a single step reaction, producing combustion products (Elghobashi and Pun 1974; Elghobashi 1979). The ensuing simple chemical reaction system (SCRS) relates the thermo-chemical state of a flame with a conserved scalar, known as the mixture fraction through algebraic relations. The main problem of determining the chemical reaction rate is thus reduced to determining the mixing of the mixture fraction. The "brush" like thick reaction zone, often the concern in early research, was determined through incorporating the influence of turbulent fluctuations. Following the work of Spalding (1971a), who first demonstrated the incorporation of the calculations of turbulent fluctuations in a turbulent jet issuing into stagnant surroundings, the incorporation of the turbulent fluctuations into combustion modelling through a probability density function (pdf) was demonstrated by Elghobashi and Pun (1974), Elghobashi (1979), Lockwood and Naguib (1975). An alternative relation between the thermo-chemical state and the mixture fraction through chemical equilibrium formed the basis for determining the minor species CO and pollutants NO (Jones and Priddin 1978; Jones 1980). Though the equilibrium model was successful in predicting temperature and major species, it failed to predict the correct level of CO in hydrocarbon fuels. The equilibrium model also underpredicted the NO level by a wide margin. Jones (1980) speculated that the probability density function may be a source of errors, but according to him, a more widely accepted explanation is the equilibrium assumptions of atom O. The O atom can be a order of magnitude higher than the equilibrium values (Jones 1980). Despite the shortcomings, the conserved scalar model has been widely used for a number of applications: furnace and gas turbine simulations (Smith and Smoot 1981; Shyy et al. 1988; Nikjooy et al. 1988), finite element based combustion simulations (Kim and Chung 1987; Elkaim et al. 1993), three dimensional jet diffusion flames in a surface layer (Hernández et al. 1995), study of the effects of turbulence model on combustion (Gran et al. 1997), combustion including radiation heat transfer (Abbas et al. 1984; Ramamurthy et al. 1994) and the flow structure in bluff body flames (Dally et al. 1998) to mention a few.
In the eddy break-up (EBU) model, the problematic reaction rate term in turbulent combustion is modelled by considering the hydrodynamic features rather than the chemical kinetic features. The model was first formulated by Spalding (1971b) with some modifications later (Spalding 1976). However, the most popular of the eddy-break models is the one proposed by Magnussen and Hjertager (1976). In the eddy break-up model, the reaction rate of the fuel is given by the rate of dissipation of the eddies containing the species of fuel, oxidiser and the products. The eddy break-up model of Magnussen and Hjertager (1976) differs from the original model of Spalding (1971b) in relating the dissipation of the eddies to the mean concentrations instead of the concentration fluctuations. The EBU model has been shown to make reasonable predictions in a number of applications (Khalil et al. 1975; Magnussen and Hjertager 1976). In order to retain finite rate effects, Nikjooy et al. (1988) combined the eddy break-up expression with the Arrhenius type expression. Though the model looks promising, it lacks a sound theoretical foundation. An advanced eddy break-up model, commonly known as the eddy dissipation concept (EDC) model, treats the small scale eddies where the reaction takes place, as a perfectly stirred reactor (Gran 1994). This facilitates the incorporation of the finite rate effects in the combustion calculations. The importance of the finite rate effects in the EDC model is demonstrated by Gran and Magnussen (1996b). Their work shows that the fast chemistry EDC model is inferior to the conserved scalar model, but the finite rate EDC model improves the prediction considerably. The popularity of the EBU/EDC model lies in the fact that the model is simple and straightforward to implement. Bressloff et al. (1996) have shown an application of the EBU model where the combustion is treated with the simple EBU model while the complex issues of soot and radiation modelling are described in great detail.

The laminar flamelet model is a very powerful model which includes the finite rate chemistry effects in the turbulent non-premixed combustion calculations without increasing the computational load considerably. From the application point of view, the laminar flamelet model uses the same computational framework as the conserved scalar model. The instantaneous relationship between the mixture fraction and all the scalar variables, such as the species mass fractions and the temperature, is computed from the laminar diffusion flame. The realistic reaction mechanism and the transport of species can be included in the flamelet model as the flamelet profiles are calculated off-line. The mathematical background and the formulation of the laminar flamelet model can be found in Bray and Peters (1994), Peters (1984) and Peters (1986). The improvement
in prediction by the laminar flamelet model over the equilibrium model was first demonstrated by Liew et al. (1984). Their calculation successfully predicted the presence of $O_2$ at the axis of the fuel jet which results from non-equilibrium effects. However, the prediction of $CO$ was somewhat deteriorated. Drake et al. (1988) have shown that the flamelet model produces good predictions of temperature, mass fractions of $CO_2$, $CO$, $H_2O$ for a syngas jet flame. Their calculations have predicted the super-equilibrium OH level in the near field of the jet, but also predicted a rapid decay of OH towards equilibrium at the downstream location of the jet. Haworth et al. (1988) have shown that the history effect is important for the prediction of OH and using an equivalent steady strain rate to include the transient effect, they have predicted accurate levels of OH at the downstream location for the same syngas jet flame. The calculations of Lentini (1994) however contradict the findings of both Drake et al. (1988) and Haworth et al. (1988) for OH prediction. Lentini (1994) using the steady flamelet model has shown that the OH prediction in the upstream level is comparable to the predictions of Drake et al. (1988) and Haworth et al. (1988). More importantly, the prediction does not show a rapid decay towards the equilibrium level at the downstream location as observed by Drake et al. (1988). The laminar flamelet model is shown to be successful in predicting the complex chloromethane fuel combustion (Lentini and Puri 1995). The flamelet model has also been used for the prediction of a number of various practical issues such as NO formation (Sanders et al. 1997), soot (Brookes and Moss 1999), lift-off phenomenon (Sanders and Lamers 1994), partial premixing (Rogg et al. 1986) and transient effects (Pitsch et al. 1998) with varying degrees of success.

The pdf transport/Monte-Carlo model is the most promising combustion model for incorporating finite rate chemistry effects. The chemical reaction term is treated exactly without any modelling, but the model suffers from the modelling of the mixing term. The pdf transport/Monte-Carlo model is very resource-intensive. To minimise computational burden, often the reduced mechanism, ILDM mechanism, partial equilibrium and flamelet models are used to describe the thermo-chemical state instead of the full reaction mechanisms. A detailed description of the pdf transport/Monte-Carlo formulation can be found in Pope (1985) and Pope (1990). Because of the computational resources required, this model is still not viable for industrial applications.

The conditional moment closure (CMC) model developed by Bilger (1993) has shown good results for including finite-rate chemistry effects. The CMC model has been successful in predicting the emission of NO (Smith et al. 1992; Barlow et al.
An assessment of the flamelet and CMC models against direct numerical simulation (DNS) data has shown the superiority of the CMC model (Swaminathan and Bilger 1999). Borghi’s group (Obounou et al. 1994) have developed a finite rate chemistry model where diffusion is modelled by using the interaction by exchange with the mean (IEM) and the reaction rate term includes a time delay which is compared with a mixing time scale. The IEM model has been successful in a number of applications including the prediction of the scaling behaviour of NO (Schlatter et al. 1996). These new modelling approaches are still in their early stages of development and have not yet gained popularity.

1.3 Objectives of this study

The objectives of the thesis are three fold; the first objective is to evaluate the performance of the non-premixed turbulent combustion models for predicting bluff body flames. The second objective is to assess the predictive capabilities of a flamelet based NO model and the final objective is to present a flamelet based radiation modelling strategy.

The use of modern laser based diagnostic systems for combustion measurements has resulted in a number of well documented experimental data available through the world wide web which are suitable as bench mark problems (Masri 1997; Barlow and Frank 1997; Hassel 1997). This in turn resulted in renewed interest in the validation studies of combustion models. The International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames (TNF) are solely dedicated to different issues related to combustion modelling with special emphasis on the turbulence-chemistry interaction. The comparison of the combustion model calculations with a set of well documented experimental data made available through the simultaneous applications of Raman scattering, Rayleigh scattering and laser induced fluorescence (LIF) is essential in identifying the strengths or weaknesses of the combustion models under different situations. Validation studies are also necessary for further development of combustion models. In this regard it is important to isolate different submodels that are involved with the overall combustion calculations. To accomplish this, it is necessary to understand the differences in model predictions that result from using different combustion models, different fluid dynamics models, different model constants, different numerical schemes, different thermo-fluid properties and different radiation models. The empha-
sis of the present study is not only to identify a suitable model that fares well under different conditions but also to identify the influences of different submodels.

The combustion models evaluated here are the conserved scalar with flame sheet and equilibrium chemistry, eddy break-up and laminar flamelet models. The first three combustion models are based on fast chemistry assumption, while the last one is a non-equilibrium model. All the combustion models are assessed using the same turbulence model, numerical schemes, boundary conditions and CFD code, allowing a more direct comparison of the models for turbulence-chemistry interaction. Furthermore, the turbulence model constants are adjusted to achieve a better agreement of the flow field. This strategy is adopted in recognition of the well known fact that the turbulence model is not universal and that fine tuning is necessary to account for differences in flow geometries and situations. This strategy is consistent with the objective of the study, which is to compare the submodels of turbulence-combustion interaction, rather than to test the true predictive accuracy of the turbulence model. With regard to this approach, the work reported here is closely aligned with the TNF workshop. The experimental data and some of the submodels are taken from the TNF workshop web site (TNF 1996).

The good predictions of temperature and major species are no longer sufficient, the combustion model should also be able to predict minor species, radicals and emissions of pollutants. The growing concerns about environmental pollution and the strict regulations regarding pollutant emissions make it necessary to find a suitable predictive tool for emissions calculation. The prediction of NO poses the most stringent test of the combustion models because the NO production rate is very sensitive to the accurate prediction of temperature and concentration of O. In this regard, it is also important to study the influence of radiation heat transfer on the temperature and minor species. With this objective in view, the flamelet based NO prediction and the flamelet based radiation modelling study are undertaken.

The configuration selected in this study is a bluff body combustor. The reason behind this selection is that the flow in a bluff body bears great similarity to practical combustors used in industrial applications. The bluff body is therefore a suitable compromise as a model problem because the burner, with its one or two recirculation zones, has some of the complications of industrial furnaces, while retaining the relatively simple and well-defined initial and boundary conditions. The bluff body combustor also provides a controlled environment for the study of turbulence-chemistry interaction.
1.4 Outline of the thesis

The mathematical formulations of different physical and chemical processes are described in chapter 2. This chapter starts with a brief description of the governing equations of mass, momentum, energy and species. The time averaged form of the differential equations are given and a brief description of the turbulence and combustion models is provided. Chapter 3 describes the methods for solving the governing differential equations and for implementing the combustion models in a general CFD algorithm. Chapter 4 is devoted to the description of generation of the flamelet library using different methods. The flamelet libraries for different fuels used in the study are also given.

The results of the numerical study of the bluff body flames are discussed in chapters 5 and 6. The results obtained by using different combustion models are compared to one another and to the available experimental data in these chapters. These chapters also give general discussions on the structure of the flames and different aspects of turbulent-chemistry interaction. The flamelet based NO modelling is described in chapter 7. Chapter 8 presents a flamelet based radiation modelling technique. The thesis is closed with a discussion of the main conclusions of the present work in chapter 9.
This chapter presents a brief description of the mathematical models for the solution of turbulent non-premixed combustion problem. The mathematical models incorporate a number of assumptions about the physical and chemical processes to keep the problem in a tractable form. Despite the simplifications, a complete set of mathematical formulation should provide the relevant quantities in turbulent flames at different points in space and time with sufficient accuracy. The main focus of this chapter is to present the mathematical tools that describe the interaction between the turbulence and chemistry by employing different thermo-chemical descriptions.

First, the general transport equations of mass, momentum, energy and species concentrations are introduced and the difficulties associated with the solution of the equations for turbulent reacting flows are described. The averaging concept for variable density flows are discussed and the time-averaged transport equations are presented. Finally, the modelling approaches for the turbulence as well as the combustion models utilised in the present study are described.

2.1 Transport equations

The starting point for any analysis of turbulent reacting flows is the conservation equations of fluid mechanics. These equations are well established and are given in many fluid mechanics texts. In addition to these equations, the species conservation equations are required which are considered in details in combustion texts (Kuo 1986; Warnatz et al. 1996a). Here only a brief description of these governing equations is stated.

The governing equations describing the flow of fluid can be derived from the conservation of mass, momentum and energy. These equations are written below using the Cartesian tensor notation:
Chapter 2. Mathematical Models

Continuity:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 \] (2.1)

Momentum:

\[ \rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\tau_{ij}}{\partial x_j} + \rho g_i \] (2.2)

where \( \tau_{ij} \) is the viscous stress tensor defined by:

\[ \tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \rho}{\partial x_k} \right) \] (2.3)

and where \( p \) is the pressure, \( \mu \) is the mixture viscosity, \( \delta_{ij} \) is the Kronecker delta and \( g_i \) is the gravitational acceleration vector.

Energy:

\[ \rho \frac{\partial h}{\partial t} + \rho u_j \frac{\partial h}{\partial x_j} = \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i} \left( \mu \frac{\partial h}{\partial x_i} + \mu \left( \frac{1}{Sc} - \frac{1}{\sigma} \right) \sum_{\alpha=1}^{N} h_{\alpha} \frac{\partial Y_{\alpha}}{\partial x_i} \right) \] (2.4)

where \( h \) is the specific mixture enthalpy, \( Y_{\alpha} \) is the mass fraction, \( Sc \) and \( \sigma \) are the Schmidt and Prandtl numbers of the mixture respectively. Low Mach number flows (\( Ma << 1 \)) are considered and as a consequence the terms associated with the kinetic energy of the mixture and the viscous dissipation rate are neglected. Fourier's and Fick's laws of molecular fluxes are employed. The term \( \frac{\partial p}{\partial x_i} \) is negligible in many practically occurring situations, e.g. jets, gas turbines and furnaces (Jones and Kakhi 1996). The Lewis number, defined as the ratio of the Schmidt and Prandtl numbers are close to unity for combusting flows. The assumption of unity Lewis number leads to the simplification of the energy equation to:

\[ \rho \frac{\partial h}{\partial t} + \rho u_j \frac{\partial h}{\partial x_j} = \frac{\partial}{\partial x_i} \left( \mu \frac{\partial h}{\partial x_i} \right) \] (2.5)

and the species conservation to:

\[ \rho \frac{\partial Y_{\alpha}}{\partial t} + \rho u_j \frac{\partial Y_{\alpha}}{\partial x_j} = -\frac{\partial J_{\alpha}}{\partial x_i} + \omega_{\alpha} \quad \text{for} \quad \alpha = 1, \ldots, N \] (2.6)

where \( \omega_{\alpha} \) is the net rate of formation of species \( \alpha \) per unit volume. \( J_{i,\alpha} \) is the mass
molecular flux of species $\alpha$. In combusting flows many species with widely disparate molecular weights participate with the consequence that the proper treatment of the molecular fluxes involves the full array of diffusion coefficients characterising the diffusion of species $\alpha$ into a mixture involving species $i, i = 1, 2, \ldots, N$ (Libby and Williams 1994). However, when Eq. (2.6) is applied for turbulent flows, the complete treatment of the molecular diffusion flux is less important and Fick’s law of diffusion, $J_i, \alpha = -D_\alpha \frac{\partial \rho \alpha}{\partial x_i}$ is used to represent the molecular diffusion flux.

To obtain the chemical source term, a system involving $N$ chemical species and $R$ reaction steps is considered, of the form (Libby and Williams 1994):

$$
\sum_{\alpha=1}^{N} v'_{\alpha \beta} M_\alpha = \sum_{\alpha=1}^{N} v''_{\alpha \beta} M_\alpha \quad \beta = 1, \ldots, R
$$

(2.7)

where $M_\alpha$ is the chemical symbol of species $\alpha$, $v'_{\alpha \beta}$ and $v''_{\alpha \beta}$ are the stoichiometric coefficients of species $\alpha$ in the reaction step $\beta$. The chemical source term $\omega_\alpha$ is the net result of the construction and destruction of species $\alpha$ due to each reaction step $\beta$, i.e.

$$
\omega_\alpha = \sum_{\beta=1}^{R} \omega_{\alpha \beta}
$$

(2.8)

where $\omega_{\alpha \beta} = 0$, if species $\alpha$ does not participate in the reaction step $\beta$. In any particular reaction step, the rate of formation of species $\alpha$, is the net rate of formation of $\alpha$ due to forward and backward reaction steps in reaction $\beta$:

$$
\omega_{\alpha \beta} = W_\alpha \left(v''_{\alpha \beta} - v'_{\alpha \beta}\right) \left(k_{f_{\beta}} p_{m_{\beta}} \prod_{\alpha=1}^{N} \left(\frac{Y_\alpha}{W_\alpha}\right)^{v'_{\alpha \beta}} - k_{b_{\beta}} p_{l_{\beta}} \prod_{\alpha=1}^{N} \left(\frac{Y_\alpha}{W_\alpha}\right)^{v''_{\alpha \beta}}\right)
$$

(2.9)

where $m_{\beta} = \sum_{i=1}^{N} v'_{\alpha \beta}$ and $l_{\beta} = \sum_{i=1}^{N} v''_{\alpha \beta}$ are the orders of the forward and backward reactions respectively. $k_{f_{\beta}}$ and $k_{b_{\beta}}$ are the rate constants of the forward and backward reactions. The rate constants are expressed as:

$$
k_{f_{\beta}} = B_\beta T^{m_{\beta}} a_\beta \exp \left(-\frac{E_\beta}{RT}\right)
$$

(2.10)

where $B_\beta$ is the pre-exponential factor, $a_\beta$ is a constant exponent, $E_\beta$ is the activation energy and $R$ is the universal gas constant.

Combustion influences the flow field through density and the equation of state for ideal gases is used to express density:
The equations described so far constitute a closed set of equations and in principle they can be solved numerically with appropriate initial and boundary conditions. However, the direct numerical simulation (DNS) requires large computer memory and cpu time to resolve very small spatial and time scales. For example, the number of grid points needed in the DNS is proportional to $Re_t^{3/4}$, where $Re_t$ is the turbulence Reynolds number, for three dimensional inert mixing layer flows (Libby and Williams 1994). The extension of the techniques of DNS to reacting turbulent flows is in the early stages of development (Libby and Williams 1994). The traditional approach for treating high Reynolds number turbulent flows has been to average the conservation equations with the consequence that all fine details of the flow do not require spatial and temporal resolution.

### 2.2 Time averaged equations

As explained in the previous section, the governing equations are averaged to treat turbulent flows. The standard practice is to decompose the instantaneous equations into their mean and fluctuating parts and then to average them. Different types of averaging can be applied, but it is now widely accepted that Favre-averaging, i.e. mass weighted averaging is the convenient means for obtaining the governing equations for turbulent flows with significant density variations. With Favre-averaging the velocity and scalars (but not density and pressure) are decomposed according to $u_i = \bar{u}_i + u''_i$ and $\phi_\alpha = \bar{\phi}_\alpha + \phi''_\alpha$. In Favre-averaging, $\bar{\rho}u''_i = \bar{\rho}\phi''_\alpha = 0$, whereas for Reynolds averaging, $u_i = \bar{u}_i + u'_i$ and $\phi_\alpha = \bar{\phi}_\alpha + \phi'_\alpha$ and where $\bar{u}_i = \bar{\phi}_\alpha = 0$. The Favre-averaging results in conservation equations that do not include terms involving density fluctuations. Therefore, the resultant equations are easier to interpret and model than their Reynolds averaged counterpart.

Applying Favre averaging to Eqs. (2.1), (2.2), (2.5) and (2.6) leads to the following conservation equations:

\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j}{\partial x_j} = 0
\]  

(2.12)
\[
\frac{\partial}{\partial t} (\bar{p} \bar{u}_i) + \frac{\partial}{\partial x_j} (\bar{p} \bar{u}_j \bar{u}_i) = - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \bar{p} \bar{u}_j' \bar{u}_i' \right) + \bar{p}g_i \tag{2.13}
\]

\[
\frac{\partial}{\partial t} (\bar{p} \bar{h}) + \frac{\partial}{\partial x_j} (\bar{p} \bar{u}_j \bar{h}) = \frac{\partial}{\partial x_i} \left( \bar{p} \bar{u}_i'' h'' \right) \tag{2.14}
\]

\[
\frac{\partial}{\partial t} (\bar{p} \gamma_{\alpha}) + \frac{\partial}{\partial x_j} (\bar{p} \bar{u}_j \gamma_{\alpha}) = \frac{\partial}{\partial x_i} \left( \bar{p} \bar{u}_i'' \gamma_{\alpha}'' \right) + \overline{\omega}_{\alpha} \quad \text{for} \quad \alpha = 1, \ldots, N \tag{2.15}
\]

These equations are written for high Reynolds numbers, so that the averaged molecular fluxes are neglected in comparison to the turbulent fluxes \( \bar{p} \bar{u}_j' \bar{u}_i' \) (Reynolds stress) and \( \bar{p} \bar{u}_j'' \phi_{\alpha}'' \) (scalar flux). These equations have identical form to the equations of constant density flows. The unknown terms in the above equations are the Reynolds stress, scalar flux, density and mean reaction rate. The first two unknowns are calculated from the turbulence model, while combustion models are required to calculate the last two unknowns.

### 2.3 Turbulence model

Several models have been proposed to model Reynolds stress. Among these, the relatively simple \( k - \varepsilon \) model has been widely used for turbulent combustion calculations (Brookes and Moss 1999; Biagioli 1997; Sanders and Lamers 1994; Liew et al. 1984; Lentini 1994). The \( k - \varepsilon \) model has shown a number of shortcomings, such as its inability to correctly represent the anisotropy of the Reynolds stresses and its overprediction of the spreading rate of jet and bluff body flows (Dally et al. 1998). Many of these shortcomings are eliminated in higher order closure formulations such as second moment closure and Reynolds-stress closure. Over the last few years, several second moment closure models have been developed and applied in a number of turbulent combusting flows (Jones 1994). However, the simple \( k - \varepsilon \) model can capture the characteristics of flow fields of bluff body flames reasonably accurately (Dally et al. 1998). The present study focuses at the prediction of the thermo-chemistry in bluff body flames by different chemistry models. For that purpose, the \( k - \varepsilon \) description is sufficient.

Most of the work in turbulence modelling is based on constant density flows (Jones and Whitelaw 1982). The modelling of inert turbulent flows is significantly complex.
without the inclusion of the variable density contributions introduced by combustion. In turbulent combustion, large density fluctuations arise and must be accounted for in the modelling. The common approach for modelling variable density flows is to recast the Reynolds averaged model in terms of Favre-averaged quantities with the assumption that the density variations are accounted for by averaging. The extension of the constant density $k - \varepsilon$ model for variable density flows is described in Kuo (1986) and Jones and Whitelaw (1982). The starting point for modelling the Reynolds stress is the eddy viscosity model:

$$\bar{\rho}u_i'u_j' = -\mu_t \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) + \frac{2}{3} \bar{\rho} \bar{k} \delta_{ij} + \frac{2}{3} \mu_t \bar{u}_i \delta_{ij} \quad (2.16)$$

The turbulent viscosity $\mu_t$ is assumed to be proportional to the product of a turbulent velocity scale and a length scale. In the $k - \varepsilon$ model, these velocity and length scales are obtained from two parameters, the turbulent kinetic energy, $k$, and the dissipation rate of turbulent kinetic energy, $\varepsilon$. The velocity scale is taken to be $\sqrt{k}$ and the length scale is taken to be $\sqrt{\varepsilon}$. Thus, the eddy viscosity $\mu_t$ is given by:

$$\mu_t = \bar{\rho} C_{\mu} \frac{k^2}{\varepsilon} \quad (2.17)$$

where $C_{\mu}$ is a proportionality constant. The modelled equations for the turbulent kinetic energy and energy dissipation rate are given by:

$$\frac{\partial}{\partial x_j} (\bar{\rho} \bar{k}) = \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{\sigma_k} \frac{\partial \bar{k}}{\partial x_j} \right) + G - \bar{\rho} \bar{\varepsilon} \quad (2.18)$$

and

$$\frac{\partial}{\partial x_j} (\bar{\rho} \bar{\varepsilon}) = \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{\sigma_\varepsilon} \frac{\partial \bar{\varepsilon}}{\partial x_j} \right) + C_{\varepsilon_1} \frac{\varepsilon}{k} G - C_{\varepsilon_2} \bar{\rho} \frac{\varepsilon^2}{k} \quad (2.19)$$

where $C_{\varepsilon_1}, C_{\varepsilon_2}$ are the empirical constants and $\sigma_k$ and $\sigma_\varepsilon$ are the Prandtl numbers governing the turbulent diffusion of $k$ and $\varepsilon$, $G$ is the rate of production of turbulent kinetic energy:

$$G = \mu_t \left( \frac{\partial \bar{u}_j}{\partial x_i} + \frac{\partial \bar{u}_i}{\partial x_j} \right) \frac{\partial \bar{u}_i}{\partial x_i} \quad (2.20)$$

The constants are calibrated in simple (constant density) flows, such as decaying grid turbulence ($\Rightarrow C_{\varepsilon_2}$), near wall flows (assuming production=dissipation and $u'v'/k \approx$
constant \( \rightarrow C_{e1}, C_{\mu} \). The constants are assigned values with computer optimisation so that the widest range of flows possible can be predicted. The following values are recommended: \( C_{\mu} = 0.9; C_{e1} = 1.44; C_{e2} = 1.92; \sigma_{k} = 1.0; \sigma_{e} = 1.3 \). For free flows \( \sigma_{f} = 0.7 \) and near wall flows \( \sigma_{f} = 0.9 \) (Libby 1996).

The standard \( k - \varepsilon \) model does not produce the correct spreading rate of a single axisymmetric jet issuing into a co-flowing or stagnant environment. Several empirical modifications of the model constants have been proposed to remedy this shortcoming (McGuirk and Rodi 1979; Pope 1978; Thies and Tam 1996). The overprediction of the spreading rate is also observed for the case of bluff body flames (Gran and Magnussen 1996a; Correa and Gulati 1992; Gran et al. 1997). The modifications similar to those for the jet flow and also a simple modification in the value of \( C_{e1} \), i.e. \( C_{e1} = 1.60 \) have been implemented for a bluff body flame (Dally et al. 1998). Dally et al. (1998) have shown that the simple modification of \( C_{e1} \) is sufficient to produce a good prediction of the spreading rate of the jet of the bluff body flow. The value of \( C_{e1} \) has been adjusted from 1.44 to 1.60 and has been implemented as standard for the bluff body target flame in the third TNF workshop (TNF3 1998).

### 2.4 Combustion models for non-premixed combustion

The averaging of the species concentration equation leads to the mean reaction rate term (see Eq. 2.15). Direct closure of the mean reaction rate term through Taylor series expansion is not feasible for highly exothermic combustion reactions (Williams 1985). No suitable deterministic method is available to date to determine the mean reaction rate term. However, a number of combustion models are available, which do not require the specification of the mean reaction rate. These models reduce the turbulent reacting flow problem to a tractable form by introducing a single scalar that characterises the thermo-chemistry of the reacting mixture.

#### 2.4.1 Conserved scalar models

In conserved scalar models of non-premixed combustion, the instantaneous thermo-chemical state of the mixture is determined by a single conserved scalar. Detailed formulation and the analysis of the conserved scalar model can be found in many texts,
e.g. Kuo (1986), Williams (1985) and more recently in Warnatz et al. (1996a). With the assumptions of equal diffusivity, unity Lewis number and adiabatic combustion, all the conserved scalars (elemental mass fractions and enthalpy) can be related to a single normalised conserved scalar, the mixture fraction. Thermo-chemical models are then required to specify the relationship between the mixture fraction and the scalar variables (temperature, species concentrations). These models are based on the "fast" chemical reaction, e.g. the time required to complete reaction is much shorter than the convection and diffusion time in the turbulent flame. A brief description of the conserved scalar models is given in following sections.

**Flame sheet model**

This is the simplest reaction scheme which assumes that the reaction takes place in a thin flame sheet at an infinitely fast rate. The flame sheet is located at the stoichiometric mixture fraction. Outside the flame sheet, inert mixing between the reactants and the products takes place. The model calculates the species concentrations and temperature from algebraic equations based on the reaction stoichiometry, without any information of reaction rate or equilibrium condition. The species concentrations and temperature are calculated from (Lockwood and Naguib 1975; Chung 1993):

\[ 0 \leq Z \leq Z_{st} \quad Y_{fu} = 0.0 \quad Y_{ox} = Y_{ox,A} \frac{Z_{st} - Z}{Z_{st}} \quad (2.21) \]

\[ Z_{st} \leq Z \leq 1.0 \quad Y_{ox} = 0.0 \quad Y_{fu} = Y_{fu,F} \frac{Z - Z_{st}}{Z_{st}} \quad (2.22) \]

where, the mixture fraction is defined as:

\[ Z = \frac{(sY_{fu} - Y_{ox}) + Y_{ox,A}}{sY_{fu,F} + Y_{ox,A}} \quad (2.23) \]

and the stoichiometric mixture fraction as:

\[ Z_{st} = \frac{Y_{ox,A}}{sY_{fu,F} + Y_{ox,A}} \quad (2.24) \]

Here, \( Y_{fu} \) and \( Y_{ox} \) denote the mass fraction of fuel and oxidiser respectively; \( s \) is the stoichiometric oxygen required to burn 1 kg of fuel and the subscripts A and F denote the air and fuel stream respectively.
The mass fraction of the product can be obtained from the conservation of mass as:

\[ Y_{pr} = 1.0 - (Y_{ox} + Y_{fu}) \]  

(2.25)

For adiabatic combustion, the enthalpy is also a conserved scalar and with the assumption of unity Lewis number, the instantaneous enthalpy and thermo-chemical properties are related to the instantaneous mixture fraction according to the relations:

\[ h(Z) = Z h_p + (1 - Z) h_A \]  

(2.26)

\[ \int_0^T C_p \, dT = h(Z) - Y_{fu} H_{fu} \]  

(2.27)

\[ C_p(Z) = \sum_{\alpha} Y_{\alpha}(Z) C_{p\alpha}(Z) \]  

(2.28)

\[ \rho(Z) = \frac{P W(Z)}{R T(Z)} \]  

(2.29)

\[ \frac{1}{W(Z)} = \frac{Y_{fu}(Z)}{W_{fu}} + \frac{Y_{ox}(Z)}{W_{ox}} + \frac{Y_{pr}(Z)}{W_{pr}} \]  

(2.30)

where, \( H_{fu} \) is the heating value of fuel, \( C_p \) is the specific heat and \( W \) is the molecular weight and \( R \) is the universal gas constant.

An obvious shortcoming of the flame sheet model is that it does not calculate intermediates, minor species and radicals. In many applications, it is desirable to have an insight into the behaviour of these species. Moreover, the absence of these radicals in the mixture can give a substantial underestimation of the specific heat, which consequently leads to an overprediction of the temperature.

The flame sheet model was developed in the early 70's. Some of the earlier work can be found in Elghobashi and Pun (1974), Lockwood et al. (1974) and Elghobashi (1979). Because of its simplicity, the flame sheet model is still being used in combustion calculations (Dally et al. 1998; Chung 1993). In applications where only the mean flame structure, temperature and major species are required without precise accuracy, this model is a good choice as the model is very simple and subsequently, required computational resources are small.
Equilibrium model

In the equilibrium chemistry model, the gas mixture is assumed to be at chemical equilibrium at every location and time in the flame. The equilibrium composition and temperature of the flame are calculated as a function of mixture fraction based on the minimisation of Gibbs free energy (Kuo 1986; Wamatz et al. 1996a). An important advantage of the chemical equilibrium model is that it can provide information about the minor species and radicals without a detailed knowledge of the reaction kinetics.

The chemical equilibrium model is valid only if the characteristic Damköhler numbers are much larger than unity, e.g. the reaction processes are much faster than the convection and diffusion processes of the flow. However, in many practical and laboratory flames, only part of the reaction processes are fast enough to reach chemical equilibrium. The slower, lower Damköhler number reactions interact with the convection and diffusion processes of the flows. Such finite rate chemistry effects lead to the abundance of the species involved. The mass fraction of these species can not be adequately represented by the equilibrium model. A well known example of this is provided by the super-equilibrium concentrations of OH radicals found in the upstream part of turbulent flames (Drake et al. 1984; Masri et al. 1996; Barlow et al. 1990). Here, the consumption of OH is governed by three body recombination reactions which are relatively slow and do not reach the equilibrium condition in the upstream part of flames where intense mixing occurs. The resultant balance of production, consumption, convection and diffusion is such that the OH level can be in excess of the equilibrium level by a factor of 5.

Constrained equilibrium model

The chemical equilibrium approach has been widely used and reasonable temperature and major species concentrations can be obtained. The major shortcoming of the equilibrium model is related to its prediction of unrealistically high level of CO in the fuel rich mixture of hydrocarbon flames (Jones 1980). The constrained equilibrium model is an empirical modification to the equilibrium model to reproduce the realistic level of CO in the fuel rich mixture. The model is based on the idea that reactions in hydrocarbon flames occur primarily in a small zone around the stoichiometric mixture fraction. Outside this zone, if the temperature is too low or the mixture is too rich or lean, the fuel will not burn.
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In the present study, the commercial CFD code FLUENT is used to obtain constrained equilibrium concentrations for the hydrocarbon fuel. In the calculation, the equilibrium condition is applied for mixture leaner than the rich flammability limit, for mixture richer than the rich flammability limit the flame is extinguished and the unburned fuel mixes with the equilibrium composition at the rich flammability limit.

An alternative constrained equilibrium model is also available (Bilger and Ståner 1983) where the thermochemistry is described by a reaction zone at the stoichiometric mixture fraction and a by a fuel breakup/pyrolysis sheet at a slightly higher mixture fraction. A portion of the hydrocarbon fuel breaks up into intermediate hydrocarbons in a one-step, irreversible and infinitely fast reaction at the fuel breakup/pyrolysis sheet. These intermediates are considered to be consumed at the stoichiometric mixture fraction surface. The concentration of other species are computed from the equilibrium approximation taking into account the constraints for the fuel and the intermediate species.

The presumed shape pdf method

The nonlinearity of the instantaneous relationship between the mixture fraction and the scalar variables, \( \phi(Z) \), implies that the mean scalar variables in a turbulent field can not be obtained from \( \bar{\phi} = \phi(\bar{Z}) \). The mean scalar variables in a turbulent field are thus obtained by introducing a probability density function \( P(Z) \) (Jones and Whitelaw 1982):

\[
\bar{\phi} = \int_0^1 \phi(Z)P(Z)dZ
\] (2.31)

The shape of the probability density function is presumed and is given in terms of the mean, \( \bar{Z} \), and variance, \( \bar{Z}'' \), of the mixture fraction. The values of the mean and variance of mixture fraction are obtained from their respective modelled transport equations:

\[
\frac{\partial}{\partial x_j} (\bar{\rho}u_j \bar{Z}) = \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{\sigma_t} \frac{\partial \bar{Z}}{\partial x_j} \right) \tag{2.32}
\]

\[
\frac{\partial}{\partial x_j} (\bar{\rho}u_j \bar{Z}''^2) = \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{\sigma_t} \frac{\partial \bar{Z}''^2}{\partial x_j} \right) + C_{g1} \mu_t \left( \frac{\partial \bar{Z}''^2}{\partial x_j} \right)^2 - C_{g2} \frac{\bar{\epsilon}}{k} \bar{Z}''^2 \tag{2.33}
\]

where \( C_{g1} \) and \( C_{g2} \) are model constants with values of 2.0 and 2.8 respectively. The
common types of assumed pdf shape used in combustion calculations are the double delta pdf (Khalil et al. 1975), clipped Gaussian distribution (Lockwood and Naguib 1975) and beta pdf (Jones and Priddin 1978). In a comparative study of the above pdf functions, Jones (1980) have shown that the double delta function gives unrealistic double peak values in the radial temperature profiles. Both the clipped Gaussian and beta pdfs have produced similar results and accurately predicted temperature and species mass fraction profiles. The implementation of the clipped Gaussian function requires an iterative procedure. The beta pdf does not require arbitrary clipping in order to satisfy the bounds of the mixture fraction as with the clipped Gaussian pdf and the implementation is particularly straightforward. Hence the beta pdf is utilised in the present study.

2.4.2 Laminar flamelet model

The laminar flamelet model views the turbulent flame as an ensemble of laminar locally one dimensional structures embedded within the turbulent flow fields (Bray and Peters 1994). The theoretical background of the laminar flamelet concept can be found in Liew et al. (1984), Peters (1984), Peters (1986) and more recently in Bray and Peters (1994) and Lentini (1994) and the references therein. The laminar flamelet model has been presented as a non-equilibrium version of the classical Burke-Schumann limit (Bray and Peters 1994). The approach is based on the notion that, if the chemical time scales are much shorter than the characteristic turbulence time scales, reaction takes place in locally thin one dimensional structures. These structures are assumed to be the same as available in a laminar flame. In non-premixed turbulent combustion, the reaction zone is attached to the high temperature region close to stoichiometric mixture and advected and diffused with the mixture fraction field (Bray and Peters 1994). Consequently, the flame fronts encountered in the non-premixed flames have no intrinsic, flow field dependent length scale; the flame thickness is determined solely by the mixture fraction field. Based on these observations, Bray and Peters (1994) and Peters (1991) have introduced a phase diagram for the regimes of non-premixed turbulent combustion using two parameters. The first parameter is the Damköhler number and the second one is the mixture fraction fluctuations around the flame front. The separated flamelets exist when the turbulent fluctuations of mixture fraction are higher than the flame thickness in the mixture fraction space; otherwise connected reaction zones exist. The flamelet
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regime is observed when the value of the Damkohler number is greater than one and the mixture fraction variance along the flame front is greater than the flame thickness in the mixture fraction space. Figure 2.1 shows regimes of turbulent non-premixed combustion and variation of local conditions in a typical non-premixed turbulent jet flame according to Bray and Peters (1994).

As stated earlier, the laminar flamelet model is presented as a non-equilibrium model. The scalar dissipation rate is identified as a characteristic quantity to describe the departure from chemical equilibrium (Bray and Peters 1994). Based on an asymptotic analysis of a flamelet structure for quasi-steady unity Lewis number flames, Bray and Peters (1994) have concluded that the scalar dissipation rate should account for non-equilibrium effects caused by both convection and diffusion (Bray and Peters 1994). Some other effects, such as rapid unsteady changes, large local differences between convection and diffusion time scales, flamelet curvature, strong variations of the scalar dissipation within the flamelet structure require more detailed analysis.

As mentioned above, the thermo-chemical state in the turbulent non-premixed flame is represented by an ensemble of laminar diffusion flamelets. Most of the studies use a counter flow diffusion flame for obtaining laminar flame data, conveniently known as flamelet library. Alternatively, flamelet equations on the conserved scalar space can be

![Figure 2.1: Regimes of non-premixed turbulent combustion with local conditions in a typical turbulent non-premixed flame](image-url)
used to generate flamelet library (Lentini 1994; Mauss et al. 1990). In the present study, both methods are used. A brief description of both methods for generating flamelet library is presented in the following subsections.

Method 1: Generation of flamelet library by Counter flow diffusion flame (Tsuji burner)

The counterflow diffusion flame consists of a laminar fuel flow issuing from a porous cylinder of radius \( R \) and a laminar air stream in the opposed direction as shown in Fig. 2.2. A stable reaction zone is established in the forward stagnation region of the cylinder. The fuel and oxidiser diffuse toward the reaction zone with velocities proportional to the concentration gradients. There is a strong coupling between the fluid mechanics (fuel–air mixing rate) and chemical kinetics (reaction rates) leading to the reaction zone structures which are strong functions of the velocity gradients.

The flow in the stagnation region is given by (Drake and Blint 1988; Peters 1984):

\[
    u = ax \tag{2.34}
\]

\[
    v = -ay \tag{2.35}
\]
where $x$ and $y$ are the coordinates parallel and perpendicular to the burner surface respectively, $u$ and $v$ are the corresponding velocity components and $a$ is the velocity gradient. Dimensionless velocities $f'$ and $V$ together with a density weighted $y$ coordinate are often introduced where:

$$f' = \frac{u}{u_e} \quad (2.36)$$

$$V = \frac{\rho v}{\sqrt{\rho u_e a}} \quad (2.37)$$

and non-dimensional distance $\eta$ may be expressed as:

$$\eta = \sqrt{\frac{a}{\rho u_e c_p}} \int_0^1 \rho dy \quad (2.38)$$

Since there is no tangential fuel velocity, $f' = 0$ at the burner wall. Since $u \rightarrow u_e$ as $y \rightarrow \infty$, $f' = 1$ in the air stream. Along the stagnation point streamline direction ($x = 0$), the following differential equations apply:

**Continuity:**

$$f' + \frac{dV}{d\eta} = 0 \quad (2.39)$$

**Momentum:**

$$(f')^2 + V \frac{dV}{d\eta} - \frac{\rho}{\rho_e} = \frac{d}{d\eta} \left( C \frac{df'}{d\eta} \right) \quad (2.40)$$

where

$$C = \frac{\rho \mu}{\rho_e u_e} \quad (2.41)$$

**Species:**

$$V \frac{dY_\alpha}{d\eta} - \frac{\omega_\alpha W_\alpha}{\rho} + \frac{1}{\sqrt{\rho u_e c_p} \ \rho \ c_p} \frac{d}{d\eta} (\rho Y_\alpha V \eta) = 0 \quad \text{for} \quad \alpha = 1, \ldots, N \quad (2.42)$$

**Energy:**

$$V \frac{dT}{d\eta} = \frac{1}{\sqrt{\rho u_e c_p} \ \rho \ c_p} \frac{d}{d\eta} (\rho \frac{dT}{d\eta}) - \frac{1}{c_p \sqrt{\rho u_e c_p}} \sum_{\alpha=1}^{N} \rho Y_\alpha V \eta c_p \alpha \frac{dT}{d\eta} - \frac{1}{\rho a c_p} \sum_{\alpha=1}^{N} \omega_\alpha W_\alpha h_\alpha \quad (2.43)$$

In these equations, $Y_\alpha$ and $W_\alpha$ are the mass fraction and molecular weight of species $\alpha$, and $T$, $c_p$ and $\rho$ are the temperature, specific heat and density of the mixture. $v_{\alpha \eta}$ is
the diffusion co-efficient of the $\alpha$-th species in the $\eta$ direction. The thermal diffusion is neglected in the calculation. The chemical production rate of the $\alpha$-th species per unit volume, $\dot{\omega}_\alpha$, is calculated from:

$$\dot{\omega}_\alpha = \sum_{\beta=1}^{R} \omega_{\alpha\beta}$$  \hspace{1cm} (2.44)

where $\omega_{\alpha\beta}$ is the reaction rate of $\alpha$-th species in the $\beta$-th elementary reaction step. The reaction mechanism used in the present study is taken from (Peters 1993) and is given in appendix A.

**Method 2: Generation of flamelet library using flamelet equations**

The flamelet equations are devised, based on universal co-ordinate transformation on the mixture fraction space, in the following form (Peters 1984; Bray and Peters 1994):

$$\rho \frac{\partial Y_\alpha}{\partial t} = \rho \frac{\chi}{2} \frac{\partial^2 Y_\alpha}{\partial Z^2} + \dot{\omega}_\alpha$$  \hspace{1cm} (2.45)

$$\rho \frac{\partial T}{\partial t} = \rho \frac{\chi}{2} \frac{\partial^2 T}{\partial Z^2} - \sum_{\alpha=1}^{n} \frac{h_\alpha}{C_p} \dot{\omega}_\alpha$$  \hspace{1cm} (2.46)

where $\chi$ is the scalar dissipation rate and has to be specified as an input. This formulation has widely been used to generate flamelet library (Mauss et al. 1990; Seshadri et al. 1990; Lentini 1994).

This formulation has the advantage that it is independent of the flow field and the scalar dissipation rate $\chi$ implicitly incorporates the convection and diffusion effects normal to the surface of the stoichiometric mixture (Bray and Peters 1994). However, the formulation is derived by neglecting the higher order terms involving convection and curvature along the stoichiometric mixture fraction surface and also based on the assumption of unity Lewis number. The effects of higher order terms are sometimes important (Bray and Peters 1994). The assumption of unity Lewis number also influences the flamelet structure specially in the rich zone (Pitsch and Peters 1998). An advanced flamelet formulation which includes the differential diffusion effects has been reported recently (Pitsch and Peters 1998). This formulation is very complex and is not utilised in the present study.
Statistics of non-equilibrium parameter

In the laminar flamelet model, the thermo-chemical composition of the turbulent flame is completely determined by two parameters, the mixture fraction and a non-equilibrium parameter, the scalar dissipation rate. In turbulent flow fields, these parameters are statistically distributed. It is therefore necessary to know the statistical distribution of the mixture fraction and the scalar dissipation rate. In virtually all laminar flamelet model formulations, it is assumed that the mixture fraction and the scalar dissipation rate are statistically independent. This assumption drastically simplifies the formulations. Thus, the average value of scalar variables in a turbulent flow field is given by:

\[ \bar{\phi} = \int_0^\infty \int_0^1 \phi(Z; \chi) P(Z) P(\chi) dZ d\chi \]  

(2.47)

The pdf for mixture fraction is assumed to be a beta function (Peters 1984). The pdf of scalar dissipation rate is assumed to be a log-normal function and experimental evidence justifies this assumption (Effelsberg and Peters 1988). The mean scalar dissipation rate in the turbulent flow field is modelled according to:

\[ \bar{\chi} = C_\chi \frac{\bar{\phi}}{k} \]  

(2.48)

where \( C_\chi \) is a constant with a value of 2.0 (Liew et al. 1984). The width of the log-normal distribution is given in terms of variance, \( \sigma \) (Peters 1984). The value of \( \sigma^2 \) is assigned as 2.0 after Peters (1984).

In principle, the local and global extinction of turbulent flames can be described by the distribution of the scalar dissipation rate. Local extinction events occur when the scalar dissipation rate exceeds the extinction limit \( \chi_q \) and, since the scalar dissipation rate is distributed in turbulent fields, the probability of extinction is given by:

\[ P_{\text{ext}} = \int_0^{\chi_q} P(\chi) d\chi \]  

(2.49)

The scalar dissipation rate, and consequently the probability of extinction, depends on the flow time scales, which vary across the turbulent flame. For higher mixing rate, the value of the scalar dissipation rate is high and the pdf, \( P(\chi) \), shifts towards the higher values of the scalar dissipation rate. This results in a higher probability of extinction and the presence of a larger portion of extinguished flamelets. Percolation theory (Peters
1984; Peters 1986) predicts that when the probability of extinction exceeds a certain critical value $P_c$, the flame will no longer be interconnected and global extinction will occur. In that case, the flamelets representing the thermo-chemical state of a turbulent flame at a location in question are all extinguished. This approach has been used to analyse the lift-off phenomenon of turbulent jet diffusion flames (Sanders and Lamers 1994). In the region near the burner nozzle, the intense turbulent mixing leads to a higher scalar dissipation rate; if $P_{ext}$ exceeds $P_c$, global extinction occurs and the flame is lifted. Further downstream, where the scalar dissipation rate decreases to such a value that $P_{ext} = P_c$, the flame is stabilised.

Though the flamelet model has been successful in the predicting lift-off phenomenon, it is not yet clear whether the same formulation will be successful in predicting the local extinction phenomenon, often observed in turbulent CH$_4$ flames (Masri et al. 1996). In the present study, the laminar flamelet model is assessed for a number of fuel mixtures as well as for different Reynolds numbers to investigate its suitability for flames both near and far away from chemical equilibrium.

**Non-equilibrium parameter**

Two parameters are currently in use to describe the non-equilibrium effects: the scalar dissipation rate and the strain rate. The scalar dissipation rate is theoretically the correct parameter and should account for non-equilibrium effects caused by both convection and diffusion (Bray and Peters 1994). However, recent studies suggest that the use of strain rate is more appropriate (Sanders and Lamers 1994; Bray and Peters 1994; Bradley et al. 1990; Fairweather et al. 1991). The arguments for using the strain rate are given in Bray and Peters (1994). The scalar dissipation rate, given by Eq. (2.48), depends on two physical parameters: (1) the turbulence time scale $\tilde{\tau}$ and (2) the mixture fraction variance, $Z'^2$. According to Bray and Peters (1994), the non-equilibrium parameter used to couple the thermo-chemical state of the turbulent flame to that in the library should depend only on the turbulent time scale, represented by $\tilde{\tau}$. The mixture fraction fluctuations should not influence the chemistry as long as these do not enter into the reaction zone. This differentiation is very important for partially premixed turbulent flames where the partial mixing of fuel and air occurs before chemical reaction takes place. The flamelets in a turbulent premixed flame do not extend from pure fuel ($Z = 1$) to pure air ($Z = 0$), rather they span over a smaller part of mixture fraction space. Cor-
responding partially premixed flamelets can be constructed by moving the boundary conditions towards the reaction zone while keeping the strain rate and consequently the scalar dissipation rate constant at the reaction zone. The structure of partially premixed flamelets should depend on the temperature and the concentrations imposed on the new boundary. However, for fuels with a small stoichiometric mixture fraction such as hydrogen or methane, the flamelet profiles are not expected to be influenced by partial premixing of the fuel stream. This is because the reaction zone is still far away from the fuel boundary. However, the corresponding reduction of the mixture fraction variance across the flamelet would decrease the mean scalar dissipation rate (see Eq. 2.48), and subsequently will influence the thermo-chemical state of the turbulent flame, if the scalar dissipation rate is used as the non-equilibrium parameter. Based on above analysis, Bray and Peters (1994) have proposed to use the strain rate as the non-equilibrium parameter and to relate its mean to turbulent time scales as:

\[ \bar{\alpha} = \frac{\bar{\varepsilon}}{k} \]  

(2.50)

Correspondingly, a new scalar dissipation rate, producing an equivalent coupling between the time scales of the turbulent flame and the library, can be defined according to Bray and Peters (1994). The expression for the modified scalar dissipation rate is given by:

\[ \chi = C \frac{\bar{\varepsilon}}{k} (\Delta Z)^2 \]  

(2.51)

The scalar dissipation rate defined by the above expression differs from the standard scalar dissipation rate defined by the Eq. (2.48) in the mixture fraction variance term. The new relation is based on a fixed mixture fraction variance, \( \Delta Z \), rather than on the actual mixture fraction variance, \( Z''^2 \), which varies along the turbulent flame. \( \Delta Z \) is the thickness of the laminar flamelets in the mixture fraction space and it contains the reaction zone and surrounding diffusive layers. For fuel with small stoichiometric mixture fraction, \( \Delta Z \) can be taken as \( \Delta Z = 2Z_{st} \) as a first approximation (Bray and Peters 1994). The use of the strain rate as well as the new definition of the scalar dissipation rate has been very successful in predicting the lift-off phenomenon (Sanders and Lamers 1994; Bray and Peters 1994). However, the flamelet model using the strain rate as the non-equilibrium parameter has failed to predict the scaling behavior of NO\(_x\) (Sanders and Gokalp 1995; Schlatter et al. 1996). Sanders et al. (1997) have investigated the effects
of different non-equilibrium parameter on the NOx scaling behavior by using the strain rate, the standard scalar dissipation rate defined by Eq. (2.48) and the modified scalar dissipation rate defined by Eq. (2.51). They found that only the use of the standard scalar dissipation rate, defined by Eq. (2.48), as the non-equilibrium parameter, can produce the correct trend of NOx scaling. Thus, the question of the correct parameter for accounting the non-equilibrium effect is still open and it is further investigated in the present study.

2.4.3 Eddy break-up model

Eddy break-up modelling approach is very different from the modelling approaches described so far specially with respect to chemistry modelling and the turbulence-chemistry interaction modelling. The eddy break-up model is an empirical model for expressing the mean chemical reaction rate in the transport equations of the mean mass fractions. Spalding (1971b) has observed that the reaction rate in a premixed flame is only weakly dependent on temperature, pressure and mixing strength, instead the reaction process is controlled by turbulence mixing. Based on these observations, he proposed a model for the reaction rate which did not account explicitly the effects of chemical kinetics. This model is known as the eddy break-up model. According to the model, the mean reaction rate is proportional to the rate at which larger eddies are broken into smaller eddies. The expression for the mean reaction rate of fuel according, to this model, is given by:

\[
\overline{\omega_f} = C_{EBU} \frac{\bar{\varepsilon}}{k} \left( \bar{\gamma}_f^2 \right)^{1/2}
\]

where \( \bar{\gamma}_f^2 \) is the fluctuation of fuel mass fraction and \( C_{EBU} \) is the model constant.

This model faces difficulties in determining the fluctuations of fuel concentrations. Models similar to the original eddy break-up model have been proposed by a number of researchers. The most popular of these models is the one proposed by Magnussen and Hjertager (1976).

The expression for the mean reaction rate in the eddy break-up model proposed by Magnussen and Hjertager (1976), which is popularly known as Magnussen’s model, is given by:
where $Y_{fu}$, $Y_{ox}$ and $Y_{pr}$ are the concentration of fuel, oxygen and products respectively, $s$ is the stoichiometric oxygen fuel ratio. $A$ and $B$ are model constants with values of 4.0 and 2.0 respectively. The crucial difference between this model and the original eddy break-up model is that this model relates the dissipation of eddies with the mean concentrations of intermittent quantities instead of the fluctuating concentrations. This model also recognises that the dissipation of eddies containing different species can be rate determining for different conditions. Magnussen's eddy break-up model has been widely used for calculations of industrial flows and is also implemented and evaluated in the present study. An extended version of the model known as the eddy dissipation concept (EDC) model is also available which can further include finite rate chemistry effects (Gran 1994).

Several options are available in the numerical application of the EBU model. In one method, as utilised in Magnussen and Hjertager (1976), the transport equation for the fuel mass fraction is solved with the rate of reaction available from the EBU model. An additional equation of mixture fraction is solved from where remaining species are calculated. The second method, as used in the commercial code FLUENT, is to solve the transport equations of all the species involved in the combustion process. The EBU model gives the source term for fuel and the source terms for the remaining species are calculated from the reaction rate expression with an appropriate stoichiometric relation. The second method is implemented in the present study. In this method, the following transport equations are solved for mass fraction of fuel, oxygen, product and enthalpy:

Mass fraction of fuel:

$$\frac{\partial}{\partial x_j} (\bar{u} \bar{Y}_{fu}) = \frac{\partial}{\partial x_j} \left( \mu_t \frac{\partial \bar{Y}_{fu}}{\partial x_j} \right) - \bar{p} \bar{\omega}_f$$  \hspace{1cm} (2.54)

Mass fraction of oxygen:

$$\frac{\partial}{\partial x_j} (\bar{u} \bar{Y}_{ox}) = \frac{\partial}{\partial x_j} \left( \mu_t \frac{\partial \bar{Y}_{ox}}{\partial x_j} \right) - s \bar{p} \bar{\omega}_f$$  \hspace{1cm} (2.55)
Mass fraction of product:

\[
\frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_j \bar{Y}_{pr}) = \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{\sigma_t} \frac{\partial \bar{Y}_{pr}}{\partial x_j} \right) + (1 + s) \bar{\rho} \bar{\omega}_f \tag{2.56}
\]

Enthalpy:

\[
\frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_j \bar{h}) = \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{\sigma_t} \frac{\partial \bar{h}}{\partial x_j} \right) \tag{2.57}
\]

where, \( Y_{fu} \), \( Y_{oz} \) and \( Y_{pr} \) are mass fraction of fuel, oxygen and product respectively; \( s \) is the stoichiometric mass of oxygen, and the fuel rate of fuel burning, \( \bar{\omega}_f \), is given by Eq. 2.53.

The mean temperature is found from:

\[
\bar{h} = \sum_{\alpha=1}^{N} \bar{Y}_{\alpha} h_{\alpha}(\bar{T}) \tag{2.58}
\]

and the mean density is determined from the equation of state for a mixture of perfect gases:

\[
\bar{\rho} = \frac{\bar{P}}{\bar{T} R \sum_{\alpha=1}^{N} \frac{Y_{\alpha}}{M_{\alpha}}} \tag{2.59}
\]
Numerical Implementation

This chapter summarises the numerical methods employed to implement the various mathematical models presented in chapter 2. The numerical methods are of crucial importance in the detailed study of combustion processes. A reliable and accurate numerical method is needed so that the errors associated with the numerics do not prevent the evaluation of the underlying mathematical models. There are a large number of numerical methods available in the literature for solving the governing equations of flow, heat transfer and combustion (Patankar 1980; Versteeg and Malalasekera 1995; Ferziger and Peric 1996). A brief description of the widely used numerical method is given in the following sections. First, the solution method for the flow field calculations is described without any reference to combustion models. The incorporation of the combustion model into the general flow calculations is described in later sections.

3.1 Governing equations

The physical and chemical processes of combustion can be described by the governing equations of conservation of mass, momentum, turbulence kinetic energy, energy dissipation rate, mixture fraction and mixture fraction variance equations. All conservation and transport equations have the following generalised form:

\[ \frac{\partial}{\partial x_j} (\rho u_j \phi) = \frac{\partial}{\partial x_j} (\Gamma_\phi \frac{\partial \phi}{\partial x_j}) + S_\phi \]  

(3.1)

where \( \phi \) is the general dependent variable. These equations differ only in the form of the source term, \( S_\phi \) and their diffusive transport coefficient, \( \Gamma_\phi \).

Along with the boundary conditions, these elliptic equations are solved numerically.
by a standard finite volume method. The detailed derivation and formulation of the finite volume method can be found in Patankar (1980) and Versteeg and Malalasekera (1995). Here only a brief description of the general make-up of the method is provided.

### 3.2 Finite difference equations: general remarks

The differential equations can be reduced to a set of algebraic equations by integration over small control volumes or cells. The calculation domain is divided into a finite number of such control volumes to form a computational grid system. Numerical values of the scalar variables and pressure are determined at the intersection of these mesh lines (grid nodes). The velocities are calculated at a point half-way between these grid nodes. This "staggered" location for velocities makes the calculation of the pressure gradients easy and necessitates the adoption of different control volumes for each of the velocity component. Figure 3.1 shows such control volumes for a 2-D case in Cartesian coordinates. The integration of Eq. (3.1) over the corresponding control volume for the variable in question together with appropriate assumptions about the way in which the quantities vary between grid nodes leads to algebraic equations of the following form:

$$ a_P \phi_P = \sum_{i=E,W,N,S} \alpha_i \phi_i + S_C \quad (3.2) $$

where, $P$ is the central node and $E,W,N,S$ are the neighbour nodes of the control volume. In the integration procedure, the source term, $S_\phi$, in Eq. (3.1) is linearised as:

$$ S_\phi = S_P \phi_P + S_C \quad (3.3) $$

where, $S_P$ is selected in such a way that it is unconditionally negative. The coefficient of the central node is given by:

$$ a_P = \sum \alpha_i - S_P \quad (3.4) $$

The neighbour coefficients $\alpha_i$ contain the influence of the convective and diffusive fluxes through the cell faces. The ratio of convective to diffusive flux at a given cell face is conventionally known as a cell Peclet number e.g. for a face with surface normal to the
Figure 3.1: Control volume for (a) scalar cell, (b) staggered velocity cells

In the $x$-direction, the cell Peclet number is defined as:

$$Pe_{\phi,x} = \frac{\rho u \Delta x}{\Gamma_\phi} \quad (3.5)$$

### 3.2.1 Discretisation schemes

The integration of the convective terms on the left hand side of Eq. (3.1) leads to the need to interpolate the $\phi$ values at the cell faces from the adjacent nodal values. This interpolation practice constitutes the most problematic element of the discretisation scheme (the diffusive fluxes are always discretised using second order accurate central differencing). The discretisation of the convection terms with the central differencing scheme (CDS) produces unphysical oscillations (Patankar 1980). The hybrid (of upwind differencing scheme and CDS) scheme eliminates these oscillations, however the scheme has known tendency to introduce numerical diffusion because of switching to the first order upwind scheme for $Pe > 2$. The numerical diffusion is specially prominent in the presence of skewness (i.e. when the flow is not aligned to the grids) (Patankar 1980). Minimisation of the artificial diffusion by refining grids incurs unacceptable computational penalty. The higher order schemes, such as the third-order upstream weighted QUICK scheme of Leonard (1979) may overcome this drawback. Although the higher order discretisation schemes avoid the problems associated with
first-order upwinding, they are more unstable and do not necessarily improve the solutions. For instance, during a comparative study of different discretisation schemes, Lien and Leschziner (1994) and Alvarez and Jones (1993) confirmed that the second-order TVD scheme and the third-order QUICK scheme yield identical solution and the TVD scheme is much more stable and computationally efficient. In any case, higher order schemes have little influence in computations involving turbulence models, such as the $k-\varepsilon$ model which are generally dominated by the production and destruction terms rather than the convection term (Lien and Leschziner 1994; Alvarez and Jones 1993). The modelling of the turbulent reacting flows is subjected to a number potential of sources of error. These include those arising from the turbulence model, those arising from the combustion model and those which results from discretisation of the resulting set of differential equations. It is clearly of the utmost importance to isolate the error associated with the discretisation scheme in order to draw definitive conclusions on the performance of calculation methods. In order to investigate the numerical error associated with the discretisation scheme three different schemes are used in the current work. These are:

**Hybrid:** The hybrid scheme is a combination of central differencing and upwind scheme. It uses central differencing when the Peclet number is small ($Pe < 2$) and switches to upwind scheme for large Peclet numbers ($Pe > 2$). This scheme produces a realistic solution and is highly stable. The hybrid scheme has been widely used for predicting practical flows. The disadvantage is that this scheme is first order accurate and produces false diffusion.

**Power law:** The power law differencing scheme of Patankar (Patankar 1980) is a curve fit to the exact solution of a one dimensional, steady state, convection-diffusion flow problem. In this scheme, the diffusion is set to zero when the cell $Pe$ exceeds 10. If $0 < Pe < 10$, the flux is evaluated by using a polynomial expression. This scheme produces better result than the hybrid scheme, but it also suffers from the problem of false diffusion.
TVD: The total variation diminishing (TVD) scheme, first devised for gas dynamics problems, has also been used in the turbulent combusting flows (Jones 1994). The TVD scheme is stable, second order accurate and is easy to implement. In this scheme, the cell face values needed in the differencing of the convection term are written as upwind values plus correction terms which overall lead to second order accuracy, but where the correction is limited to prevent spatial oscillations by means of a limiter. The are a wide range of limiters available in the literature (Van Leer 1974; Chakravarthy and Osher 1983; Lien and Leschziner 1994). In the present study, Van Leer’s (Van Leer 1974) and UMIST (Upstream Monotonic Interpolation for Scalar Transport) (Lien and Leschziner 1994) limiters are employed. In the TVD scheme, the upwind contribution is included in the neighbouring coefficients, while the anti diffusive flux is implemented via a ”deferred correction” source term $S^{PC}_\phi$.

Figure 3.2 shows a two dimensional control volume and associated nodal stencil. The coefficients of the discretised Eq. (3.2) that result from applying the above mentioned schemes are given in Table 3.1.

Figure 3.2: Two dimensional control volume and associated nodal stencil
Table 3.1: Coefficients for different scheme

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hybrid scheme</td>
<td>$a_E = \max[-F_e, (D_e - F_e/2), 0]$</td>
</tr>
<tr>
<td></td>
<td>$a_W = \max[F_w, (D_w + F_w/2), 0]$</td>
</tr>
<tr>
<td></td>
<td>$a_N = \max[-F_n, (D_n - F_n/2), 0]$</td>
</tr>
<tr>
<td></td>
<td>$a_S = \max[F_s, (D_s + F_s/2), 0]$</td>
</tr>
<tr>
<td>Power law scheme</td>
<td>$a_E = D_e \max{0, (1 - 0.1</td>
</tr>
<tr>
<td></td>
<td>$a_W = D_w \max{0, (1 - 0.1</td>
</tr>
<tr>
<td></td>
<td>$a_N = D_n \max{0, (1 - 0.1</td>
</tr>
<tr>
<td></td>
<td>$a_S = D_s \max{0, (1 - 0.1</td>
</tr>
<tr>
<td>TVD scheme</td>
<td>$a_E = D_e + \max(-F_e, 0)$</td>
</tr>
<tr>
<td></td>
<td>$a_W = D_w + \max(F_w, 0)$</td>
</tr>
<tr>
<td></td>
<td>$a_N = D_n + \max(-F_n, 0)$</td>
</tr>
<tr>
<td></td>
<td>$a_S = D_s + \max(F_s, 0)$</td>
</tr>
<tr>
<td></td>
<td>$S_f^{DC} = \left[ F_e^+ - \Psi(r_e^-) / 2 - F_e^+ \Psi(r_e^+ / 2) \right] (\phi_E - \phi_P)$</td>
</tr>
<tr>
<td></td>
<td>$+ \left[ F_w^+ \Psi(r_w^- / 2 - F_w^+ \Psi(r_w^+ / 2) \right] (\phi_P - \phi_W)$</td>
</tr>
<tr>
<td></td>
<td>$+ \left[ F_n^+ \Psi(r_n^- / 2 - F_n^+ \Psi(r_n^+ / 2) \right] (\phi_N - \phi_P)$</td>
</tr>
<tr>
<td></td>
<td>$+ \left[ F_s^+ \Psi(r_s^- / 2 - F_s^+ \Psi(r_s^+ / 2) \right] (\phi_P - \phi_W)$</td>
</tr>
<tr>
<td></td>
<td>where, $r_e^+ = \frac{\phi_P - \phi_W}{\phi_P - \phi_E}$, $r_e^- = \frac{\phi_E - \phi_W}{\phi_E - \phi_P}$, $r_w^+ = \frac{\phi_W - \phi_W}{\phi_W - \phi_E}$, $r_w^- = \frac{\phi_E - \phi_W}{\phi_E - \phi_P}$</td>
</tr>
<tr>
<td></td>
<td>$r_n^+ = \frac{\phi_P - \phi_W}{\phi_P - \phi_N}$, $r_n^- = \frac{\phi_N - \phi_W}{\phi_N - \phi_P}$, $r_s^+ = \frac{\phi_P - \phi_W}{\phi_P - \phi_S}$, $r_s^- = \frac{\phi_S - \phi_W}{\phi_S - \phi_P}$</td>
</tr>
</tbody>
</table>

In the expressions, $F = \rho u$, $D = \frac{F}{\delta t}$, $Pe = \frac{F}{D}$
3.3 Boundary conditions

The transport equations of the scalar variables are all of elliptic type (Patankar 1980). The solution of elliptic partial differential equations requires information to be provided at all points on a closed boundary surrounding the solution domain. The specification of these conditions varies according to the type of boundary and the dependent variables under consideration. The treatment and implementation of boundary conditions are given in great details in Versteeg and Malalasekera (1995). Here, a brief description is provided.

3.3.1 Inlet boundary

The values of each variables are assigned for each grid node at the entry plane. These values must be known from measurements, from the problem specifications or from estimates of conditions prevailing in the inflow stream. The mean flow properties at the inlet are usually known, while some or all turbulence properties have to be estimated. In the absence of Reynolds stresses at the inlet, the turbulent kinetic energy is estimated as:

\[
    k_{in} = \frac{3}{2}(iU_m)^2
\]

where, \(U_m\) is bulk velocity, and \(i\) is the turbulence intensity with values ranging form 1%-10%. The scalar dissipation rate \(\varepsilon\) on the other hand has to be estimated and is usually estimated from length scale as:

\[
    \varepsilon_{in} = \frac{C_{\mu}^{3/4} k_{in}^{3/2}}{l_m}
\]

where \(l_m\) is the turbulent mixing length. For a pipe flow, \(l_m = 0.07 \times \text{Radius}\).

3.3.2 Plane or axis of symmetry

The normal components of the convective and diffusive fluxes are zero at a plane of symmetry, i.e. there is no transport across a plane of symmetry. The normal velocity component is zero. The implementation of this boundary condition is straight forward and can be set by assigning the appropriate coefficient \(a_i\) to zero.
3.3.3 Outlet boundary

The outlet boundary is placed far way from the region of interest so that the flow is fully developed and is in the direction out of the solution domain. The usual approach is to use upwinding at the out-flow surface and then to apply zero gradient condition at the boundary. This is sufficient for all variables except for the normal velocity. Overall continuity imposes a constraint and the outlet velocity should be such that the overall mass conservation is preserved over the complete solution domain. One way to ensure this is to calculate the mass flux going out of the domain $M_{out}$ by first applying zero gradient. The velocity at the outlet is then scaled by the multiplying factor $\frac{M_{in}}{M_{out}}$, where $M_{in}$ is the inlet mass flow rate.

3.3.4 Solid wall

The no-slip condition is the appropriate boundary condition at a solid wall. However, the turbulent flow over a solid surface is characterised by the presence of a very thin viscous sublayer adjacent to the wall along which rapid variations of the mean velocity and turbulent properties exist. The number of grid points required to resolve the viscous sublayer is prohibitively large. The log-law of the wall is used to overcome the mesh resolution problem. The implementation of the log-law condition has been done in many different ways (Versteeg and Malalasekera 1995; Jones 1994). Table 3.2 shows the optimal near wall relationships according to Versteeg and Malalasekera (1995). These relationships are used in conjunction with the universal log-law of the wall:

$$ u^+ = \frac{1}{k} \ln(Ey^+) $$  (3.8)

Some of the notations of the near wall relationships of Table 3.2 are given in Fig. 3.3, which shows a u-cell near the solid wall. The relationships of Table 3.2 are implemented in the discretised equations through the source terms $S_C$ and $S_P$. 
Table 3.2: Near wall relationship for the $k-\varepsilon$ model

<table>
<thead>
<tr>
<th>Equation Type</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Momentum equation tangential to the wall:</td>
<td></td>
</tr>
<tr>
<td>wall shear stress $\tau_w = \rho C_{\mu}^{1/4} k_p^{1/2} u_p / u^+$</td>
<td></td>
</tr>
<tr>
<td>wall force $F_s = -\tau_w A_{cell} = -(\rho C_{\mu}^{1/4} k_p^{1/2} u_p / u^+) A_{cell}$</td>
<td></td>
</tr>
<tr>
<td>Momentum equation normal to the wall:</td>
<td></td>
</tr>
<tr>
<td>normal velocity=0</td>
<td></td>
</tr>
<tr>
<td>Turbulence kinetic energy:</td>
<td></td>
</tr>
<tr>
<td>generation of turbulent kinetic energy, $G = (\tau_w u_p - \rho C_{\mu}^{3/4} k_p^{3/2} u^+) \Delta V / \Delta y_p$</td>
<td></td>
</tr>
<tr>
<td>Dissipation rate equation:</td>
<td></td>
</tr>
<tr>
<td>net nodal value, $\varepsilon_p = C_{\mu}^{3/4} k_p^{3/2} / (\kappa \Delta y_p)$</td>
<td></td>
</tr>
</tbody>
</table>

Figure 3.3: Control volume for u-velocity at a solid wall
3.4 Solution Algorithm

The equations for mass conservation, momentum and the coupled scalar variables are solved by using the SIMPLE algorithm (Patankar 1980). The description of the SIMPLE algorithm can be found in many texts (Patankar 1980; Versteeg and Malalasekera 1995; Ferziger and Peric 1996) and is not repeated here. The combustion models are incorporated into the algorithm as follows:

1. Guess the initial conditions for all variables.
2. Update the boundary conditions.
3. Solve the momentum equations.
4. Solve the pressure correction equations.
5. Correct the pressure and velocities.
6. Solve the $k$ equation.
7. Solve the $\varepsilon$ equation.
8. Solve the other scalar equations (for combustion modelling).
9. Calculate the density.
10. Use the new values as the initial conditions and repeat steps 2 to 8 until convergence is reached.
11. Calculate the temperature and mass fraction of species after convergence is reached.

The set of algebraic equations are solved by repeated sweeps of a line by line application of the well known tri-diagonal matrix algorithm (TDMA) (Patankar 1980). The equations are solved along constant $x_i$ and in doing so the variables located along adjacent lines are kept constant. The coefficient $a_i$ and source term, $S_C$ in Eq. (3.2) are evaluated using values of the variables at the start of the TDMA sweep and are not changed during the TDMA solution. The solution is regarded as converged when the residual source term scaled against a representative inflow flux is small (typically $10^{-5}$) for all variables.
The combustion models are incorporated in the steps 8, 9 and 11 of the algorithm and are described below.

### 3.4.1 Flame sheet/Equilibrium model

The incorporation of the flame sheet and equilibrium models in the general solution algorithm is similar. The relationship, $\phi = \phi(Z)$, calculated either by the flame sheet model or by the equilibrium chemistry model, is tabulated in a file. The data file is used as an input to the CFD code. As explained earlier, the beta pdf used to incorporate the influence of the turbulent fluctuations is given by (Jones 1994):

$$ P(Z) = \frac{Z^{a-1}(1-Z)^{b-1}}{\int_0^1 Z^{a-1}(1-Z)^{b-1} dZ} = \frac{Z^{a-1}(1-Z)^{b-1}}{\Gamma(a)\Gamma(b)} $$

(3.9)

where the values of the exponents $a$ and $b$ are given by:

$$ a = Z \left[ \frac{\bar{Z}(1-\bar{Z})}{Z^r} - 1 \right] $$

(3.10)

$$ b = (1-\bar{Z}) \frac{a}{\bar{Z}} $$

(3.11)

and where, the mean, $\bar{Z}$, and the variance, $Z^{\eta_2}$, of the mixture fraction are obtained from the solution of their respective transport equations.

Because $P(Z)$ is a density-weighted pdf, mean values are given by:

$$ \bar{\phi} = \int_0^1 \phi(Z)P(Z) dZ = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \int_0^1 \phi(Z)Z^{a-1}(1-Z)^{b-1} dZ $$

(3.12)

$$ \bar{\phi} = \bar{\rho} \int_0^1 \phi(Z) \frac{P(Z)}{\rho(Z)} dZ $$

(3.13)

and

$$ \bar{\rho} = \left[ \int \frac{P(Z)}{\rho(Z)} dZ \right]^{-1} $$

(3.14)

The flame sheet/equilibrium model enters the general solution algorithm in steps 8, 9 and 11 as follows:
Chapter 3. Numerical Implementation

Step 8:

8a: Solve the transport equation for mean mixture fraction, Eq. (2.32).

8b: Solve the transport equation for mean mixture fraction variance, Eq. (2.33).

Step 9:

9: Calculate the density from Eq. (3.14).

Step 11:

11: Calculate the temperature, mass fraction of species and other scalar variables from Eq. (3.13).

The integration in Eqs. (3.12), (3.13) and (3.14) is evaluated by the Romberg's method with the midpoint approximation (Press et al. 1993). The \( \phi(Z) \) at the intermediate point of the data file required for the integration is obtained from interpolation. The end points \( (Z = 0, 1) \) of the integration become singular in the numerical calculation procedure when the parameter \( a \) or \( b \) is less than unity. This singularity is eliminated analytically according to the method suggested by Bray et al. (1994) and Chen et al. (1994). According to them, the integration in Eq. (3.12) is approximated by:

\[
\int_0^1 \phi(Z)Z^{a-1}(1-Z)^{b-1}dZ \cong \frac{\xi^a}{a} \phi(0) + \int_{\xi}^{1-\xi} \phi(Z)Z^{a-1}(1-Z)^{b-1}dZ + \frac{\xi^b}{b} \phi(1) \quad (3.15)
\]

where, \( \xi \) represents a very small number (say \( 10^{-30} \)).

Another numerical difficulty is that the computed value of \( a \) and \( b \) in Eqs. (3.10) and (3.11) may approach magnitudes of several hundred thousands in the iteration process (Chen et al. 1994). This problem in turn leads to overflow in the calculation of \( P(Z) \). According to the characteristic of the beta function, the \( P(Z) \) will be close to a delta function when either value of exponent \( a \) and \( b \) is adequately large (see Fig. 3.4). In the present calculation, when the value of \( a \) or \( b \) is very large (say, 500), the \( P(Z) \) is approximated by a delta function, \( P(Z) = \delta(Z - \bar{Z}) \). The mean scalar variable is then given by:

\[
\bar{\phi} = \int_0^1 \phi(Z)P(Z)dz = \int_0^1 \phi(Z)\delta(Z - \bar{Z})dz = \phi(\bar{Z}) \quad (3.16)
\]
3.4.2 Laminar flamelet model

The laminar flamelet model has been described in section 2.4.2. According to this model, the scalar variables depend on two parameters, the mixture fraction and the scalar dissipation rate, so that $\phi = \phi(Z; \chi)$. The mean value of the scalar variable is given by:

$$\bar{\phi} = \int_0^\infty \int_0^1 \phi(Z; \chi) P(Z) P(\chi) dZ d\chi$$  \hspace{1cm} (3.17)

The double integration in Eq. (3.17) is simplified by using a limited number of flamelet libraries each represented by the scalar dissipation rate $\chi_l$. The integration range in $\chi$ is divided into $L$ subranges $[\chi_{l-1/2}, \chi_{l+1/2}]$, with $l = 1, 2, \ldots, L$ (in particular $\chi_{1/2} = 0$), such that $\chi_l$ is a representative value for the corresponding interval. The integration is evaluated by means of the approximation (Lentini 1994):
\[
\int_0^\infty \int_0^1 \phi(Z; \chi) P(Z) P(\chi) dZ d\chi \cong \sum_{i=1}^L \int_{\chi_{i-1/2}}^{\chi_{i+1/2}} P(\chi) d\chi \int_0^1 \phi(Z; \chi_i) dZ
\]  
(3.18)

The integration of \( \int_0^1 \phi(Z; \chi) dZ \) is similar to that explained in the previous section 3.4.1. The evaluation of \( \int_{\chi_{i-1/2}}^{\chi_{i+1/2}} P(\chi) d\chi \) is explained here. The integration requires the specification of the pdf shape in \( \chi \) space. As mentioned earlier, the pdf \( P(\chi) \) is assumed to be log-normal:

\[
P(\chi) = \frac{1}{\chi \sigma \sqrt{2\pi}} \exp \left[ -\frac{1}{2\sigma^2} (\ln \chi - \mu)^2 \right]
\]  
(3.19)

where the parameters \( \mu \) and \( \sigma \) are related to the mean value of \( \chi \) by:

\[
\bar{\chi} = \exp(\mu + \frac{1}{2} \sigma^2)
\]  
(3.20)

The integration \( \int_{\chi_{i-1/2}}^{\chi_{i+1/2}} P(\chi) d\chi \) is thus simplified in the form:

\[
\int_{\chi_{i-1/2}}^{\chi_{i+1/2}} P(\chi) d\chi = \frac{1}{\sqrt{\pi}} \int_{\theta_{i-1/2}}^{\theta_{i+1/2}} \exp^{-\theta^2} d\theta
\]  
\[
= \frac{1}{2} [\text{erf}(\theta_{i+1/2}) - \text{erf}(\theta_{i-1/2})]
\]  
(3.21)

where \( \text{erf} \) denotes the error function.

Finally, the mean value of density and scalar variable given by Eq. (3.17) is rewritten as:

\[
\bar{\rho} = \left[ \sum_{i=1}^L \frac{1}{2} [\text{erf}(\theta_{i+1/2}) - \text{erf}(\theta_{i-1/2})] \int_0^1 \frac{P(Z)}{\rho(Z, \chi_i)} dZ \right]^{-1}
\]  
(3.22)

\[
\bar{\phi} = \sum_{i=1}^L \frac{1}{2} [\text{erf}(\theta_{i+1/2}) - \text{erf}(\theta_{i-1/2})] \int_0^1 \phi(Z, \chi_i) P(Z) dZ
\]  
(3.23)

\[
\bar{\phi} = \bar{\rho} \left[ \sum_{i=1}^L \frac{1}{2} [\text{erf}(\theta_{i+1/2}) - \text{erf}(\theta_{i-1/2})] \int_0^1 \frac{\phi(Z, \chi_i)}{\rho(Z, \chi_i)} P(Z) dZ \right]
\]  
(3.24)

where arguments of the error function are given explicitly in terms of the computed quantities as follows:
and the scalar dissipation rate is given by:

\[
\chi = C_x \frac{\overline{e}}{k} \overline{Z'/Z_r^2} \tag{3.26}
\]

The flamelet library is represented by the inert mixing state for \( \chi > \chi_q \) indicating an extinguished flamelet. In order to accurately account for the contribution of the extinguished flamelet, the integration range is divided into subranges in such a way that \( \chi L - 1/2 = \chi_q \) and \( \chi L + 1/2 = \infty \). Further details of the integration method can be found in Lentini (1994).

The laminar flamelet model is incorporated into the general algorithm in steps 8, 9 and 11 as follows:

**Step 8:**

8a: Solve the transport equation for mean mixture fraction, Eq. (2.32).

8b: Solve the transport equation for mixture fraction variance, Eq. (2.33).

**Step 9:**

9a: Calculate the scalar dissipation rate from Eq. (3.26).

9b: Calculate the arguments of the error function from Eq. (3.23).

9c: Calculate the density from Eq. (3.22).

**Step 11:**

11: Calculate the temperature, mass fraction of species and other scalar variables from Eq. (3.24).

### 3.4.3 Eddy break-up model

The eddy break-up model is an empirical model for expressing the mean chemical reaction rate in the transport equations of the mean mass fractions. The EBU model is described in section 2.4.3. Here, the numerical implementation of the EBU model in the CFD code is described. The EBU model enters in steps 8, 9 and 11 as follows:
Step 8:

8a: Solve the transport equation for the mean enthalpy, Eq. (2.57).

8b: Solve the transport equations for the mean mass fraction of the species, Eqs. (2.54), (2.55) and (2.56).

Step 9:

9: Calculate the density from the equation of state, Eq. (2.59).

Step 11:

11: Calculate the temperature from Eq. (2.58) and other scalar variables.

With the EBU model, an ignition procedure is required as initially the product of combustion is absent throughout the flow field. The ignition is achieved by assigning a small amount of mass fraction of product near the fuel jet entry.
The laminar flamelet model requires as an input a library of flamelet profiles. The accuracy of the model in many ways depends on the accuracy of the flamelet library. Experimental data can be used as the flamelet library as in Liew et al. (1984). However, more detailed information can be obtained by generating the flamelet profiles from the numerical solution of laminar flames. As explained earlier, there are two different approaches available for calculating the flamelet profiles. The first method is based on the numerical solution of a counterflow diffusion flame (Peters 1984; Rogg et al. 1986; Drake et al. 1988; Lentini and Puri 1995). The second method is the solution of the flamelet equations based on the universal co-ordinate transformation (Peters 1986; Bray and Peters 1994; Pitsch and Peters 1998; Lentini 1994).

In the present study, flamelet profiles are calculated using both methods for CO/H₂/N₂ flame. For H₂/CO and CH₄/H₂ flames, only the counterflow diffusion flame method is employed.

4.1 Computation of flamelet library

The mathematical formulations for generating flamelet library are given in section 2.4.2. The flamelet libraries used in the simulation of turbulent non-premixed flames of the present study consist of 7 flamelets. Liew et al. (1984), Sanders and Lamers (1994) and Gran et al. (1994) have used 2 flamelets in their calculations, Sanders and Gökalp (1997) have used 5 flamelets, Lentini (1994) have used 7 flamelets and Drake et al. (1988) have used 17 flamelets. The use of higher numbers of flamelets will certainly improve accuracy, but it will also increase the computational time considerably.
The laminar flame and flamelet code RUN-1DL (Rogg 1995) is used to compute the flamelet library. In the numerical procedure, the equations governing the laminar flamelet problem are discretised using the finite difference technique. The resulting equations are solved on a adaptive grid system, in which additional grids are added at locations where the profiles of the variables to be solved have large gradients or curvatures. The adaptive gridding strategy in the code is designed to produce a mesh that resolves the thin flame front with a reasonable number of grid points.

The flamelet equations are solved with detailed reaction mechanism of Warnatz (Peters 1993). The reaction mechanism is given in appendix A. The reaction mechanism involves 12 species (CO, O_2, CO_2, H_2O, H_2O_2, HO_2, H, OH, O, H_2, HCO, N_2) for H_2/CO and CO/H_2/N_2 fuels and 17 species (CH_4, O_2, H_2O, CO_2, CO, H_2, H, OH, O, HO_2, CH_3, HCO, CH_2O, H_2O_2, CH, CH_2, N_2) for CH_4/H_2 fuel.

The flamelet profiles calculated by the counterflow diffusion flame method are on the physical space, which should be converted to the mixture fraction space to use in the laminar flamelet modelling. The mixture fraction can be defined in terms of atomic mass of element presents in the system as:

\[ Z = \frac{Z_m - Z_{m,0}}{Z_{m,F} - Z_{m,0}} \]  

(4.1)

where \( Z_m \) is the mass fraction of element \( m \) and subscripts \( O \) and \( F \) refer to air and fuel streams respectively. Different researchers have used different elements for the definition of mixture fraction. Lentini and Puri (1995) have used N-element and Sanders and Gökcalp (1997) have used H-element for the definition of mixture fraction. However, the mixture fractions calculated from the C, H, O and N element mass fractions generally differ by some amount because of the differences in the molecular transport of different species (Drake and Blint 1988). Bilger (1988) proposed an overall mixture fraction which is a linear combination of the elemental mixture fractions. Bilger’s formula is used in the present study:

\[ Z = \frac{2(Z_C - Z_{C,O})/W_C + 2(Z_H - Z_{H,O})/2W_H - 2(Z_O - Z_{O,O})/W_O}{2(Z_{C,F} - Z_{C,O})/W_C + 2(Z_{H,F} - Z_{H,O})/2W_H - 2(Z_{O,F} - Z_{O,O})/W_O} \]  

(4.2)

where subscripts O and F refer to air and fuel streams respectively. \( W_\beta \) is the atomic weight of element \( \beta \). This definition yields the correct stoichiometric mixture frac-
tion, even in the presence of the differential diffusion effect. Bilger's formula has been widely accepted for the definition of mixture fraction in the laminar flamelet modelling (Pitsch and Peters 1998) as well as analysing the experimental data (Masri et al. 1996; Dally et al. 1998) in the past few years.

The scalar dissipation rate is another parameter to characterise the flamelets. For the counterflow geometry, the scalar dissipation rate is approximated as a function of mixture fraction, assuming constant density and diffusivity, by (Bray and Peters 1994):

\[ \chi = \frac{a}{\pi} \exp\{-2[erfc^{-1}(2Z)]^2\} \]  

(4.3)

where \( a \) is the strain rate and \( erfc^{-1} \) is inverse of the complementary error function. Clearly, the scalar dissipation rate varies along the counterflow flame, but it is convenient to have a single value of the scalar dissipation rate to represent each flamelet. The scalar dissipation rate at the stoichiometric location is used in the present study to represent each flamelet. In some studies, the value of the scalar dissipation rate at the maximum temperature has been used (Liew et al. 1984; Lentini 1994). Choosing the value of the scalar dissipation rate at the maximum temperature is not expected to give significantly different results in turbulent combustion calculations.

### 4.2 Flamelet library for CO/H\(_2\)/N\(_2\) flame

The counterflow diffusion flame on Tsuji burner is simulated by keeping the normalised fuel velocity fixed at 6.4, while varying the strain rate at the air stream side. Dixon-Lewis et al. (1984) have shown that the normalised fuel velocity (see, Eq. 2.37) only affects the location of the stagnation point and the flame relative to the cylinder without disturbing the flame structure. The syngas fuel consists of 27.5% CO, 32.3% H\(_2\) and 40.2% N\(_2\) by volume. The flamelet profiles for temperature and mass fractions of CO, H\(_2\), H\(_2\)O, CO\(_2\) and OH are shown in Figs. 4.1-4.6. The flamelet profiles are generated with full molecular transport of the species and for the strain rate values of 0.1, 10.0, 100.0, 500.0, 2000.0 and 4900.0 /s. The corresponding scalar dissipation rate are 0.026, 2.576, 25.76, 128.80, 515.20 and 1262.241 s. The last value corresponds to the extinction limit. The peak temperatures at the scalar dissipation rates of \( \chi_{st} = 0.026 /s \) and \( \chi_{st} = 0.2576 /s \) are higher than the equilibrium temperature of 2161 K (equilibrium temperature is calculated by CHEMKIN-II code). The peak temperatures in
excess of equilibrium temperature at lower scalar dissipation rate are caused by the differential diffusion effect. The preferential diffusion of H2 leads to the enrichment of H2 at the flame front relative to the initial fuel mixture and subsequently results in higher temperature. Only for higher scalar dissipation rate does the flamelet temperature fall below the equilibrium temperature. The effect of stretching of the flamelets is clearly evident from these figures. The influence of the scalar dissipation rate on the temperature is high. The peak temperature falls from 2415 K at $\chi_{st} = 0.026$ /s to 1375 K at $\chi_{st} = 1262.24$ /s. The effect of scalar dissipation rate on the H2 and CO mass fractions is very small and its effect is only observed near the stoichiometric mixture fraction. The H2O mass fraction profiles are moderately influenced by the scalar dissipation rate. The CO2 mass fraction on the other hand is considerably influenced by the scalar dissipation rate. The peak CO2 is reduced by almost 50% at the extinction limit and also the location of the peak shifts towards the fuel rich zone. With the increase of scalar dissipation rate, the OH level first increases and then starts to decrease as the scalar dissipation rate approaches the extinction limit. The peak values of OH for $\chi_{st} = 0.026$ /s and $\chi_{st} = 1262.24$ /s are similar, but at $\chi_{st} = 1262.24$ /s, the width of the OH profile is much higher.

In order to investigate the effect of differential diffusion, the flamelet profiles are generated by setting $Le=1.0$ for all the species. The flamelet profiles are obtained for the strain rate values of 0.1, 10.0, 100.0, 2000.0 and 4000.0 /s with corresponding scalar dissipation rate of 0.026, 2.576, 25.76, 128.80, 515.20 and 1030.4 /s. The extinction limit is reduced for the unity Lewis number case as compared to the differential diffusion case. The flamelet profiles for the unity Lewis number are shown in Figs. 4.7-4.12. The peak temperature at the lowest scalar dissipation rate is 2151 K, which is 10 K below the equilibrium temperature of 2161 K. With the increase of scalar dissipation rate, the location of the peak temperature shifts towards the fuel rich side. The peak temperature at the extinction condition is almost equal to that with the full molecular transport. The level of H2O profiles decreases by about 30%, while the level of CO2 increases by about 60% as compared to the flamelets with full molecular transport. The OH flamelet profiles show slight reduction of the peak values when compared to those of the flamelet with the differential diffusion effect.

The flamelet profiles generated by the flamelet equations based on the conserved scalar space are shown in Figs. 4.13-4.18. In this method, the scalar dissipation rate has to be specified as an input data. Calculations are performed for the values of $\chi_{st}$.
of 0.48, 3.66, 33.27, 155.41, 600.46 and 1436.0 /s. The last value corresponds to the extinction limit $\chi_q$. The peak temperature at the lowest scalar dissipation rate is 2023 K, which is less than the equilibrium temperature of 2161 K. The flamelet profiles for species concentrations are similar to those obtained by the counterflow diffusion flame with Le=1.0.
Figure 4.1: Flamelet profiles for temperature for CO/H₂/N₂ fuel obtained from counter flow diffusion flame method with differential diffusion effects. 

- \( \chi = 0.026 \),  
- \( \chi = 2.576 \),  
- \( \chi = 25.76 \),  
- \( \chi = 128.80 \),  
- \( \chi = 515.20 \) to \( \chi = 1262.24 \) /s

Figure 4.2: Flamelet profiles for mass fraction of CO for CO/H₂/N₂ fuel obtained from counter flow diffusion flame method with differential diffusion effects for CO/H₂/N₂ fuel. 

- \( \chi = 0.026 \),  
- \( \chi = 2.576 \),  
- \( \chi = 25.76 \),  
- \( \chi = 128.80 \),  
- \( \chi = 515.20 \) to \( \chi = 1262.24 \) /s
Figure 4.3: Flamelet profiles for mass fraction of H$_2$ for CO/H$_2$/N$_2$ obtained from counter flow diffusion flame method with differential diffusion effects.

- $\chi = 0.026$,
- $\chi = 2.576$,
- $\chi = 25.76$,
- $\chi = 128.80$,
- $\chi = 515.20$,
- $\chi = 1262.24$ /s

Figure 4.4: Flamelet profiles for mass fraction of H$_2$O for CO/H$_2$/N$_2$ fuel obtained from counter flow diffusion flame method with differential diffusion effects.

- $\chi = 0.026$,
- $\chi = 2.576$,
- $\chi = 25.76$,
- $\chi = 128.80$,
- $\chi = 515.20$,
- $\chi = 1262.24$ /s
Figure 4.5: Flamelet profiles for mass fraction of CO$_2$ for CO/H$_2$/N$_2$ fuel obtained from counter flow diffusion flame method with differential diffusion effects. $\chi = 0.026$, $\chi = 2.576$, $\chi = 25.76$, $\chi = 128.80$, $\chi = 515.20$, $\chi = 1262.24$ /s

Figure 4.6: Flamelet profiles for mass fraction of OH for CO/H$_2$/N$_2$ fuel obtained from counter flow diffusion flame method with differential diffusion effects. $\chi = 0.026$, $\chi = 2.576$, $\chi = 25.76$, $\chi = 128.80$, $\chi = 515.20$, $\chi = 1262.24$ /s
Figure 4.7: Flamelet profiles for temperature for CO/H$_2$/N$_2$ fuel obtained from counter flow diffusion flame method with unity Lewis number.

- $\chi = 0.026$
- $\chi = 2.576$
- $\chi = 25.76$
- $\chi = 128.80$
- $\chi = 515.20$
- $\chi = 1030.40$ s

Figure 4.8: Flamelet profiles for mass fraction of CO for CO/H$_2$/N$_2$ fuel obtained from counter flow diffusion flame method with unity Lewis number.

- $\chi = 0.026$
- $\chi = 2.576$
- $\chi = 25.76$
- $\chi = 128.80$
- $\chi = 515.20$
- $\chi = 1030.40$ s
Figure 4.9: Flamelet profiles for mass fraction of H₂ for CO/H₂/N₂ fuel obtained from counter flow diffusion flame method with unity Lewis number. --- χ = 0.026, --- χ = 2.576, ··· · χ = 25.76, ····· χ = 128.80, --- χ = 515.20 ··· · χ = 1030.40/s

Figure 4.10: Flamelet profiles for mass fraction of H₂O for CO/H₂/N₂ fuel obtained from counter flow diffusion flame method with unity Lewis number. --- χ = 0 026, --- ... χ = 25.76, ····· χ = 128.80, --- χ = 515.20 ··· · χ = 1030.40/s
Figure 4.11: Flamelet profiles for mass fraction of CO$_2$ for CO/H$_2$/N$_2$ fuel obtained from counter flow diffusion flame method with unity Lewis number. $\chi = 0.026$, $\chi = 2.576$, $\chi = 25.76$, $\chi = 128.80$, $\chi = 515.20$, $\chi = 1030.40$ /s

Figure 4.12: Flamelet profiles for mass fraction of OH for CO/H$_2$/N$_2$ fuel obtained from counter flow diffusion flame method with unity Lewis number. $\chi = 0.026$, $\chi = 2.576$, $\chi = 25.76$, $\chi = 128.80$, $\chi = 515.20$, $\chi = 1030.40$ /s
Figure 4.13: Flamelet profiles for temperature for CO/H$_2$/N$_2$ fuel obtained from flamelet equations on mixture fraction space. --- $\chi = 0.048$, -- - $\chi = 3.66$, - - - $\chi = 33.27$, - - - - $\chi = 155.41$, -- - $\chi = 600.46$ - - - $\chi = 1436.34$ /s

Figure 4.14: Flamelet profiles for mass fraction of CO for CO/H$_2$/N$_2$ fuel obtained from flamelet equations on mixture fraction space. --- $\chi = 0.048$, -- - $\chi = 3.66$, - - - $\chi = 33.27$, - - - - $\chi = 155.41$, -- - $\chi = 600.46$ - - - $\chi = 1436.34$ /s
Figure 4.15: Flamelet profiles for mass fraction of H₂ for CO/H₂/N₂ fuel obtained from flamelet equations on mixture fraction space. ——— χ = 0.048, —— χ = 3.66, ···· χ = 33.27, ····· χ = 155.41, ——— χ = 600.46 —····· χ = 1436.34/s

Figure 4.16: Flamelet profiles for mass fraction of H₂O for CO/H₂/N₂ fuel obtained from flamelet equations on mixture fraction space. ——— χ = 0.048, —— χ = 3.66, ···· χ = 33.27, ····· χ = 155.41, ——— χ = 600.46 —····· χ = 1436.34/s
Figure 4.17: Flamelet profiles for mass fraction of CO\textsubscript{2} for CO/H\textsubscript{2}/N\textsubscript{2} fuel obtained from flamelet equations on mixture fraction space.  \( \chi = 0.048, \) \( \chi = 3.66, \) \( \chi = 33.27, \) \( \chi = 155.41, \) \( \chi = 600.46 \) \( \chi = 1436.34 \text{ /s} \)

Figure 4.18: Flamelet profiles for mass fraction of OH for CO/H\textsubscript{2}/N\textsubscript{2} fuel obtained from flamelet equations on mixture fraction space.  \( \chi = 0.048, \) \( \chi = 3.66, \) \( \chi = 33.27, \) \( \chi = 155.41, \) \( \chi = 600.46 \) \( \chi = 1436.34 \text{ /s} \)
4.3 Flamelet library for H₂/CO flame

This fuel consists of 66.67 % H₂ and 33.33 % CO by volume. The flamelets are generated with a normalised fuel velocity of 3.5 and by the counterflow diffusion flame method on the Tsuji burner. Figures 4.19-4.22 and 4.23-4.26 show the flamelet profiles with and without the differential diffusion effect respectively. The flamelets are generated for the strain rates of 1.0, 100.0, 400.0, 2000.0, 6000.0, 12800.0 /s (extinction limit) with the differential diffusion effects and 1.0, 100.0, 400.0, 2000.0, 6000.0, 10500.0 /s (extinction limit) without the differential diffusion effects. The temperature is significantly influenced by the scalar dissipation rate. The peak temperature is reduced by about 1300 K for the differential diffusion flamelets and by about 800 K for Le=1.0 flamelets when the scalar dissipation rate is increased to the extinction limit. The effect of the scalar dissipation rate on the mass fraction of CO₂ is also significant. The mass fraction of H₂O is less influenced by the scalar dissipation rate. In can be seen from these figures that the differential diffusion has substantial effects on the magnitude and trend of the species concentrations. The peak mass fraction of CO₂ increases from about 0.05 to about 0.15 when equal diffusivities and unity Lewis number are assumed. The location of the peak also shifts from Z = 0.35 to Z = 0.15, overlapping with the location of temperature and H₂O peaks.
Figure 4.19: Flamelet profiles for temperature for H\textsubscript{2}/CO fuel obtained from counter flow diffusion flame method with differential diffusion effects. 

\[ \chi = 0.094, \quad \chi = 9.436, \quad \chi = 37.745, \quad \chi = 188.728, \quad \chi = 566.1848, \quad \chi = 1208.32 \text{ s} \]

Figure 4.20: Flamelet profiles for mass fraction of H\textsubscript{2}O for H\textsubscript{2}/CO fuel obtained from counter flow diffusion flame method with differential diffusion effects. 

\[ \chi = 0.094, \quad \chi = 9.436, \quad \chi = 37.745, \quad \chi = 188.728, \quad \chi = 566.1848, \quad \chi = 1208.32 \text{ s} \]
Figure 4.21: Flamelet profiles for mass fraction of CO$_2$ for H$_2$/CO fuel obtained from counter flow diffusion flame method with differential diffusion effects. $\chi = 0.094$, $\chi = 9.436$, $\chi = 37.745$, $\chi = 188.728$, $\chi = 566.1848$ $\chi = 1208.32$ /s

Figure 4.22: Flamelet profiles for mass fraction of OH for H$_2$/CO fuel obtained from counter flow diffusion flame method with differential diffusion effects. $\chi = 0.094$, $\chi = 9.436$, $\chi = 37.745$, $\chi = 188.728$, $\chi = 566.1848$ $\chi = 1208.32$ /s
Figure 4.23: Flamelet profiles for temperature for H$_2$/CO fuel obtained from counter flow diffusion flame method with unity Lewis number. 

- $\chi = 0.094$, 
- $\chi = 9.436$, 
- $\chi = 37.745$, 
- $\chi = 188.728$, 
- $\chi = 566.1848$, 
- $\chi = 990.82$ /s

Figure 4.24: Flamelet profiles for mass fraction of H$_2$O for H$_2$/CO fuel obtained from counter flow diffusion flame method with unity Lewis number. 

- $\chi = 0.094$, 
- $\chi = 9.436$, 
- $\chi = 37.745$, 
- $\chi = 188.728$, 
- $\chi = 566.1848$, 
- $\chi = 990.82$ /s
Figure 4.25: Flamelet profiles for mass fraction of CO₂ for H₂/CO fuel obtained from counter flow diffusion flame method with unity Lewis number.

- - - \( \chi = 0.094 \), ---- \( \chi = 9.436 \), - · - \( \chi = 37.745 \), · · · · \( \chi = 188.728 \),

- - - \( \chi = 566.1848 \) --- \( \chi = 990.82 \) /s

Figure 4.26: Flamelet profiles for mass fraction of OH for H₂/CO fuel obtained from counter flow diffusion flame method with unity Lewis number.

- - - \( \chi = 0.094 \), ---- \( \chi = 9.436 \), - · - \( \chi = 37.745 \), · · · · \( \chi = 188.728 \),

- - \( \chi = 566.1848 \) --- \( \chi = 990.82 \) /s
4.4 Flamelet library for CH$_4$/H$_2$ flame

The CH$_4$/H$_2$ fuel consists of 50 % CH$_4$ and 50 % H$_2$ by volume. The flamelet profiles are generated for the strain rates of 3.0, 20.0, 100.0, 500.0, 1800.0, 3600.0 /s (extinction value) with the full molecular transport and 3.0, 20.0, 100.0, 500.0, 1000.0, 1800.0 /s (extinction value) with the equal mass diffusivities flamelets. The extinction limit is halved when equal mass diffusivities are assumed for this flame. Figures 4.27-4.31 and 4.32-4.36 show the flamelet profiles with and without the differential diffusion effects. Unlike CO/H$_2$/N$_2$ and H$_2$/CO fuels, CH$_4$/H$_2$ fuel is less influenced by the scalar dissipation rate. The peak temperature is reduced by about 600 K for the differential diffusion flamelets and by about 400 K for the unity Lewis number flamelets. The peak temperature at the extinction condition is about 1800 K with and without the differential diffusion effect, which is about 500 K more than the peak temperatures of CO/H$_2$/N$_2$ and CO/H$_2$ flames at the extinction. The effect of the differential diffusion is observed in varying degrees for temperature and mass fractions of H$_2$O, OH and CO. The mass fractions of H$_2$ and OH are slightly reduced and the mass fraction of CO is slightly increased in the unity Lewis number flamelets as compared to the the differential diffusion flamelets. The CO$_2$ levels are almost doubled for the unity Lewis number case. The peak CO$_2$ for this fuel is located at the the stoichiometric mixture fraction, Z = 0.05, both with or without the differential diffusion effect.
Figure 4.27: Flamelet profiles for temperature for CH$_4$/H$_2$ fuel obtained from counter flow diffusion flame method with differential diffusion effects.

- $\chi = 0.064$, $\cdot \cdot \cdot \chi = 0.428$, $\cdot \cdot \cdot \chi = 2.139$, $\cdot \cdot \cdot \cdot \chi = 10.695$, $\cdot \cdot \cdot \cdot \cdot \chi = 38.505 - \cdot \cdot \chi = 77.01$ /s

Figure 4.28: Flamelet profiles for mass fraction of H$_2$O for CH$_4$/H$_2$ fuel obtained from counter flow diffusion flame method with differential diffusion effects.

- $\chi = 0.064$, $\cdot \cdot \cdot \chi = 0.428$, $\cdot \cdot \cdot \chi = 2.139$, $\cdot \cdot \cdot \chi = 10.695$, $\cdot \cdot \cdot \chi = 38.505 - \cdot \cdot \chi = 77.01$ /s
Figure 4.29: Flamelet profiles for mass fraction of CO$_2$ for CH$_4$/H$_2$ fuel obtained from counter flow diffusion flame method with differential diffusion effects. --- $\chi = 0.064$, ----- $\chi = 0.428$, ······ $\chi = 2.139$, ······ $\chi = 10.695$, ----- $\chi = 38.505$ ·· ·· $\chi = 77.01$ /s

Figure 4.30: Flamelet profiles for mass fraction of OH for CH$_4$/H$_2$ fuel obtained from counter flow diffusion flame method with differential diffusion effects. --- $\chi = 0.064$, ----- $\chi = 0.428$, ······ $\chi = 2.139$, ······ $\chi = 10.695$, ----- $\chi = 38.505$ ·· ·· $\chi = 77.01$ /s
Figure 4.31: Flamelet profiles for mass fraction of CO for CH$_4$/H$_2$ fuel obtained from counter flow diffusion flame method with differential diffusion effects. 

\[ \chi = 0.064, \quad \chi = 0.428, \quad \chi = 2.139, \quad \chi = 10.695, \quad \chi = 21.31 \cdot \cdot \cdot \chi = 38.502 / \text{s} \]

Figure 4.32: Flamelet profiles for temperature for CH$_4$/H$_2$ fuel obtained from counter flow diffusion flame method with unity Lewis number. 

\[ \chi = 0.064, \quad \chi = 0.428, \quad \chi = 2.139, \quad \chi = 10.695, \quad \chi = 21.31 \cdot \cdot \cdot \chi = 38.502 / \text{s} \]
Figure 4.33: Flamelet profiles for mass fraction of H$_2$O for CH$_4$/H$_2$ fuel obtained from counter flow diffusion flame method with unity Lewis number. $\chi = 0.064$, $\chi = 0.428$, $\chi = 2.139$, $\chi = 10.695$, $\chi = 21.31$ $\chi = 38.502$/s

Figure 4.34: Flamelet profiles for mass fraction of CO$_2$ for CH$_4$/H$_2$ fuel obtained from counter flow diffusion flame method with unity Lewis number. $\chi = 0.064$, $\chi = 0.428$, $\chi = 2.139$, $\chi = 10.695$, $\chi = 21.31$ $\chi = 38.502$/s
Figure 4.35: Flamelet profiles for mass fraction of OH for CH$_4$/H$_2$ fuel obtained from counter flow diffusion flame method with unity Lewis number. 

$\chi = 0.064, \quad \chi = 0.428, \quad \chi = 2.139, \quad \chi = 10.695,$

--- $\chi = 21.31 \cdots \chi = 38.502$/s

Figure 4.36: Flamelet profiles for mass fraction of OH for CH$_4$/H$_2$ fuel obtained from counter flow diffusion flame method with unity Lewis number. 

$\chi = 0.064, \quad \chi = 0.428, \quad \chi = 2.139, \quad \chi = 10.695,$

--- $\chi = 21.31 \cdots \chi = 38.502$/s
CHAPTER 5

Modelling of Correa and Gulati
Bluff Body Flame

In this chapter, an assessment of combustion models is presented for the simulation of a bluff body flame. The combustion models evaluated are the flame sheet, equilibrium, eddy break-up and laminar flamelet models. The combustion of syngas fuel (27.5% CO, 32.3% H₂ and 40.2% N₂ by volume) is investigated. The syngas fuel has a relatively high stoichiometric mixture fraction \( Z_{st} = 0.323 \) and as a result, the flame front lies in the shear layer. The high stretching rate at the shear layer prevents reactions from reaching the chemical equilibrium condition. This flame thus provides a suitable test case for the study of turbulence-chemistry interaction.

A brief description of the experimental setup is given first, followed by a description of some previous predictions for this flame. The results of the present predictions are then described. The effects of different flamelet profiles are presented in a separate section. The influence of discretization scheme on the predicted results is also discussed. Finally, a general discussion on the flame structure is given.

5.1 Experimental setup

The experiment of Correa and Gulati (1992) on a bluff body stabilised flame is simulated in the present study. The schematic drawing of the bluff body combustor is shown in Fig. 5.1. The fuel jet is located at the center of a 15 cm x 15 cm square wind tunnel. The diameter of the fuel jet is 3.18 mm and the diameter of the bluff body is 38.1 mm. The syngas fuel consisted of 27.5% CO, 32.3% H₂ and 40.2% N₂ by volume. The fuel and air jet velocities were 80.0 m/s and 6.5 m/s respectively. Temperature was 300 K for both the streams.
A detailed description of the experimental technique employed for the measurement of temperature and species concentrations has been reported in Correa and Gulati (1992). Raman scattering was used to determine concentrations of N₂, O₂, H₂, CO and CO₂. Among the major species, CO and CO₂ were the most difficult to measure with the Raman system. The values of the mixture fraction were calculated from the species concentrations using Bilger's formula (Bilger 1988). The radial profiles of temperature and species concentrations were reported at the downstream locations of the recirculation zone. In addition, the temperature-mixture fraction scatter plots were presented at x/d=5, x/d=10 and x/d=40 (where, x is the axial distance and d is the diameter of the fuel jet). These scatter plots showed significant non-equilibrium effects at x/d=5. At x/d=10, the deviation from the equilibrium condition was substantially small and at x/d=40, the flame was essentially equilibrated. Localised extinction was not observed at any axial location in the scatter plots. Thus, this flame provides a suitable test case for evaluating combustion models without considering the complex transient effects of local extinction, reignition and partial premixing. There were no reported measurements of mean or fluctuating velocity for this flame.
5.2 Previous predictions

This test case and data have widely been used to assess, validate and develop combustion models (Correa and Gulati 1992; Correa and Pope 1992; Gran and Magnussen 1996a; Gran et al. 1997; Biagioli 1997). Correa and Gulati (1992) used a partial equilibrium combustion and the $k-\varepsilon$ turbulence models to perform their own prediction. Their calculations showed an overprediction of the spreading rate of the fuel jet, especially at the downstream locations. This overprediction also resulted in poor predictions of species concentrations and temperature. They attributed this discrepancy to the shortcomings of the $k-\varepsilon$ model. Correa and Pope (1992) employed a hybrid Monte Carlo/finite volume method. In their calculations, the turbulence was modelled by the $k-\varepsilon$ model and the thermo-chemical condition was described by the same partial equilibrium model of Correa and Gulati (1992). Their predictions showed better agreements in general than those of Correa and Gulati (1992). An assessment of the standard $k-\varepsilon$, low Reynolds number $k-\varepsilon$ and Reynolds stress (RSM) models for this combustor geometry was reported by Gran et al. (1997). They used the flame-sheet model for combustion modelling. In their calculations, both the standard $k-\varepsilon$ and the low Reynolds number $k-\varepsilon$ models produced overprediction of the fuel jet and the RSM model provided better predictions. Gran and Magnussen (1996b) reported an assessment of the fast and the finite rate chemistry eddy dissipation concept (EDC) combustion models, the partial equilibrium model and the pdf transport method. According to their calculations, the EDC model with the finite rate chemistry provided an excellent agreement. Biagioli (1997) compared the partial equilibrium and the pdf transport models. His results were similar to those reported in other studies.

All previous predictions have shown that the effect of turbulence modelling is very important. The standard $k-\varepsilon$ model overpredicted the spreading rate of the fuel jet and therefore the correct evaluation of combustion models became difficult. The advanced turbulence models such as the RSM model yielded better predictions. In the present study, the $k-\varepsilon$ model with $C_{e1} = 1.60$ provides a very good prediction of the flow field. Thus in the present work, the assessment of combustion models is less influenced by the inaccuracy of the flow field calculation.
5.3 Present prediction

5.3.1 Numerical details

The combustion models are implemented within an in-house finite volume CFD code. The CFD code employs a non-uniform structured mesh system with staggered velocity control volumes. Two grid arrangements employing 97 (axial) x 87 (radial) and 122 (axial) x 87 (radial) non-uniform grids are used in the calculation. The grid arrangement is shown in Fig. 5.2. The grid lines are concentrated in the high shear region behind the bluff body. The influence of discretisation scheme is studied by employing hybrid, power law and TVD schemes.

There are some uncertainties in the specification of inlet conditions as experimental inlet data are not available. The velocity at the inlet is considered to be uniform according to Correa and Gulati (1992). The inlet turbulence parameters are specified as

\[ k_{in} = i U_i^2 \]  
\[ \varepsilon_{in} = \frac{C_{mu}^{1/4} k_{in}^{3/2}}{\lambda R} \]

where \( i \) is the turbulence intensity and \( \lambda \) is the length scale. In the present study, \( i = 0.01 \) and \( \lambda = 0.07 \) are used. Correa and Gulati (1992) mentioned that the effect of inlet condition was negligible for this flame as the turbulence generated in this flow rapidly overwhelmed the inlet level.
Figure 5.2: Grid arrangement; (a) 97x87 grids, (b) 122x87 grids
5.3.2 Comparison with previous studies

The results of the laminar flamelet combustion model calculations are compared with the predictions of Correa and Gulati (1992) and Gran and Magnussen (1996a). Correa and Gulati (1992) used the partial equilibrium model for combustion and the $k-\varepsilon$ model for turbulence. Gran and Magnussen (1996a) used the eddy dissipation concept (EDC) model for combustion and the $k-\varepsilon$ model for turbulence. In the present study, turbulence is modelled by the $k-\varepsilon$ model. The comparison of axial mixture fraction profile is shown in Fig. 5.3. The present study underpredicts the mixture fraction profile, but is in good agreement with the other predictions. The figure shows that three very different combustion models produce almost similar results. The discrepancy in the calculations were attributed to the turbulence modelling (Correa and Gulati 1992; Gran and Magnussen 1996a; Gran et al. 1997). The standard $k-\varepsilon$ turbulence model is known to overpredict the spreading rate of the jet. The turbulence model group of the International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames (TNF) (The Turbulence Model Group 1996) has recommended the use of the $k-\varepsilon$ model with $C_{t1} = 1.60$ for bluff body flames. The use of the $k-\varepsilon$ model with $C_{t1} = 1.60$ remarkably improves the prediction as shown in the same graph.
Chapter 5. Modelling of Correa and Gulati Bluff Body Flame

5.3.3 Comparison of combustion models

In this subsection, the results obtained by using the flame sheet, equilibrium, eddy break-up (EBU) and flamelet models are compared with each other and with the experimental data. In all the calculations, the $k-\varepsilon$ model with $C_{\varepsilon}=1.60$ was used for the turbulence closure. The hybrid discretisation scheme with 97 (axial) x 87 (radial) grids was used in the calculations. The effects of different discretisation schemes and the grid size are presented in subsection 5.3.5. For the laminar flamelet model, the flamelet libraries are generated with full molecular transport of the species.

The axial mixture fraction calculated by four combustion models are shown in Fig. 5.4. The mixture fraction values are overpredicted up to $x/d=10$ by all the models. This overprediction may be caused by the uncertainties of the inlet conditions. The flamelet model gives good prediction between $x/d=10$ and $x/d=20$ and then overpredicts further down stream. Other models overpredict the mixture fraction, though slightly, after $x/d=10$.

The radial mixture fraction profiles at two axial locations $x/d=10$ and $x/d=20$ are shown in Fig. 5.5. There is little difference among the calculations by four combustion models and the agreement is generally very good.
The good agreement of the mixture fraction profiles sets the stage for a meaningful evaluation of combustion models for the prediction of temperature and species concentrations. The radial temperature profiles are shown in Fig. 5.6. There are significant differences in the peak temperatures calculated by different combustion models at both the locations. The eddy break-up model overpredicts the peak temperature by about 400 K, the flame sheet model by about 200 K, the equilibrium model by about 150 K. The flamelet model overpredicts the peak temperature by about 100 K. The peak experimental temperature is approximately 1600 K, which is several hundreds below the equilibrium temperature of 2161 K (this equilibrium temperature is calculated by CHEMKIN-II code). This clearly indicates that the flame does not reach the equilibrium condition at these locations. The flamelet model incorporates the non-equilibrium effects and as a result, it provides a better agreement of the peak temperature. The combustion model based on the fast chemistry and one step reaction, such as the eddy break-up and flame sheet models, is found inadequate to reproduce peak temperature.

The mass fraction of H\textsubscript{2} is shown in Fig. 5.7. The prediction by all four models are similar, expect by the laminar flamelet model which underpredicts the centerline value at x/d=20. It is shown in the subsection 5.3.4 that the differential diffusion effect included in the flamelet library is responsible of this discrepancy. Figure 5.8 shows CO mass fraction profiles. All four combustion models overpredict the centerline value at x/d=10. The eddy break-up model predicts a narrower width of the CO profiles. The peak value of H\textsubscript{2}O is underpredicted by all the models as shown in Fig. 5.9, except by the laminar flamelet model. The flamelet model overpredicts the peak value as well as the fuel lean value. This behavior is consistent with the overprediction of temperature. The flame-sheet, equilibrium and EBU models overpredict temperature, but underpredict H\textsubscript{2}O mass fraction. This inconsistency was also reported by Correa and Gulati (1992).
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Figure 5.4: Axial mixture fraction profiles; comparison of combustion models

Figure 5.5: Radial mixture fraction profiles; comparison of combustion models
Figure 5.6: Radial profiles of temperature; comparison of combustion models

Figure 5.7: Radial profiles of mass fraction of H\textsubscript{2}; comparison of combustion model
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Figure 5.8: Radial profiles of mass fraction of CO; comparison of combustion models

Figure 5.9: Radial profiles of mass fraction of H2O; comparison of combustion models
5.3.4 Effects of flamelet profiles

The influence of different flamelet profiles on predictions by the laminar flamelet model is presented in this subsection. The flamelet profiles are generated by three different methods. These three methods are flamelet with differential diffusion effect, flamelet with unity Lewis number and flamelet equations based on conserved scalar space.

Figure 5.10 shows the comparison of different flamelets for the prediction of axial mixture fraction profiles. The agreement between the predicted and the experimental data is generally good for all the flamelets, but the initial core length is overpredicted. The differences among different flamelets are small up to x/d=20. After x/d=20, the differences start to emerge. The flamelet with differential diffusion effect overpredicts the mixture fraction after x/d=20, whereas the flamelet equations based on conserved scalar overpredicts up to x/d=20. The flamelet with Le=1.0 gives better prediction over the whole axial distance except over the initial core length.

The radial mixture fraction profiles at x/d=10 and x/d=20 are shown in Fig. 5.11. The predicted mixture fractions by different flamelets are very similar and are in very good agreement with the experimental data.

The radial temperature profiles are shown in Fig. 5.12. At both locations, the peak temperatures and the fuel lean temperatures are overpredicted by the flamelet with differential diffusion effect, underpredicted by the flamelet equations based on conserved scalar space and well predicted by the flamelet with unity Lewis number.

Figure 5.13 shows the radial mass fraction profiles of CO. Reasonably good agreement is obtained by all the flamelets. The radial mass fraction profiles of H₂ is shown in Fig. 5.14. The prediction by the flamelet with unity Lewis number and the flamelet equations based on conserved scalar space are identical and better than the prediction by the flamelet with differential diffusion effect. In the calculation of flamelet library with the differential diffusion effects, H₂ diffuses out of the fuel stream and diffuses towards the flame front because of the higher diffusion coefficient. This results in a lower concentration of H₂ in the fuel rich region. The radial mass fraction profiles of H₂O is shown in Fig. 5.15. The peak value of H₂O is underpredicted by the flamelet with unity Lewis number and the flamelet equations on conserved scalar space. The flamelet with the differential diffusion effect overpredicts the H₂O profiles. This overprediction of H₂O can be partly explained by the differential diffusion effects. As explained earlier, the higher diffusion of H₂ towards the flame front in the flamelet calculations results in
higher temperature and H₂O mass fraction. The comparison of the predicted results and the experimental data reveals that overall the flamelet model with unity Lewis number provides a better prediction and it also implies that the unity Lewis number is a better representation of the diffusion of species in turbulent flames. Recent experimental evidence also corroborates that the effects of differential diffusion is small in turbulent flames (Barlow and Frank 1998).
Figure 5.10: Axial mixture fraction profiles; effects of flamelet profiles

Figure 5.11: Radial mixture fraction profiles; effect of flamelet profiles
Figure 5.12: Radial temperature profiles; effect of flamelet profiles

Figure 5.13: Radial mass fraction of CO; effect of flamelet profiles
Figure 5.14: Radial mass fraction of $\text{H}_2$; effect of flamelet profiles

Figure 5.15: Radial mass fraction of $\text{H}_2\text{O}$; effect of flamelet profiles
5.3.5 Comparison of discretisation schemes

Three different discretisation schemes are used in order to assess the numerical error associated with the discretisation of the convection term. Three discretisation schemes used in the present study are the hybrid, power law and TVD schemes. Figure 5.16 shows the predicted results of the mean mixture fraction along the centreline. The predicted mean mixture fraction varies little among different schemes. The figure also shows the predicted axial mixture fraction by using the hybrid scheme with 122x87 grids. The figure shows that the effect of the refined grid size is small. Figure 5.17 shows radial profiles of the mean mixture fraction at two axial locations. Again, it is noted that the variations in the predicted results by using different schemes and the fine grid are small. Therefore, it can be concluded that the spatial discretisation error is small enough to allow the underlying mathematical models to be evaluated.

Figure 5.16: Axial mixture fraction profiles; comparison of discretisation schemes
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5.4 Discussion

Based on the results of the simulations, a number of general remarks can be made on the characteristic of the interactions between the turbulent flow field and the chemistry. From the predicted results of the mass fraction of H₂, CO and to a certain extent H₂O, it can be argued that the relatively simple equilibrium, eddy break-up or even the flame-sheet model is sufficient to produce very good predictions. However, that can not be argued for the temperature prediction. From the physical and chemical point of view, temperature is a very important quantity. In many practical applications, it is essential to obtain a correct temperature field. Only the laminar flamelet model has yielded good predictions of temperature profiles.

The predicted contour plots of the streamline, mixture fraction and temperature, calculated by the laminar flamelet model with Le=1.0, reveal the complex nature of the bluff body flame as shown in Figs. 5.18-5.20. An important region of the flame is the recirculation zone where the flame is stabilised. Unfortunately, no experimental data is available at this region to assess the performance of combustion models. The predicted recirculation zone at the face of the bluff body extends up to x/d=8. The mixture fraction contours show that the flame spreads like a jet and the stoichiometric mixture fraction (Z_{st} = 0.323) lies inside the shear layer. The predicted flame length is estimated to be
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\(x/d=44\) (where stoichiometric mixture fraction meets the center line). The recirculation zone contains lean mixtures and as a result, the temperature inside the recirculation zone is very low (see Fig. 5.20). Along the flame front, the temperature varies from 1600 K to 1700 K between \(x/d=5\) and \(x/d=20\). Figure 5.21 shows the predicted mean scalar dissipation rate. High values of the mean scalar dissipation rates are found near the fuel jet nozzle and in the shear layer between the fuel jet and the recirculation zone. The scalar dissipation rate varies between approximately \(50.0-110.0/\text{s}\) along the flame front in the region of \(x/d=5\) to \(x/d=20\). These high values of scalar dissipation rate prevent the chemical reactions from reaching the equilibrium condition. The flamelet profiles shown in the previous chapter indicates that the temperature is very sensitive to the scalar dissipation rate. The mass fraction of \(\text{H}_2\) and \(\text{CO}\) is not influenced by the scalar dissipation rate, whereas the mass fraction of \(\text{H}_2\text{O}\) is moderately sensitive to the scalar dissipation rate. This explains why the predicted results of mass fraction of \(\text{H}_2\), \(\text{CO}\) and to a certain extent \(\text{H}_2\text{O}\) by the flamelet model are similar to those calculated by the flame sheet, eddy break-up and equilibrium models, but the predicted results of temperature by the laminar flamelet model are different from those calculated by other models. The influence of the scalar dissipation rate incorporated in the flamelet model results in the predicted temperature of 1600 K-1700 K between \(x/d=5\) and \(x/d=20\) in comparison to the equilibrium temperature of 2161 K. At down stream locations, the scalar dissipation rate along the flame front is relaxed and the flame temperature approaches the equilibrium value. The peak temperature is located around \(x/d=44\) near the centerline.
Figure 5.18: Predicted contours of streamlines. The laminar flamelet model with unity Lewis number flamelet is used in the prediction.

Figure 5.19: Predicted contours of mixture fraction. The laminar flamelet model with unity Lewis number flamelet is used in the prediction. Note the location of the flame front where $Z = Z_{st}$.
Figure 5.20: Predicted contours of temperature in Kelvin. The laminar flamelet model with unity Lewis number flamelet is used in the prediction.

Figure 5.21: Predicted contours of the scalar dissipation rate in /s. The laminar flamelet model with unity Lewis number flamelet is used in the prediction.
5.5 Summary

1. The standard $k - \varepsilon$ model overpredicts the spreading rate of the fuel jet and that makes the meaningful evaluation of combustion models difficult. The $k - \varepsilon$ model with $C_{\varepsilon 1} = 1.60$ gives the accurate spreading rate of the fuel jet.

2. The peak experimental temperature at $x/d=10$ and $x/d=20$ is less than the equilibrium temperature. The flamelet model provides a very good prediction of the non-equilibrium peak temperature. All other models overpredict the peak temperature.

3. The predictions of major species (CO, H$_2$, H$_2$O etc.) by all four models are similar.

4. The flamelet model is found to be better than the other models assessed in the present study. It predicts temperature, major and minor species more accurately.

5. Among the flamelet profiles, the flamelet with unity Lewis number and the flamelet on the conserved scalar space provide better predictions. There is little difference between the predicted results of mass fractions of major species by the flamelet with unity Lewis number and by the flamelet equations based on the conserved scalar space. However, the temperature is slightly underpredicted by the flamelet equations based on the conserved scalar space.

6. The numerical errors associated with discretisation scheme are negligible.
In this chapter, the predictions of Sydney bluff body flames are presented. Results obtained with different combustion models are compared to one another and to the available experimental data. Fuels ranging from simple H₂/CO to complex CH₄/H₂ are investigated for different fuel inlet velocities to study the effect of turbulence-chemistry interaction. Unlike the bluff body flame presented in the previous chapter, experimental data are available inside the recirculation zone for these flames. These flames are well suited for the evaluation of combustion models as a compromise between a model problem and practical combustion situations.

First, a brief description of the experimental set up is given. Then, the inlet boundary conditions used in the simulation are described. The numerical details of the present work is presented next. The evaluation of combustion models for H₂/CO and CH₄/H₂ fuels are then presented. The effect of differential diffusion on the laminar flamelet model predictions is analysed. The sensitivity of the laminar flamelet models to different non-equilibrium parameters are presented next. Finally, some important aspects of the application of the combustion models are discussed and conclusions are drawn.

6.1 Experimental setup

An extensive set of experimental data documented and published by Dally et al. (1998) is used here to assess combustion models. The schematic drawing of the bluff body burner and corresponding measurement locations are shown in Fig. 6.1. The figure was obtained from Masri (1997). The bluff-body burner has an outer diameter $D_B = 50$ mm
Table 6.1: Fuels studied and relevant parameters

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Flame</th>
<th>$U_f/U_c$</th>
<th>$Re_f$</th>
<th>% BO</th>
<th>$T_{in}$</th>
<th>$Z_{st}$</th>
<th>$T_{ad}$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_2/CO$ (2:1)</td>
<td>HCl</td>
<td>134/40</td>
<td>17500</td>
<td>18</td>
<td>298</td>
<td>0.135</td>
<td>2400</td>
</tr>
<tr>
<td></td>
<td>HC2</td>
<td>321/40</td>
<td>41990</td>
<td>43</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$CH_4/H_2$ (1:1)</td>
<td>HM1</td>
<td>118/40</td>
<td>15800</td>
<td>50</td>
<td>298</td>
<td>0.05</td>
<td>2265</td>
</tr>
<tr>
<td></td>
<td>HM2</td>
<td>178/40</td>
<td>23900</td>
<td>75</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>HM3</td>
<td>214/40</td>
<td>28700</td>
<td>91</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

¹ BO stands for Blow off

and a concentric jet diameter $D_j = 3.6$ mm. The burner was placed in a wind tunnel of $254 \times 254$ mm cross section. The single point Raman/Rayleigh/LIF technique was used to measure temperature, concentration of CO$_2$, CO, H$_2$O, H$_2$, O$_2$, N$_2$, OH and NO. Fuels ranging from simple $H_2/CO$ to complex $CH_4/H_2$ were investigated by Dally et al. (1998) at various mean fuel inlet velocities. The complete data set is available from the world wide web (Masri 1997). Two different fuels are investigated in the present study: $H_2/CO$ (2:1 by volume) and $CH_4/H_2$ (1:1 by volume) for different fuel inlet velocities. $H_2/CO$ flames did not show localised extinction for the velocities studied, while $CH_4/H_2$ flames showed considerable local extinction at the neck zone for higher velocities. A list of the flames investigated in the present study and some relevant parameters are given in Table 6.1 according to Dally et al. (1998). These flames provide an ideal situation for the study of turbulence-chemistry interaction for flames far from equilibrium and for flames with local extinction.

### 6.1.1 Measurements uncertainty

In order to evaluate any mathematical model quantitatively against the experimental data it is very important to know the error associated with the measurements. Dally et al. (1998) reported that the error associated with the bluff body flame were resulted from many factors such as shot noise, electronic noise, error associated with optical set up, spatial resolution error, the cross talk between the Raman signals, the fluorescence interference from soot precursors and other molecules and the interpolation of the Raman calibration factors. An estimate of the precision of the single-point measurements given in Dally et al. (1998) for two typical samples of a $CH_4/H_2$ flame are reproduced in the Table 6.2. The errors associated with the interference and the spatial resolution were not given as these errors are difficult to quantify (Dally et al. 1998). The fluo-
Chapter 6. Modelling of Sydney Bluff Body Flames

Figure 6.1: Schematic drawing of a bluff body stabilised flame and measurement locations
Table 6.2: Sample estimates of error associated with measured species concentrations for two typical sample compositions

<table>
<thead>
<tr>
<th>Sample</th>
<th>Temperature</th>
<th>Species</th>
<th>% Mass Fraction</th>
<th>% Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lean</td>
<td>1900</td>
<td>O₂</td>
<td>4.0</td>
<td>10.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>N₂</td>
<td>75.0</td>
<td>0.8</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CO₂</td>
<td>8.0</td>
<td>4.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CO</td>
<td>2.0</td>
<td>9.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>H₂</td>
<td>0.5</td>
<td>12.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>H₂O</td>
<td>11.0</td>
<td>5.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>OH</td>
<td>0.3</td>
<td>3.8</td>
</tr>
<tr>
<td>Rich</td>
<td>1400</td>
<td>CH₄</td>
<td>18.0</td>
<td>2.3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>N₂</td>
<td>57.0</td>
<td>1.1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CO₂</td>
<td>5.5</td>
<td>5.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CO</td>
<td>5.5</td>
<td>8.3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>H₂</td>
<td>2.5</td>
<td>4.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>H₂O</td>
<td>12.0</td>
<td>4.0</td>
</tr>
</tbody>
</table>

rescence interference affects only selected species. The fluorescence interference from soot precursors is very low for these flames. Hydrocarbon flames are most affected by the interference and CO line suffers the highest interference levels. The error associated with fluorescence interference is generally less than 10% (Dally et al. 1998). The spatial resolution error estimates are also given in Dally et al. (1998). According to them, the maximum resolution error is 9% at X/D_B = 0.0 and r/R_b = 0.06. At all locations where r/R_b ≥ 0.25 the error is less than 4%. The maximum error associated with the NO measurements was reported to be approximately 10% (Dally et al. 1998).

6.2 Numerical details

6.2.1 Initial and boundary conditions

The experimental data can only be fully exploited for the evaluation of the numerical models if reliable and accurate boundary conditions are available for use in the simulation. The specification of the boundary conditions at symmetry axis, solid wall and outlet plane is well defined as explained in section 3.3. The specification of inlet conditions requires information from measurements, which is described below.

The measured mean velocity \( \bar{u} \) and its rms fluctuations \( u' \) are provided in Masri et al. (1996). Figure 6.2 shows these experimental inlet conditions. Both the mean velocity
and the rms velocity fluctuations are taken as zero on the bluff body wall. The inlet velocity specified in Masri et al. (1996) for modelling deviates slightly from the actual experimental data as the sharp changes are intentionally avoided for numerical stability. However, Masri et al. (1996) argued that the momentums are within 2% of the specified value. When the specified initial profiles are used, the calculation underpredicted the mean mass flow rate and calculated momentum flow rate for the fuel jet. The underprediction is also evident in the radial velocity profiles as shown in Fig. 6.4. The fuel jet nozzle extends to more than 40 diameters upstream of the burner surface. Thus the flow may be considered to be fully developed at the exit of the jet. The fully developed profiles as shown in Fig. 6.3 are then specified at the inlet. The fully developed inlet specification provides a better prediction of velocity as shown in Fig. 6.4. Dally et al. (1998) also specified the fully developed profiles at the inlet instead of the experimental initial conditions of Masri et al. (1996) in their simulation.

6.2.2 Computational grids

To compute the flow field around the bluff-body, the computational domain is extended to 170 mm in the radial direction and 216 mm in the axial direction. Two grid arrangements employing 99 (axial) x 89 (radial) and 217 (axial) x 197 (radial) grids are used in the calculations. The grid arrangement is shown in Fig. 6.5. The grids are concentrated near the fuel exit to resolve the shear layers. The differences in the predicted results between the two grid arrangements are small and are discussed later. The results obtained by using the coarse grid are found to be accurate enough for the evaluation of performance of different combustion models.
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Figure 6.2: Experimental initial conditions for (a) mean velocity and (b) its rms fluctuations

Figure 6.3: Fully developed initial conditions for (a) mean velocity and (b) its rms fluctuations
Figure 6.4: Comparison of radial velocity profiles at different axial locations.

- Experimental data, —— fully developed inlet profiles, —— experimental inlet velocity profiles
Figure 6.5: Grid arrangement; (a) 99x89 grids and (b) 217x197 grids
6.3 Evaluation of combustion models

The combustion models are evaluated by comparing radial profiles of mean mixture fraction, variance of mixture fraction, temperature and concentrations of major and minor species at different axial locations. These locations lie inside the recirculation zone as well as at the neck zone. It is important to have some idea about the structure of the flame in order to evaluate and explain the results of the predictions. A description of the flame structure in the bluff body burner of the present work is given by Dally et al. (1998). The bluff body stabilised flames are characterised by three distinct zones: recirculation zone, neck zone and jet-like zone. The recirculation zone is formed at the face of the bluff body, extends about one bluff body diameter downstream. The recirculation zone has a larger vortex on the air side and depending on jet velocity a smaller vortex close to the fuel jet. With increasing fuel jet velocity relative to the coflow air stream, the fuel jet expands and shifts the core of the inner vortex downstream until it loses its recirculation pattern. The outer vortex becomes shorter and smaller. Downstream of the recirculation zone is the neck zone. The neck zone is characterised by intense mixing. Non equilibrium effects and when the jet velocity is sufficiently high, local extinction is observed at this zone. The third zone is the rest of the flame which spreads in a jet like manner.

The combustion models assessed are the flame sheet, equilibrium and laminar flamelet models. The equilibrium model has known shortcomings for hydrocarbon fuels. Therefore, the constrained equilibrium model is also assessed for the CH\textsubscript{4}/H\textsubscript{2} flames. Details of the combustion models are described in chapter 2. The predicted results of each flame are described separately beginning with the H\textsubscript{2}/CO flames.

6.3.1 H\textsubscript{2}/CO flames

Predicted results are presented for two flames, first with a fuel jet velocity of 134 m/s (HC1), the second with one of 321 m/s (HC2). These velocities correspond to about 18 % and 43 % of the velocity at global extinction.
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HC1 flame

The HC1 flame consists of H$_2$/CO (2:1 by volume) and the flame has a mean inlet velocity of 134 m/s. This flame does not show local extinction.

Figure 6.6 shows the radial mixture fraction profiles at four axial locations. The predicted length of the recirculation zone for this flame is $x/D=1.3$. Therefore the first three locations are inside the recirculation zone and the last location is at the neck zone. Predictions by all four models are very similar at $x/D=0.26$, $x/D=0.6$ and $x/D=1.8$. At $x/D=0.9$, the laminar flamelet model with the differential diffusion effect shows lower values compared to those shown by the other models near the centre of the fuel jet. At $x/D=0.26$, the experimental mixture fraction has a flat profile in the outer region between $r=5$ mm to $r=23$ mm. This region contain slightly lean mixtures. The calculations by all the combustion models however do not reproduce the experimental flat profile in the outer region. The mixture fraction profile is overpredicted until $r=10$ mm and then underpredicted further away. At $x/D=0.6$, the mixture fraction is again overpredicted until $r=10$ mm and then underpredicted further away. The same behaviour of the predicted results are also observed at $x/D=0.9$, where the predicted mixture fractions cross the experimental value at $r=7$ mm. At $x/D=1.8$, the mixture fraction is underpredicted until $r=14$ mm and then the agreement is very good further away.

Radial profiles of mixture fraction variance are shown in Fig. 6.7. Again, it is shown that the differences among different combustion model predictions are small. Three distinct mixing layers are evident from these profiles inside the recirculation zone ($x/D<0.9$) by the presence of multiple maxima of mixture fraction variance. The outer mixing layer lies around $r=23$ mm on the outer edge of the outer vortex where mixing between this vortex and the coflowing air occurs. The location of the outer mixing layer as well as the peak value of the mixture fraction variance is well predicted. The second layer of mixing lies between the inner and outer vortex region and is characterised by the gradual increase of mixture fraction variance. This intermediate mixing layer is clearly evident at $x/D=0.6$ and $x/D=0.9$. At $x/D=0.26$, this mixing layer is not evident in the measurements, as the lower part of both inner and outer vortices are well mixed. The peak value of rms fluctuations is overpredicted for this mixing layer and the location of the mixing layer is also underpredicted. The third layer lies between the fuel jet and the inner vortex. This layer has the highest rms fluctuations of the mixture fraction. The location of this zone is well predicted, although the peak rms value of the mix-
ture fraction fluctuations is overpredicted. Outside the recirculation zone ($x/D > 0.9$), the mixture fraction variance is characterised by a single peak in the shear layer of the jet-like flow. The location of the peak is slightly underpredicted.

Radial profiles of $H_2$ and CO are shown in Figs. 6.8 and 6.9. These profiles are similar to the mixture fraction profiles and indicate that the fuel break down rate is reasonably well represented.

Radial temperature profiles are shown in Fig. 6.10. At $x/D=0.26$, the location of the peak temperature is reasonably well predicted by all the combustion models. The predicted peak temperature by the flame sheet model is more closer to the experimental peak. All other models underestimate the peak value. These underpredictions of the peak temperature are caused by the overprediction of the mixture fraction fluctuations. Only the flamelet model with differential diffusion effect provides a good agreement in the fuel lean zone. At $x/D=0.6$, the peak temperature as well as the location of the peak value is accurately predicted by the flame sheet model. The other models underpredict the peak temperature. The temperature in the lean side is reasonably well predicted by the flamelet with differential diffusion effects and underpredicted by the all other models. The temperature is reasonably well predicted by all the models at $x/D=0.9$. At $x/D=1.8$, the flame sheet model overpredicts the peak temperature by about 400 K, the equilibrium model overpredicts by about 350 K, the flamelet model with the differential diffusion effect overpredicts by the about 150 K and the flamelet model with unity Lewis number overpredicts by about 100 K.

Figure 6.11 shows the radial profiles of the mass fraction of $H_2O$. The equilibrium and the laminar flamelet model with unity Lewis number produce similar mass fraction profiles of $H_2O$ and both the models underpredict the $H_2O$ profiles at $x/D=0.26$, $x/D=0.6$ and $x/D=0.9$. At $x/D=1.8$, the equilibrium and the laminar flamelet model with unity Lewis number produce good predictions. The flamelet model with the differential diffusion effect overpredicts the $H_2O$ mass fraction and the flame sheet model produces underprediction at all locations.

Radial profiles of mass fraction of $CO_2$ is shown in Fig. 6.12. At $x/D=0.26$, the experimental data shows a flat profile of $CO_2$ mass fraction in the outer zone, which is not evident in the temperature and $H_2O$ mass fraction profiles. The flamelet model with the unity Lewis number and the equilibrium model reproduce this flat $CO_2$ profile reasonably well. The equilibrium model however produces an unrealistic peak in the fuel rich zone. The flame sheet model yields a sharp peak at $r=5$ mm, which is not seen
in the measured data. The flamelet model with full molecular transport underpredicts
the peak value by about 75% at \( x/D = 0.26 \) and at other locations, the level of underpre-
diction is slightly reduced. The predictions by the flamelet model with the unity Lewis
number are very good at \( x/D = 0.9 \) and reasonably good at \( x/D = 1.8 \) and \( x/D = 0.9 \). The
predictions of the mass fraction of CO\(_2\) by the equilibrium model suffer from producing
the unrealistic double peaks at \( x/D = 0.6 \) and \( x/D = 0.9 \). However, the equilibrium predic-
tion is good at \( x/D = 1.8 \). The flame sheet model overpredicts the peak level of CO\(_2\) and
the overprediction is specially severe at \( x/D = 1.8 \).

The last quantity used to evaluate the combustion models is the OH concentrations.
The OH concentrations are shown to be present in super-equilibrium quantities in the
upstream part of the flames (Drake et al. 1984; Correa and Gulati 1988; Barlow et al.
1990). The radicals are formed in the two-body reaction involving two reactants and
(usually) two products. These reactions generally have high Damköhler numbers, i.e.
they are fast compared to the flow process. The radicals are consumed in three-body
recombination reactions. The Damköhler number associated with the recombination
reactions are considerably lower. As a result, the radical concentrations will gener-
ally be substantially above the equilibrium levels. One of the stringent tests of com-
bustion models is whether it can predict the OH level accurately. Figure 6.13 shows
predicted OH profiles together with the experimental data. The OH levels predicted
by the equilibrium model are 2-3 times lower than the measured value. The laminar
flamelet model predicts qualitatively the super-equilibrium level of OH. The flamelet
model with \( Le = 1.0 \) predicts accurately the peak value of OH, but the OH level is un-
derpredicted in the fuel lean zone except at \( x/D = 1.8 \). The underprediction is specially
severe at \( x/D = 0.6 \). The measured OH profiles decay towards the equilibrium value at
the downstream locations. This decay is well predicted by the laminar flamelet model.
Figure 6.6: Radial profiles of mixture fraction in the HCl flame. 
- measurements, —— flame sheet, ······ equilibrium, —— flamelet with differential diffusion, ——— flamelet with Le=1.0
Figure 6.7: Radial profiles of mixture fraction variance in the HCl flame.

- Measurements, --- flame sheet, ······ equilibrium, --- flamelet with differential diffusion, - - - flamelet with Le=1.0
Figure 6.8: Radial profiles of mass fraction of H₂ in the HCl flame.

O measurements, —— flame sheet, ····· equilibrium, --- flamelet with differential diffusion, ····· flamelet with $Le=1.0$
Figure 6.9: Radial profiles of mass fraction of CO in the HCl flame.
- Measurements, --- flame sheet, ····· equilibrium, -- flamelet with differential diffusion, ····· flamelet with Le=1.0
Figure 6.10: Radial profiles of temperature in the HCl flame.
○ measurements, −−−− flame sheet, ····· equilibrium, −−−− flamelet with differential diffusion, −−−−− flamelet with Le=1.0
Figure 6.11: Radial profiles of mass fraction of H$_2$O in the HCl flame.
- measurements, --- flame sheet, · · · · equilibrium, -- flamelet with differential diffusion, · · · · flamelet with Le=1.0
Figure 6.12: Radial profiles of mass fraction of CO\textsubscript{2} in the HCl flame.
- Measurements, --- flame sheet, ----- equilibrium, ---- flamelet with differential diffusion, ----- flamelet with Le=1.0
Figure 6.13: Radial profiles of mass fraction of OH in the HCl flame. 
○ measurements, ······ equilibrium, --- flamelet with differential diffusion, - - - flamelet with Le=1.0
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HC2 flame

The flame considered here consists of H2/CO (2:1 by volume) and has an inlet velocity of 321 m/s. This velocity is 43 % of the blow-off velocity.

Figure 6.14 shows the radial profiles of the mean mixture fraction at different axial locations. The predicted results of the mixture fraction by all the combustion models are similar. Inside the recirculation zone (x/D<0.9), the experimental mixture fraction in the outer region is less than that in the HC1 flame. The mixture fraction at the outer zone is slightly underpredicted at x/D=0.26, x/D=0.6 and x/D=0.9. At x/D=1.8, the agreement between the predictions and the measurements is reasonably good.

Radial profiles of mixture fraction variance are shown in Fig. 6.15. At x/D=0.26, three mixing layers are observed from the mixture fraction fluctuations. The location of the outer mixing layer as well as the value of the rms fluctuations is well predicted by all the combustion models. The intermediate mixing layer is lost because the lower part of the outer vortex is well mixed with the inner vortex. The predictions of the rms fluctuations in this zone are much improved than those in the HC1 flame at the same location. The location of the inner mixing layer is also well predicted. However, the peak value of the rms fluctuations is overpredicted by 80 % by the flame sheet and equilibrium models and by 60 % by the laminar flamelet model with and without the differential diffusion effect. At x/D=0.6, the peak value of the mixture fraction variance is overpredicted by all the combustion models, however, the trend of the mixture variance is well predicted. The predictions at x/D=0.9 are similar to those at x/D=0.6. At x/D=1.8, the predicted results are more closer to the measurements. The differences among the predictions obtained from different combustion models are also observed at this location and the laminar flamelet model with the differential diffusion effect produces a better prediction. The overprediction of the peak values of the mixture fraction variance is a result of the shortcomings of the \( k - \varepsilon \) turbulence model. It is well known that the \( k - \varepsilon \) model overpredicts turbulence levels inside the recirculation zone.

Figures 6.16 and 6.17 show mass fraction of CO and H2 profiles. Predictions of mass fraction of CO and H2 are reasonably good by all the combustion models.

Radial temperature profiles are shown in Fig. 6.18. At x/D=0.26, the flame sheet model overpredicts the peak temperature by about 500 K and the equilibrium model overpredicts by about 400 K. The laminar flamelet model with both the differential diffusion and Le=1.0 overpredict the peak temperature in the range of 200 K. The dif-
ference in temperature predicted by the flamelet model with and without the differential diffusion effect is comparatively small. At all other locations, the peak temperature is reasonably well predicted by the laminar flamelet model and overpredicted by the flame sheet and equilibrium models. The experimental temperature inside the recirculation zone \((x/D<0.9)\) and at the outer outer region is about 800 K less than that found in the HCl flame. The temperature at this region is underpredicted by all the combustion models. The reason behind the underprediction of temperature is the underprediction of mixture fraction in these regions. A slight underprediction of the mixture fraction has resulted in about 300 K underestimation of temperature. This behaviour is however consistent with the observation that the temperature is very sensitive to the mixture fraction in the lean side. It is estimated, from the flamelet library of H\(_2\)/CO fuel described in section 4.3, that an error of 0.012 in the mixture fraction leads to an error of about 300 K in the temperature. Therefore it is essential to obtain a very good prediction of the mixture fraction in the lean side in order to achieve a good prediction of temperature.

Radial mean mass fraction profiles of H\(_2\)O are shown in Fig. 6.19. The shape of the H\(_2\)O profiles is similar to that of the temperature. At \(x/D=0.26\), the peak value of H\(_2\)O mass fraction is overpredicted by the laminar flamelet model with differential diffusion effect by about 33\%, the equilibrium model by about 16\%, the laminar flamelet model with \(Le=1.0\) by about 6\%. The flame sheet model provides a good agreement. The laminar flamelet model with differential diffusion effect provides a good prediction in the fuel lean zone. All the other models underpredicts in the fuel lean zone. At \(x/D=0.6\), the flame sheet model underpredicts the peak value slightly and the flamelet model with \(Le=1.0\) overpredicts by the same amount. The equilibrium and the flamelet model with differential diffusion effect overpredict the peak value by varying degrees. At \(x/D=0.9\), the prediction of the peak H\(_2\)O is reasonably good by the equilibrium and the flamelet model with \(Le=1.0\). The flame sheet model provides underprediction and the flamelet model with differential diffusion effects provides overprediction of the peak value of H\(_2\)O. The mass fraction of H\(_2\)O is underpredicted in the fuel lean zone by all the combustion models at \(x/D=0.6\) and \(x/D=0.9\). The flame sheet model yields a very good agreement at \(x/D=1.8\). The equilibrium and the flamelet model with \(Le=1.0\) overpredict the H\(_2\)O profile slightly. The flamelet model with differential diffusion effect produces significant overprediction.

Large differences in the predicted results obtained by different combustion models are observed in the CO\(_2\) profiles as shown in Fig. 6.20. The flamelet model with the
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differential diffusion effect underpredicts the CO₂ level by approximately 75% and the flame sheet model overpredicts by about 50% at all locations. The laminar flamelet model with unity Lewis number yields reasonably good agreement at x/D=0.6 and x/D=0.9. At both x/D=0.26 and x/D=1.8, the laminar flamelet model with and without the differential diffusion effect gives overprediction. The predictions of the peak CO₂ and the lean value by the equilibrium model are comparable to those by the laminar flamelet model with unity Lewis number. However, the equilibrium model produces an unrealistic peak in the fuel rich side.

Figure 6.21 shows the mass fraction profiles of OH. Like the HCl flame, the HC2 flame shows super-equilibrium quantity of OH. The laminar flamelet model with unity Lewis number provides a very good prediction of the OH levels at x/D=0.26, x/D=0.6 and x/D=0.9. At x/D=1.8, the laminar flamelet model with unity Lewis number overpredicts the peak value. The experimental data show a gradual decay of the OH level from x/D=0.26 to x/D=1.8. The laminar flamelet model with unity Lewis number underestimates this decay rate. The laminar flamelet model with differential diffusion effect correctly predicts the width of the OH profiles at all the locations, but the model overestimates the peak value of OH by about 25%. The predicted OH levels by the equilibrium model are 2-3 times lower than the experimentally measured levels.
Figure 6.14: Radial profiles of mixture fraction in the HC2 flame.
- measurements, — flame sheet, · · · · equilibrium, — flamelet with differential diffusion, · · · flamelet with Le=1.0
Figure 6.15: Radial profiles of mixture fraction variance in the HC2 flame.

- Measurements, —— flame sheet, ····· equilibrium, —— flamelet with differential diffusion, ··· flamelet with Le=1.0
Figure 6.16: Radial profiles of mass fraction of H₂ in the HC2 flame.

- ○ measurements,
- -- flame sheet,
- ···· equilibrium,
- --- flamelet with differential diffusion,
- ···· flamelet with Le=1.0
Figure 6.17: Radial profiles of mass fraction of CO in the HC2 flame.
- measurements, —— flame sheet, ····· equilibrium, —— flamelet with differential diffusion, —— flamelet with Le=1.0
Figure 6.18: Radial profiles of temperature in the HC2 flame. 
- measurements, --- flame sheet, ···· equilibrium, --- flamelet with differential diffusion, ···· flamelet with $Le=1.0$
Figure 6.19: Radial profiles of mass fraction of $\text{H}_2\text{O}$ in the HC2 flame. 
$\bigcirc$ measurements, $\cdots$ flame sheet, $\cdots\cdots$ equilibrium, $\cdots\cdots\cdots$ flamelet with differential diffusion, $\cdots\cdots\cdots\cdots$ flamelet with $Le=1.0$
Figure 6.20: Radial profiles of mass fraction of CO₂ in the HC2 flame. 
- Measurements, --- flame sheet, ····· equilibrium, --- flamelet with differential diffusion, -- flamelet with Le=1.0
Figure 6.21: Radial profiles of mass fraction of OH in the HC2 flame.
- Measurements, -- flame sheet, —— equilibrium, —— flamelet with differential diffusion, ···· flamelet with Le=1.0
6.3.2 CH₄/H₂ Flames

Three different flames are presented for this fuel. These flames are the HM1 with jet velocity of 118 m/s, the HM2 with 178 m/s and the HM3 with 214 m/s. These velocities are 50%, 75% and 91% of the blow-off velocity respectively.

HM1 flame

The comparison of the measurements and the predictions for the HM1 flame is considered here. This flame does not exhibit local extinction and subsequent reignition. Figure 6.22 shows radial profiles of the mixture fraction at six axial locations. It is essential that the flow field is adequately represented in the simulation, because the mixture fraction statistics completely determine the thermo-chemistry of the flame. It is even more important for the CH₄/H₂ flame which has a low stoichiometric mixture fraction ($Z_{st}=0.05$). A small error in mixture fraction field for this fuel will lead to a large error in temperature, other species calculations and in the location of the flame front. At $x/D=0.26$, the core of the outer region contains fuel rich mixture and the stoichiometric mixture fraction exist at the edge of the outer vortex. All the combustion models produce similar predictions for the mixture fraction profiles. Though the radial mixture fraction is reasonably well predicted by all the combustion models in the fuel rich zone until $x/D=1.3$, a small amount of underprediction is observed in the outer edge of the outer vortex. Further downstream, the value near the centerline is underpredicted by all the models. Clearly, the decay rate is not well represented even after modifying the $C_{e1}$.

Radial profiles of the mixture fraction variance are shown in Fig. 6.23. As in H₂/CO flames, three distinct mixing layers inside the recirculation zone are evident from these profiles by the presence of multiple maxima. At $x/D=0.26$, the location of the outer mixing layer at $r=24$ mm as well as the peak rms value of the mixture fraction fluctuations is well predicted by all the combustion models. The predicted mixture fraction variances show a gradual decay inside the core zone of the outer vortex, whereas the measured mixture fraction profile shows a flat profile. The peak value of the mixture fraction variance in the inner mixing layer is overpredicted by all the combustion models. However, the predictions by the flamelet model with and without the differential diffusion effect are closer to the experimental data. At $x/D=0.6$, the laminar flamelet models both with and without the differential diffusion effect produce reasonably good
prediction of the mixture fraction variance at the inner mixing layer \((r=2\ \text{mm})\). The other models overpredict the mixture fraction variance. All the combustion models fail to predict correctly the location of the maxima of the measured mixture fraction variance at \(r=13\ \text{mm}\). However, all the combustion models produce good predictions at the outer mixing layer at \(r=23\ \text{mm}\). At \(x/D=0.9\), the laminar flamelet model with the differential diffusion effect and with the unity Lewis number provides a good agreement of the inner mixing layer at \(r=4\ \text{mm}\). The other models give overprediction of the rms value of the mixture fraction fluctuations. The location of the measured maxima at \(r=12\ \text{mm}\) is underpredicted by all the models and the peak value of the mixture fraction variance is also overpredicted. At \(x/D=1.3\), \(x/D=1.8\) and \(x/D=2.4\), the profiles of the mixture fraction variance show a single peak similar to jet flows. The location of the peak value is underpredicted by all the combustion models, however, the level of the peak value is reasonably well predicted at \(x/D=1.8\) and \(x/D=2.4\).

Radial profiles of \(\text{CH}_4\) and \(\text{H}_2\) are shown in Figs. 6.24 and 6.25. These profiles are similar to the mixture fraction profiles. The equilibrium model underpredicts the \(\text{CH}_4\) profiles, whereas the prediction by other models are reasonable. The slight underprediction at \(x/D=1.8\) and \(x/D=2.4\) is caused by the underprediction of mixture fraction. The profiles of \(\text{H}_2\) are again poorly predicted by the equilibrium model. The flamelet model with the differential diffusion effect underpredicts the \(\text{H}_2\) profiles in the fuel rich side.

Figure 6.26 shows the temperature profiles at different axial locations. The temperature is well predicted by all the models except the equilibrium model, and the predicted peak temperatures are within 100 K for different models at all the locations except at \(x/D=0.26\). At this location, the peak temperature is underpredicted in the range of 400 K-500 K by different combustion models. Dally et al. (1998) also reported similar underpredictions in their simulations and stated that the lower measured temperature as compared to calculations is due to the averaging effects as a result of the intermittency in the flame at this location and the underprediction is not due to the shortcomings in the simulations. The equilibrium model produces an unrealistic low temperature in the fuel rich zone at \(x/D=0.26\) and at other locations, it also produces lower temperature.

Figure 6.27 shows radial profiles of mass fraction of \(\text{H}_2\text{O}\). The flame sheet, constrained equilibrium and laminar flamelet model with \(\text{Le}=1.0\) produce very good predictions at all the locations. The equilibrium model produces unrealistic double peaks and underpredictions in the fuel rich zone. The flamelet with full molecular transport overpredicts \(\text{H}_2\text{O}\) level at all the locations.
Radial profiles of CO\textsubscript{2} mass fraction is shown in Fig. 6.28. As in H\textsubscript{2}/CO flames, large differences in the predicted results obtained by different combustion models are observed for the CO\textsubscript{2} profiles. The flame sheet model overpredicts the CO\textsubscript{2} mass fraction by about 100\% at all the locations. The laminar flamelet model with the full molecular transport underpredicts the CO\textsubscript{2} level inside the recirculation zone by about 50\%. However, the prediction by the laminar flamelet model with the full molecular transport improves further downstream. The equilibrium model shows unrealistic double peaks at x/D=0.26. Predictions at other locations by the equilibrium model are however good. The flamelet model with Le=1.0 and the constrained equilibrium model produce a reasonably good agreement inside the recirculation zone, the agreement somewhat deteriorates further downstream.

Radial profiles of OH mass fraction is shown in Fig. 6.29. The reaction zone of OH is thin in the upstream zone specially at x/D=0.26 and then it gradually increases. The thin reaction zone at x/D=0.26 is well predicted by all the combustion models. The experimental data shows a very low value of OH at x/D=0.26 and then the OH level gradually increases until x/D=0.9 and then decreases further downstream. All the combustion models overpredict the OH level at x/D=0.26. The overprediction of the OH level by the equilibrium and constrained equilibrium models are very surprising because it is shown in all other flames studied here that the calculated equilibrium profiles of OH in the upstream part of the flames are 2-3 times less than the measured value. Therefore the lower OH level at this location compared to the predicted results might be a result of intermittency in the flame similar to the temperature measurement and the overprediction of OH level by the equilibrium and constrained equilibrium models conveys a somewhat misleading conclusion. As expected, at all other locations, the equilibrium and constrained equilibrium models underpredict the OH level. The predictions by the laminar flamelet model with unity Lewis number is very good and the model also predicts the rate of decay of the OH level reasonably well. The flamelet model with the differential diffusion effect overpredicts the OH level at all the locations.

The predictions of CO profiles are very poor in general by all the combustion models as shown in Fig. 6.30. The equilibrium model severely overpredicts the CO profiles and also underpredicts the location of the peak value. The constrained equilibrium model is essentially an ad-hoc modification to the equilibrium model to reproduce the correct CO level. The constrained equilibrium model shows success at x/D=0.26 for predicting the CO level. However, at other locations it fails to reproduce the correct CO profiles.
The laminar flamelet model with both the full molecular transport and the \( \text{Le}=1.0 \) underpredict the CO level at all the locations. The scatter plot at \( x/D=1.8 \) reported in Dally et al. (1998) showed that the peak CO value reached an unrealistic high value of 25\%. This unusual high value might be results of fluorescence interferences for CO signal (Dally et al. 1998). Discounting these effects, the calculations by the flamelet model still underpredict the CO profiles. One of the possible causes for this discrepancy may be the transient effect that exists in the turbulent flame due to concentration fluctuations (Dally et al. 1998; Barlow and Chen 1992; Mauss et al. 1990).

The HMI flame was one of the target flames of the third International Workshop on Measurements and Computation of Turbulent Nonpremixed Flames (TNF3 1998). In the workshop, computations carried out by four research groups were compared with each other and with the experimental data for this flame. The results from the third TNF workshop computations are presented in appendix B. The computations of the present study are comparable with the results of the third TNF workshop. Specially, the mass fraction of OH calculated by the laminar flamelet model with unity Lewis number in the present study (see Fig. 6.29) are in better agreement with the experimental data than the TNF calculations (see Fig. B.4). In the TNF results, the flamelet model gives a higher peak value than the measured results and the CMC model gives narrower profiles of OH as well as higher peak values.
Figure 6.22: Radial profiles of mean mixture fraction in the HM1 flame.

○ measurements, —— flame sheet, · · · · · · equilibrium, · · · · constrained equilibrium —— flamelet with differential diffusion, · · · · flamelet with Le=1.0
Figure 6.23: Radial profiles of mixture fraction variance in the HMI flame.

- Measurements
- Flame sheet
- Equilibrium
- Constrained equilibrium
- Flamelet with differential diffusion
- Flamelet with $L_e=1.0$
Figure 6.24: Radial profiles of mass fraction of CH$_4$ in the HM1 flame. 
- measurements, —— flame sheet, ······· equilibrium, —······ constrained equilibrium —······ flamelet with differential diffusion, ······ flamelet with Le=1.0
Figure 6.25: Radial profiles of mass fraction of H₂ in the HM1 flame. 
- measurements, --- flame sheet, ······ equilibrium, ···· constrained equilibrium ··· flamelet with differential diffusion, ···· flamelet with $Le=1.0$
Figure 6.26: Radial profiles of temperature in the HM1 flame. O measurements, --- flame sheet, ····· equilibrium, ···· constrained equilibrium — flamelet with differential diffusion, — flamelet with Le=1.0
Figure 6.27: Radial profiles of mass fraction of H₂O in the HM1 flame. 
- measurements, —– flame sheet, ····· equilibrium, ···· constrained equilibrium —— flamelet with differential diffusion, ····· flamelet with Le=1.0
Figure 6.28: Radial profiles of mass fraction of CO$_2$ in the HM1 flame. 
- measurements, —— flame sheet, ······ equilibrium, ····· constrained equilibrium ····· flamelet with differential diffusion, ····· flamelet with Le=1.0
Figure 6.29: Radial profiles of mass fraction of OH in the HM1 flame.
O measurements, --- flame sheet, ----- equilibrium, · · · constrained equilibrium --- flamelet with differential diffusion, - - - flamelet with Le=1.0
Figure 6.30: Radial profiles of mass fraction of CO in the HM1 flame.

- ○ measurements, —— flame sheet, ····· equilibrium, —— constrained equilibrium —— flamelet with differential diffusion, —— flamelet with Le=1.0
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HM2 flame

The mean velocity of this flame is 178 m/s, which is 75 % of the blow-off velocity. This flame shows local extinction at x/D=1.8 and x/D=2.4. The comparison between experimental data and predicted results are shown in Figs. 6.31-6.39 for the HM2 flame.

Figure 6.31 shows the mean mixture fraction profiles. The overall agreement between the predictions and the measurements is reasonably good by all the combustion models. However, there is slight underpredictions at x/D=0.26 and x/D=0.6 for r>15 mm by all the models. The differences are also observed between the predicted results of different combustion models near the center line at x/D=0.6, x/D=0.9, x/D=1.3 and x/D=1.8.

Radial profiles of the mixture fraction variance are shown in Fig. 6.32. As compared to the HM1 flame, the experimental mixture fraction fluctuations are less in this flame inside the core of the outer vortex at x/D=0.26. The predicted results however, do not show a reduction of the mixture fraction variance. As in the HM1 flame, the peak mixture fraction variance at the inner mixing layer inside the recirculation zone (x/D<0.9) is overpredicted by all the combustion models. However, the predictions by the laminar flamelet model with and without differential diffusion effect are relatively better. Outside the recirculation zone, the mixture fraction variance is reasonably well predicted. The agreement between the measurements and the predictions are particularly good at x/D=2.4.

Figures 6.33 and 6.34 show CH₄ and H₂ mass fraction profiles. All the combustion models except the equilibrium model provide reasonably good predictions of CH₄ mass fraction. The equilibrium model underpredicts CH₄ mass fraction at all the locations, which clearly indicates that CH₄ breaks down into products in the fuel rich mixture, which is contrary to that observed in the experiment or in the calculations by other models. The prediction of H₂ mass fraction is reasonably good by the flame sheet, constrained equilibrium and flamelet model with unity Lewis number. The flamelet model with differential diffusion effect underpredicts the mass fraction of H₂ slightly in the fuel rich zone. The equilibrium model overpredicts the level of H₂ in the fuel rich zone at all the locations.

Figure 6.35 shows the radial temperature profiles at six axial locations. At x/D=0.26, the temperature is reasonably well predicted by all the combustion models. However, the equilibrium model underpredicts the temperature in the fuel rich side of the flame.
At both $x/D=0.6$ and $x/D=0.9$, the location of the peak temperature as well as the peak value of temperature is underpredicted by all the combustion models. This underprediction is caused by the underprediction of mixture fraction. At $x/D=1.3$, the agreement between the measurements and the predictions is very good. At $x/D=1.8$ and $x/D=2.4$, the maximum measured temperature is about 1350 K, which is considerably lower than the maximum measured temperature of about 1530 K in the HM1 flame at the corresponding locations. This lower temperature is a result of local extinction observed at these locations (Dally et al. 1998). The laminar flamelet model, at least theoretically, can predict local extinction. In the laminar flamelet model, local extinction is predicted when the scalar dissipation rate reaches a quenching limit and the blow-off of the flame occurs when the proportion of burning flamelets decreases below a certain limit. However, the flamelet model in the present study shows that this simple treatment is not adequate to predict the local extinction and subsequent lower temperature for this flame. This point is further discussed later.

The flamelet model with the differential diffusion effect provides a good prediction of $H_2O$ mass fraction inside the recirculation zone as shown in Fig. 6.36. The predictions by the flame sheet, constrained equilibrium and the flamelet model with unity Lewis number are very similar and the $H_2O$ mass fraction are underpredicted inside the recirculation zone. The flame sheet, constrained equilibrium and the flamelet model with unity Lewis number also produce very good predictions at $x/D=1.3$, $x/D=1.8$ and $x/D=2.4$ despite the localised extinction observed at these locations. The equilibrium model produces unrealistic double peaks at all the axial locations.

Figure 6.37 shows the radial mass fraction profiles of $CO_2$. The flame sheet model overpredicts and the laminar flamelet model with the differential diffusion effects underpredicts the $CO_2$ mass fraction at all the locations. The equilibrium, constrained equilibrium and the laminar flamelet models with the unity Lewis number provide a good prediction of $CO_2$ at $x/D=0.26$, $x/D=0.6$, $x/D=0.9$ and $x/D=1.3$. Contrary to the temperature predictions, the location of the peak $CO_2$ is well reproduced at $x/D=0.6$ and $x/D=0.9$. Also, the effect of the localised extinction is observed at $x/D=1.8$ and $x/D=2.4$, where the $CO_2$ level is overpredicted.

Radial mass fraction profiles of OH are shown in Fig. 6.38. At $x/D=0.26$, the experimental data shows that the OH exists at super-equilibrium level. The flamelet model with unity Lewis number provides a good prediction of the peak OH level at this location and the flamelet model with the differential diffusion effect overpredicts the peak
level. However, at both $x/D=0.6$ and $x/D=0.9$, the flamelet model with unity Lewis number underpredicts the peak level and the flamelet model with the differential diffusion effect provides a better prediction. At $x/D=1.3$, the flamelet model with unity Lewis number yields a better prediction and the flamelet model with the differential diffusion effect yields overprediction. At $x/D=0.6$ and $x/D=0.9$, the mixture fraction profiles are slightly underpredicted and the mixture fraction variance are overpredicted. Therefore, the predictions of OH at these locations are influenced by the shortcomings of the turbulence model and the direct comparison of the combustion models becomes difficult. At $x/D=1.3$, the prediction of OH does not suffer from the shortcomings of the turbulence model and thus this is a better location for comparing the combustion models. Therefore it can be concluded that the laminar flamelet model with $Le=1.0$ produces better predictions than with the differential diffusion effect. At $x/D=1.8$ and $x/D=2.4$, the effects of the localised extinction on the OH mass fraction are observed and as a consequence the flamelet model with and without the differential diffusion effect overpredicts the OH level. The equilibrium model underpredicts the OH level at all the locations.

Figure 6.39 shows the radial profiles of CO. At $x/D=0.6$ and $x/D=0.9$, the predictions of CO profiles are very poor by all the combustion models. However, at $x/D=0.9$ and $x/D=1.3$, the constrained equilibrium model yields very good predictions. Though the laminar flamelet model with and without the differential diffusion effect underpredict the CO level, the flamelet model successfully reproduces the trend. The reasonably good agreement observed by the constrained equilibrium and the flamelet models at $x/D=1.8$ and $x/D=2.4$ is somewhat misleading as none of the model reproduces the localised extinction. The equilibrium model severely overpredicts the CO level at all the locations.
Figure 6.31: Radial profiles of mean mixture fraction in the HM2 flame. O measurements, –– flame sheet, ····· equilibrium, ····· constrained equilibrium –– flamelet with differential diffusion, ····· flamelet with $Le=1.0$
Figure 6.32: Radial profiles of mixture fraction variance in the HM2 flame.  
O measurements, —— flame sheet, ····· equilibrium, ····· constrained equilibrium —— flamelet with differential diffusion, ····· flamelet with Le=1.0
Figure 6.33: Radial profiles of mass fraction of CH₄ in the HM2 flame. 
- ○ measurements, — — flame sheet, · · · · · · equilibrium, — — — constrained equilibrium — — flamelet with differential diffusion, — — — flamelet with $Le=1.0$
Figure 6.34: Radial profiles of mass fraction of H$_2$ in the HM2 flame.

- measurements, — flame sheet, ······· equilibrium, ······· constrained equilibrium ····· flames with differential diffusion, ····· flames with $Le=1.0$
Figure 6.35: Radial profiles of temperature in the HM2 flame.
- measurements, --- flame sheet, ···· equilibrium, ····· constrained equilibrium --- flamelet with differential diffusion, ···· flamelet with $Le=1.0$
Figure 6.36: Radial profiles of mass fraction of H$_2$O in the HM2 flame.

- Measurements, --- flame sheet, ···· equilibrium, - - - constrained equilibrium --- flamelet with differential diffusion, - - - flamelet with Le=1.0
Figure 6.37: Radial profiles of mass fraction of CO$_2$ in the HM2 flame. 
○ measurements, —— flame sheet, ····· equilibrium, ··· constrained equilibrium ··· flamelet with differential diffusion, ···· flamelet with Le=1.0
Figure 6.38: Radial profiles of mass fraction of OH in the HM2 flame.

- o measurements, —— flame sheet, ····· equilibrium, ····· constrained equilibrium —— flamelet with differential diffusion, ····· flamelet with $Le=1.0$
Figure 6.39: Radial profiles of mass fraction of CO in the HM2 flame. 
○ measurements, —— flame sheet, ----- equilibrium, --- constrained equilibrium --- flamelet with differential diffusion, ---- flamelet with \( L_c=1.0 \)
HM3 flame

This flame consists of CH₄/H₂ (1:1 by volume) and has an inlet velocity of 214 m/s. This velocity is 91% of the blow-off velocity. This flame shows considerable local extinction at the neck zone. A comparison of the predicted results and measurements are presented in Figs. 6.40-6.48 for the HM3 flame.

Figure 6.40 shows the mean mixture fraction profiles. At x/D=0.26, the outer vortex region contains fuel lean mixture and the flame front (where Z_{st}=0.05) moves towards the inner zone. The location of the flame front is well predicted by all the combustion models. The overall agreement between the predictions and the measurements is reasonably good by all the combustion models at other locations. The flamelet model slightly underpredicts the mixture fraction at the center line specially at x/D=0.6, x/D=0.9 and x/D=1.3.

The mixture fraction variance, as shown in Fig. 6.41, is well predicted outside the recirculation zone (for x/D > 0.9) by the flamelet model with and without the differential diffusion effect. The flame sheet, equilibrium and the constrained equilibrium model overestimates the rms value of the mixture fraction at x/D=1.3 and x/D=1.8 and produce a better agreement at x/D=2.4. The predictions of the mixture fraction variance inside the recirculation zone is poor and similar to those found in the HMI and HM2 flames.

Figures 6.42 and 6.43 show the mean mass fractions of CH₄ and H₂ respectively. The mass fractions of CH₄ and H₂ are reasonably well predicted by all combustion models except the equilibrium model. The equilibrium model underpredicts the CH₄ profiles and overpredicts the H₂ profiles in the fuel rich zone.

Radial temperature profiles are shown in Fig. 6.44. At x/D=0.26, the flame sheet and the flamelet model with the differential diffusion effect produce a good agreement. The equilibrium and constrained equilibrium models provide good predictions in the fuel lean zone and underprediction at the fuel rich zone. The flamelet model with unity Lewis number underpredicts the temperature by about 200 K. In the HMI and HM2 flames, the flame front lies at the outer edge of the outer vortex and the mixture fraction variance was well predicted at the flame front at this location. However, for the HM3 flame, the flame front lies in the inner mixing layer, where the mixture fraction variance is overpredicted. Therefore, unlike the HMI and HM2 flames, the prediction in the HM3 flame at x/D=0.26 is influenced by the overprediction of the mixture fraction.
variance and therefore a direct comparison of the combustion models and the underlying conclusions are somewhat misleading. At $x/D=0.6$, the flame sheet and the flamelet model with the differential diffusion effect accurately predict the peak temperature, but underestimate the temperature in the fuel lean zone. The flamelet model with unity Lewis number produces similar trend, but underpredicts the peak temperature by about 200 K. The equilibrium and constrained equilibrium models produce a better prediction in the lean side. At $x/D=0.9$, all the combustion models produce a reasonably good agreement. Further downstream, the peak temperature is about 1100 K, which is due to local extinction. The calculated temperature by the laminar flamelet model is considerably higher than the measured temperature, which indicates that local extinction is not reproduced by the laminar flamelet model.

Radial mass fraction profiles of $H_2O$ is shown in Fig. 6.45. The flamelet model with the differential diffusion effect provides a good agreement inside the recirculation zone. The flame sheet, constrained equilibrium and the flamelet model with unity Lewis number underpredict the $H_2O$ profiles in side the recirculation zone and the the equilibrium model shows double peaks in the fuel rich zone. The predictions out side the recirculation zone are poor due to the local extinction of the flame.

Figure 6.46 shows the comparison of different combustion models for the $CO_2$ mass fraction. As in the HM1 and HM2 flames, the equilibrium, constrained equilibrium and flamelet model with unity Lewis number provide a good prediction of the mass fraction of $CO_2$ in side the recirculation zone. The flame sheet model provides overprediction and the flamelet model with the differential diffusion effect provides underpredictions. The predictions outside the recirculation zone ($x/D>0.9$) suffer from the localised extinction observed in the experiment.

Radial profiles of OH mass fraction is shown in Fig. 6.47. The OH is present in the super-equilibrium quantity in side the recirculation zone. The equilibrium and constrained equilibrium models underestimate the OH level by a factor of 2-3. Contrary to the HM1 and HM2 flames, the reaction zone of OH is wider at $x/D=0.26$ and the reaction zone width is well predicted. The experimental data at $x/D=0.26$ and $x/D=0.9$ lie between the predicted profiles of the laminar flamelet model with and without the differential diffusion effect. At $x/D=0.6$, the flamelet model with the differential diffusion effect provides a good prediction and at $x/D=1.3$ the flamelet model with unity Lewis number yields a better prediction. As explained earlier, the predictions at $x/D=0.26$, $x/D=0.6$ and $x/D=0.9$ suffer from the overprediction of the mixture fraction variance.
and therefore, it is difficult a draw a conclusion about the predictive capabilities of the combustion models based on the predicted results at these locations. Though the OH level at $x/D=1.8$ and $x/D=2.4$ is similar to the equilibrium level, in reality local extinction at these location reduces the amount of OH. The good agreement obtained by the equilibrium and constrained equilibrium models at $x/D=1.8$ and $x/D=2.4$ is therefore misleading.

Figure 6.48 shows the radial profiles of CO mass fraction. Unlike the HM1 and HM2 flames, the constrained equilibrium model provides a very good agreement of CO profiles. The laminar flamelet model both with and without the differential diffusion effect reproduce the trend of the mass fraction profiles of CO. The equilibrium model on the other hand produces overpredictions as high as about 100%.
Figure 6.40: Radial profiles of mean mixture fraction in the HM3 flame.  
- measurements, —— flame sheet, —— equilibrium, —— constrained equilibrium —— flamelet with differential diffusion, —— flamelet with Le=1.0
Figure 6.41: Radial profiles of mixture fraction variance in the HM3 flame. 
- Measurements, flame sheet, equilibrium, constrained equilibrium, flamelet with differential diffusion, flamelet with $Le=1.0$. 

Chapter 6. Modelling of Sydney Bluff Body Flames
Figure 6.42: Radial profiles of mass fraction of CH$_4$ in the HM3 flame.

- measurements, — flame sheet, ···· equilibrium, —··· constrained equilibrium ——— flamelet with differential diffusion, —···· flamelet with Le=1.0
Figure 6.43: Radial profiles of mass fraction of H\textsubscript{2} in the HM3 flame.  
- measurements, —— flame sheet, ——— equilibrium, —— constrained equilibrium —— flamelet with differential diffusion, —— flamelet with Le=1.0
Figure 6.44: Radial profiles of temperature in the HM3 flame. 
- measurements, — flame sheet, ······ equilibrium, ···· constrained equilibrium — flamelet with differential diffusion, ···· flamelet with \( L_e=1.0 \).
Figure 6.45: Radial profiles of mass fraction of $H_2O$ in the HM3 flame. 
O measurements, — flame sheet, · · · equilibrium, · · · constrained equilibrium — flamelet with differential diffusion, · · · flamelet with $Le=1.0$
Figure 6.46: Radial profiles of mass fraction of CO₂ in the HM3 flame.

- Measurements,
- Flame sheet, 
- Equilibrium,
- Constrained equilibrium,
- Flamelet with differential diffusion,
- Flamelet with Le=1.0
Figure 6.47: Radial profiles of mass fraction of OH in the HM3 flame.

- Measurements, --- flame sheet, ⋯⋯ equilibrium, ⋯⋯⋯ constrained equilibrium
-⋯⋯ flamelet with differential diffusion, ⋯⋯⋯ flamelet with Le=1.0
Figure 6.48: Radial profiles of mass fraction of CO in the HM3 flame.
O measurements, —— flame sheet, ····· equilibrium, ····· constrained equilibrium —— flamelet with differential diffusion, ····· flamelet with Le=1.0
6.4 Effects of non-equilibrium parameters

Two parameters are currently in use to describe non-equilibrium effects in the flamelet modelling: the scalar dissipation rate and the strain rate. Here, the results obtained by using different non-equilibrium parameters are presented for the HM3 flame using the flamelet library of unity Lewis number.

The mean strain rate is calculated from \( \bar{s} = \bar{\varepsilon}/\bar{k} \) according to Bray et al. (1994). However, Sanders and Lamers (1994) and Sanders and Gökalp (1995) defined the mean strain rate by \( \bar{s} = 6.4\bar{\varepsilon}/\bar{k} \). In the HM3 flame, this definition would give the mean strain rates much above the extinction value in the recirculation zone, which is unrealistic. The fluctuations of the strain rate are incorporated by a quasi Gaussian distribution (Sanders and Lamers 1994). A modified scalar dissipation rate defined by Bray et al. (1994) is also compared here. Bray et al. (1994) argued that the flamelets are subjected to the fluctuations of the order of flamelet thickness squared, \( \Delta Z^2 \). The effective mean scalar dissipation rate acting on the flamelet is then \( \chi = 2(\Delta Z)^2/k \); where the flame thickness is \( \Delta Z = 2Z_{st} \).

The results obtained by employing different non-equilibrium parameters are compared in Figs. 6.49-6.51 for temperature, \( \text{H}_2\text{O} \) and \( \text{OH} \) mass fraction respectively. The temperature is severely underpredicted inside the recirculation zone by the strain rate formulation indicating localised extinction. The strain rate is very high at the outer edge of the vortex, whereas the value of the scalar dissipation rate is low at same location. This is because the scalar dissipation rate depends on both the strain rate and the mixture fraction variance and the value of mixture fraction variance is low at the outer edge. These two formulations predict completely opposite phenomenon; the scalar dissipation formulation predicts a flame closer to equilibrium, but the strain rate formulation predicts a locally extinguished flame. The prediction by the modified scalar dissipation rate is better than that of the strain rate, but worse than the predictions by the standard scalar dissipation rate. At \( x/D = 1.3 \), the prediction by the strain rate formulation is better than the other two formulations. The predicted temperature are very similar at \( x/D = 1.8 \) and \( x/D = 2.4 \) for all the non-equilibrium formulations. The predictions of mass fraction of \( \text{H}_2\text{O} \) by different non-equilibrium parameter are similar to those of the temperature. The strain rate, the modified scalar dissipation rate and the standard scalar dissipation rate produce reseasonable predictions for the \( \text{OH} \) level.
Figure 6.49: Effects of non-equilibrium parameter on the prediction of temperature in the HM3 flame. O measurements, —— scalar dissipation rate, --- modified scalar dissipation rate, - - - strain rate
Figure 6.50: Effects of non-equilibrium parameter on the prediction of mass fraction of H$_2$O in the HM3 flame. O measurements, — scalar dissipation rate, --- modified scalar dissipation rate, - - - strain rate
Figure 6.51: Effects of non-equilibrium parameter on the prediction of mass fraction of OH in the HM3 flame. ○ measurements, —— scalar dissipation rate, —— modified scalar dissipation rate, ——— strain rate
6.5 Effects of discretisation scheme

The results so far presented in this chapter are obtained by employing the hybrid scheme for discretisation of the convection term in the governing equations. The error associated with the discretisation scheme is assessed by employing two more schemes, power law and total variation diminishing (TVD) scheme with Van Leer and UMIST limiters. The effect of grid size is also investigated by employing a 217 (axial) x 197 (radial) grid with the hybrid scheme.

Figures 6.52-6.54 compare the results obtained by using different schemes and grid size for the HM1 flame. In the calculations of the presented figures, the combustion is accounted for by the laminar flamelet model with Le=1.0.

The differences among the predicted results of mixture fraction, mixture fraction variance and temperature are small. The maximum difference is observed in the peak temperature at x/D=0.9. The TVD scheme with the UMIST limiter produces a 3.3 % decrease of the peak temperature and the hybrid scheme with 217x197 grids produces a 2.4 % increase of the peak temperature from the peak temperature obtained by the hybrid scheme with 99x89 grids. These variations are well below the accuracy of the measurements. Therefore, it can be concluded that the spatial discretisation error is small enough to allow the underlying mathematical models to be evaluated by the hybrid scheme.
Figure 6.52: Effects of discretisation scheme on mixture fraction in the HMI flame. Measurements, hybrid scheme, power law, TVD scheme with Van Leer limiter, TVD scheme with UMIST limiter, hybrid scheme with 217x197 grids
Figure 6.53: Effects of discretisation scheme on mixture fraction variance in the HM1 flame. Measurements, hybrid scheme, power law, TVD scheme with Van Leer limiter, TVD scheme with UMIST limiter, hybrid scheme with 217x197 grids.
Figure 6.54: Effects of discretisation scheme on temperature in the HMI flame. O measurements, --- hybrid scheme, --- power law, · · · TVD scheme with Van Leer limiter, · · · TVD scheme with UMIST limiter, · · · · hybrid scheme with 217x197 grids
6.6 Discussion

The results predicted here show the complex nature of the recirculation zone of the bluff body flame. Three distinct zones: recirculation, neck and jet-like zone, as reported in Dally et al. (1998) are clearly visible in the contour plots of the streamlines (see Figs. 6.55 and 6.56). The momentum flux of the fuel jet has a strong influence on the flow structure of the recirculation zones. The recirculation zones are characterised by double vortices at lower velocities. For the HC1 flame, the predicted recirculation zone length is \( x/D = 1.3 \). Two vortices are clearly shown: the outer vortex is bigger. The centre of the vortices are: \( x/D = 0.5, r/R = 0.7 \) for the outer vortex and \( x/D = 0.7, r/R = 0.21 \) for the inner vortex. With the increased jet momentum in the HC2 flame, the length of the recirculation zone is reduced to \( x/D = 1.0 \), and the inner vortex loses its recirculation pattern. CH\(_4\)/H\(_2\) flames also show similar flow patterns. The HM1 flame has two vortices with centres at \( x/D = 0.4, r/R = 0.73 \) for the outer vortex and at \( x/D = 0.8, r/R = 0.35 \) for the inner vortex. For the HM2 flame, the length of the outer vortex reduces to \( x/D = 1.25 \) and the inner vortex moves downstream. Finally for the HM3 flame, the outer vortex loses its recirculation pattern.

Dally et al. (1998) reported that for the same geometry, the rate of momentum flux ratio defined as \( (pU^2)_{\text{fuel}}/(pU^2)_{\text{air}} \) is the only controlling parameter that effects the recirculation zone for non-reacting flows and found that the transition from double to single vortex occurs when the momentum ratio exceeds a value of 13-15 for the bluff body geometry. However, the rate of the momentum flux ratio is not the only parameter that influences the recirculation zone for the reacting flows, more parameters are needed to be considered including the heat release rate and the stoichiometric mixture fraction e.g. the type of fuel. As a result no direct correlation between different parameters and the threshold at which the transition happens was reported by them for the combusting case. Clearly, many more cases of measurements and computations of reacting flows have to be conducted before any correlation can be confidently deduced.

The increase of jet momentum also influence the flame structures as shown in the contour plots of mixture fraction in Figs. 6.57 and 6.58. At a lower jet momentum (in the HM1 flame), the stoichiometric mixture fraction lies at the outer edge of the outer vortex, which implies that the flame is burning in the outer region. The core of the outer vortex remains fuel rich. With the increase of jet momentum, the stoichiometric mixture fraction shifts from the outer edge of the outer vortex towards the inner vortex.
and the outer vortex contains fuel lean mixture. The outer vortex of the HC1 and HM3 flames contain near stoichiometric mixture. In these flames, the reaction zone is broad covering almost full width of the recirculation zone. In the HC2 and HM1 flames, the reaction occurs in a narrow zone. The reaction zone is confined at different places for the HC2 and HM1 flames: confined in the edge of the outer vortex for the HM1 flame and close to the inner vortex for the HC2 flame. The increase of jet momentum also results in a longer flame as shown from the stoichiometric contours.

The mean mixture fraction within the core of the inner vortex, $Z_{vo}$, clearly depends on the fuel jet velocity $U_j$. Its also depends on many factors such as coflow velocity $U_{co}$, diameter ratio $D_b/D_j$ and heat release rate of the fuel used and hence density ratio $\rho_f/\rho_{co}$ (Dally et al. 1998). Dally et al. (1998) have reported that there is a definite negative correlation exist between $Z_{vo}/Z_{st}$ and $U_j/U_{co}$. However, there are not enough data available to produce a convincing correlation relating all these parameters.

The influence of the momentum flux of the fuel jet on the burning pattern of the flames is more clearly shown in the contour plots of temperature as shown in Figs. 6.59 and 6.60. The peak temperature for the HC1 flame is confined in the narrow zone near the wall inside the recirculation zone. For the HC2 flame, the temperature inside the recirculation zone is around 900 K, while the peak temperature is confined in the inner vortex zone. The HM1 flame shows a closed peak temperature zone, the temperature contours for the HM2 and HM3 flames are however similar to the HC1 flame. All the contour plots of temperature also show that the reaction between $x/D \approx 1.0$ and $x/D \approx 2.0$ does not reach chemical equilibrium condition.
Figure 6.55: Contours of streamlines; (a) HC1 flame, (b) HC2 flame
Figure 6.56: Contours of streamlines; (a) HM1 flame, (b) HM2 flame, (c) HM3 flame
Figure 6.57: Contours of mixture fraction; (a) HCl flame, (b) HC2 flame. Note the location of the flame front where $Z = Z_{fl}$.
Figure 6.58: Contours of mixture fraction; (a) HM1 flame, (b) HM2 flame, (c) HM3 flame. Note the location of the flame front where $Z = Z_{flame}$. 
Figure 6.59: Contours of temperature; (a) HC1 flame, (b) HC2 flame. Unit of temperature: Kelvin
Figure 6.60: Contours of temperature; (a) HM1 flame, (b) HM2 flame, (c) HM3 flame. Unit of temperature: Kelvin
Some more general remarks on the prediction of the CO mass fraction in CH₄/H₂ flames can be made. The CO mass fraction is found to be very difficult to predict. As expected, the equilibrium chemistry model gives an extreme overprediction of CO. The constrained equilibrium model is essentially an empirical modification of the equilibrium model to reproduce the correct level of CO and the constrained equilibrium model shows limited success for predicting CO level presented here. The CO levels are underpredicted by the flamelet model with and without the differential diffusion effect. The predictions of CO by the flamelet model can be further elaborated with the help of scatter plots shown in Fig. 6.61 for the HM1 flame. The scatter plots of CO for the HM2 and HM3 flames are qualitatively similar and are not shown here. The instantaneous data for the scatter plots are obtained from Masri (1997). The CO mass fraction profiles obtained from the solution of counter flow diffusion flame with unity Lewis number at three stretch conditions are also shown for comparison. The peak CO level at all six locations are very high compared to the steady state flamelets. The measured peak level is about 25%, whereas the steady state flamelet value is about 5% at the highest strain rate. Some of this high level of CO can be attributed to the fluorescence interference (Dally et al. 1998). Discounting the fluorescence interference effects, the peak CO levels in these flames are still higher than the steady state flamelet levels. Mauss et al. (1990) have shown that the CO level in transient flamelets can be much higher than that calculated for the steady state flamelets. Based on a stochastic simulations of flamelet extinction and reignition, they concluded that the transient effects may partially explain the relatively high level of CO concentrations found in turbulent non-premixed flames. The HM2 and HM3 flames show considerable local extinction and reignition (see Fig. 6.62) and the conclusion of Mauss et al. (1990) may be applicable for these flames, but in the HM1 flame, it is unlikely that the local extinction and reignition processes occur. However, Barlow and Chen (1992) have shown that the transient flamelets where the scalar dissipation rate does not exceed the extinction limit also yield the CO level much higher than the steady state flamelets and comparable to those found in turbulent flames. These findings are however based on the solution of laminar flamelet equations. The transient flamelet model for the turbulent combustion calculations (Pitsch et al. 1998) are in the very early stage of development and it is not yet clear how the transient flamelet model will behave for predicting the CO level in turbulent flames.
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Figure 6.61: Scatter plots of mass fraction of CO for HM1 flame at (a) x/D=0.26 (b) x/D=0.6 (c) x/D=0.9 (d) x/D=1.3 (e) x/D=1.8 (f) x/D=2.4. Lines represent computed laminar diffusion flame profiles with constant mass diffusivities and $\text{Le}=1.0$. -- $a = 3.0 \text{ /s}$ ($\chi_{st} = 0.064 \text{ /s}$), · · · $a = 100.0 \text{ /s}$ ($\chi_{st} = 2.139 \text{ /s}$), · · · · · $a = 1800 \text{ /s}$ ($\chi_{st} = 38.502 \text{ /s}$)
Figure 6.62: Scatter plots of temperature at (a) $x/D=1.8$, (b) $x/D=2.4$ for HM1 flame; (c) $x/D=1.8$, (d) $x/D=2.4$ for HM2 flame; (e) $x/D=1.8$, (f) $x/D=2.4$ for HM3 flame. Lines represent computed laminar diffusion flame profiles with constant mass diffusivities and $\hat{L}e=1.0$. —— $a = 3.0 \text{ m/s} (\chi_{st} = 0.064 \text{ m/s})$, —— $a = 100.0 \text{ m/s} (\chi_{st} = 2.139 \text{ m/s})$, ······ $a = 1800.0 \text{ m/s} (\chi_{st} = 38.502 \text{ m/s})$.
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As mentioned earlier, the scalar dissipation rate provides better predictions than the strain rate as a non-equilibrium parameter in the laminar flamelet modelling. Figures 6.63 and 6.64 show the scalar dissipation rate along the flame front for the H\textsubscript{2}/CO and CH\textsubscript{4}/H\textsubscript{2} flames respectively. With the increase of jet momentum, the scalar dissipation rate increases along the flame front. The increase of the scalar dissipation rate is higher for the H\textsubscript{2}/CO flames because the flame front lies near the shear layer as the stoichiometric mixture fraction is high ($Z_{st} = 0.135$). The scalar dissipation rate along the flame front for the CH\textsubscript{4}/H\textsubscript{2} flames are well below the extinction limit as the flame front lies outside the shear layers because of the low stoichiometric mixture fraction ($Z_{st} = 0.05$). Though the mean scalar dissipation rate is well below the extinction limit, both the HM2 and HM3 flames show considerable localised extinction (see Fig. 6.62), which may be due to transient effects (Bray and Peters 1994). Clearly, the steady laminar flamelet model, in which the only coupling between the turbulent flow field and chemistry is the mean scalar dissipation rate and the extinction is predicted when the mean scalar dissipation rate exceeds the extinction limit, is not capable of predicting the localised extinction occurring in the HM2 and HM3 flames. A transient laminar flamelet model as proposed by Pitsch et al. (1998) recently may provide good results for flames with local extinction.
Figure 6.63: The variation of scalar dissipation rate for $\text{H}_2/\text{CO}$ flame; --- HC1, ---- HC2

Figure 6.64: The variation of scalar dissipation rate for $\text{CH}_4/\text{H}_2$ flame; --- HM1, ---- HM2, --- HM3
6.7 Summary

1. The performance of the flame sheet, equilibrium and laminar flamelet models were evaluated by comparing with the experimental data of H₂/CO and CH₄/H₂ fuels at different inlet velocities for a bluff body configuration.

2. The laminar flamelet model yielded better predictions than the other combustion models for predicting temperature, major and minor species.

3. The effect of the differential diffusion was studied. The effect of differential diffusion was found to be more important for the prediction of CO₂ and OH species. The unity Lewis number flamelet has provided a better representation of transport of the species.

4. The influence of different non-equilibrium parameters was evaluated and only the scalar dissipation rate was found to be suitable as a non-equilibrium parameter.

5. The laminar flamelet model failed to predict the localised extinction observed in CH₄/H₂ flames at higher velocities.

6. The predictions of CO mass fraction for CH₄/H₂ flames were found to be very difficult. The flamelet model provided severe underestimation of the CO levels, the constrained equilibrium model however showed limited success for the prediction of CO mass fraction.

7. The uncertainty of the inlet velocity profiles was investigated and the fully developed velocity profiles was shown to produce better results than the specified inlet velocity from the measurements.

8. The differences in the predicted results for different discretisation schemes was shown to be small.
CHAPTER 7

Flamelet based NO Modelling

The results presented in chapters 5 and 6 show that the laminar flamelet model provides a very good representation of the turbulent reacting flow. This model has successfully predicted the mean temperature as well as the major and minor species. The flamelet model is thus further employed to study certain practical issues like NO\(_x\) formation and radiation heat transfer which are of great importance for industrial furnaces and gas turbines. This chapter describes a flamelet based NO modelling technique and the validation against the experimental results for the HM1 and HM3 flames. The effects of radiation heat transfer is presented in the next chapter.

7.1 Flamelet based NO\(_x\) modelling

The prediction of thermal NO by the laminar flamelet model for the HM1 and HM3 flames is presented here. As explained in the previous chapters the laminar flamelet model describes the non-equilibrium chemistry by introducing the scalar dissipation rate as a parameter to account for non-equilibrium effects. However, the flamelet approach still relies on the assumption that the time scales for chemical kinetics are much shorter than the time scales for convection and diffusion. With this concept, the mean temperature, density and composition in the turbulent field is obtained by appropriately averaging scalar variable versus mixture fraction profiles of the flamelets, each of the flamelets is subjected to different level of fluid dynamic stretching characterised by the scalar dissipation rate. Combustion generated pollutants such as NO on the other hand can not be obtained from the flamelet library as the reaction rate of NO formation is slow; it is kinetically limited instead of diffusion limited. Therefore, an averaged transport equation for the mean NO-mass fraction, \(\bar{Y}_{NO}\), has to be solved. For a given \((Z, \chi)\)
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state, the source term for NO is evaluated from the corresponding chemistry states of major and minor species from the flamelet library.

So far the potential of the laminar flamelet model has not been extensively investigated for the prediction of the NO formation. The use of the laminar flamelet model for the prediction of NO has begun only in the last few years (Schlatter et al. 1996; Chen and Chang 1996; Sanders et al. 1997; Vranos et al. 1992). Sanders et al. (1997) have reported that the laminar flamelet model can reproduce the scaling behaviour of the NOx emission index when the scalar dissipation rate is used as the stretching parameter. However, the absolute level of NOx was overpredicted by a factor of 10 in their calculations. They attributed this error to many factors, including differential diffusion and radiation. The work by Sanders and Gökälp (1995) and Schlatter et al. (1996) show that the scaling behaviour of NOx emission is not reproduced when the strain rate is used as the non-equilibrium parameter. Chen and Chang (1996) and Vranos et al. (1992) have investigated the effects of differential diffusion and radiation on NO formation. The inclusion of radiation heat transfer reduced the level of NO by a factor of 2 (Chen and Chang 1996), but the NO level was still overpredicted by a large margin. Vranos et al. (1992) speculated that the overprediction of the NO level was caused by the differential diffusion effect. However, Chen and Chang (1996) disputed that speculation and argued that the overprediction of the NO level could not be explained simply by the preferential diffusion effect.

The literature review, thus, indicates that the formation of NO in turbulent flames is not fully understood yet. As a further example, Barlow and Carter (1994) have shown by using Raman/Rayleigh/LIF measurements that the peak value of NO occurs at stoichiometric levels and the previously reported rich shift (Vranos et al. 1992) is due to averaging effects. It is therefore essential that the existing laminar flamelet model is assessed against a large number of nonintrusive, spontaneous measurements to understand different factors influencing the NO formation before the predictive capability can be confidently implemented for design purposes.

7.2 Laminar flamelet calculation

The emission of NO from flames in controlled by three mechanisms: (a) thermal NO (b) prompt NO and (c) N₂O intermediate mechanism (Chen and Chang 1995; Turns 1995; Bonturi et al. 1996). The thermal NO is formed through the well known Zeldovich
mechanism. This route is enhanced by the presence of super-equilibrium O and OH, and is very sensitive to temperature. In the prompt NO mechanism, hydrocarbon fragments attack the bimolecular nitrogen, producing atomic nitrogen, cyanides and amines, which are subsequently oxidised to NO. The N\textsubscript{2}O route is analogous to the thermal route in that the O-atom attacks the molecular nitrogen. However, with the presence of a third body, the N\textsubscript{2}O is formed and which subsequently react with O atoms to produce NO. The N\textsubscript{2}O route is unimportant at low pressures (Chen and Chang 1996) and even at high pressures, the maximum contribution was reported to be slightly over 11 % for a CH\textsubscript{4}/air counterflow diffusion flame (Bonturi et al. 1996). The relative contribution from different pathways depends on fuel type, temperature, pressure and residence time (Dally et al. 1996). The high NO levels that occur in practical systems can only be reduced by reducing the thermal NO formation.

The NO formed through the thermal mechanism is considered here. The thermal NO is modelled by the Zeldovich mechanism (Sanders and Gökalp 1995) and is given in Table 7.1. The reaction rate parameters for the Zeldovich mechanism are well known and are taken from Warnatz et al. (1996b).

In Fig. 7.1 the NO source terms (\(\omega/\rho\)) are shown as a function of mixture fraction for different stretch conditions. These profiles are obtained from counterflow diffusion flame calculations on the Tsuji burner configuration. The differential diffusion effect is included in the calculation. The figure shows that the source term is very sensitive to the scalar dissipation rate. At \(\chi = 0.064 /s\), the source term is negative in the fuel rich zone, indicating consumption of NO. At \(\chi = 0.427 /s\), the negative zone of the source term almost vanishes, but the peak value remains constant. With the increase of the scalar dissipation rate, the temperature increases while the mass fraction of O first increases, then remains less sensitive to the scalar dissipation rate and finally decreases as the scalar dissipation rate approaches the extinction limit. At \(\chi = 0.427 /s\), the decrease of temperature and the increase of mass fraction of O counter balance each other and the peak source term remains almost constant. At scalar dissipation rates higher than \(\chi =

### Table 7.1: Zeldovich mechanism in units of mol, cm, s, kJ and K

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>(B_B)</th>
<th>(a_B)</th>
<th>(E_B)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(N_2+O=NO+N)</td>
<td>1.900E+14</td>
<td>0.0</td>
<td>318.7</td>
</tr>
<tr>
<td>2</td>
<td>(O+NO=N+O_2)</td>
<td>2.400E+09</td>
<td>1.0</td>
<td>161.6</td>
</tr>
<tr>
<td>3</td>
<td>(NO+H=N+OH)</td>
<td>1.300E+14</td>
<td>0.0</td>
<td>205.7</td>
</tr>
</tbody>
</table>
0.427 /s, the decrease of temperature is more prominent and that reduces the source term rapidly with the increase of the scalar dissipation rate. At $\chi = 77.01 /\text{s}$, the formation of NO almost ceases.

### 7.3 Governing equation of mass fraction of NO

As explained earlier, the concentration of NO in a turbulent flame can not be obtained from the flamelet library. The slow, kinetically limited production of NO is obtained by solving the transport equation for NO:

$$
\frac{\partial}{\partial x_j} (\rho u_j \tilde{Y}_{NO}) = \frac{\partial}{\partial x_j} \left( \frac{\mu_{\text{eff}}}{\sigma_{NO}} \frac{\partial \tilde{Y}_{NO}}{\partial x_j} \right) + \bar{\omega}_{NO}
$$

(7.1)

where $\sigma_{NO}$ is the turbulent Schmidt number, which is taken as 0.7. The mean rate $\bar{\omega}_{NO}$ is obtained by averaging the instantaneous source term $S_{NO}$ according to:
The distribution of the mixture fraction in turbulent flames is represented by the beta pdf, while that of the scalar dissipation rate is given by the log-normal distribution. The integration of Eq. 7.2 is described in 3.4.2 in greater detail.

7.4 Results of NO predictions

The comparison between the predictions and the measurements for the radial mass fraction of NO are shown in Fig. 7.2 for the HMI flame. The flamelet model with the differential diffusion effect overpredicts the NO profiles at x/D=0.26. This may be caused by the overprediction of temperature at this location (see Fig. 6.26). Further downstream, the difference between the predicted results and the measurements is reduced. The peak NO level is correctly predicted at x/D=0.9 and x/D=1.3 by the flamelet model with the differential diffusion effect. However, the prediction is poor in the fuel rich zone. The NO profiles are also overpredicted by a factor of about 1.75 at x/D=1.8 and x/D=2.4. At these locations, the overprediction of temperature as shown in Fig. 6.26 may induce this error. The flamelet with Le=1.0 underpredicts the NO level severely at every location.

The predicted radial profiles of NO together with the experimental data for the HM3 flame are shown in Fig. 7.3. At x/D=0.26, the NO profile predicted by the full molecular transport flamelet shows a peak value around r=20 mm. However, the peak is not distinct in the measured profile. The flamelet prediction with full molecular transport is very good at x/D=0.6. As in the HM1 flame, the mass fraction of NO is overpredicted in the fuel rich zone at x/D=0.9. The NO levels are overpredicted at x/D=1.3, x/D=1.8 and x/D=2.4 by a factor of 2-3. At these locations, the flame exhibits local extinction, which is not reproduced in the flamelet calculations as explained in chapter 6. The inability of the laminar flamelet model to predict the local extinction also results in the overprediction of NO. For this flame again, the flamelet with Le=1.0 severely underpredicts the NO level at all axial locations.

The predictions presented in chapter 6 indicate that the unity Lewis number flamelet provides better predictions for temperature, major and minor species. The prediction of NO mass fraction by the flamelet model with Le=1.0 is, however, very poor. In order to investigate this apparent inconsistency, the mass fraction of CH₄ is plotted against the
mass fraction of $\text{H}_2$ at different axial locations for the HM1 and HM3 flames as shown in Figs. 7.4-7.5. It is evident from these figures that neither the full molecular transport flamelet nor the equal diffusivity and $\text{Le}=1.0$ flamelet can reproduce the extent of the actual differential diffusion. The flamelet with full molecular transport overpredicts the actual of differential diffusion, while the unity Lewis number flamelet underpredicts. Though the unity Lewis number flamelet is found adequate for the prediction of temperature and species concentrations, the unity Lewis number flamelet is not the accurate representation of the extent of differential diffusion. The prediction of NO is found to be very sensitive to differential diffusion effect. It is thus important to include the actual extent of differential diffusion effect for the improved prediction of NO. To demonstrate the importance of handling the accurate differential diffusion effect, additional flamelet profiles are generated with variable Lewis number. The Lewis number for each species is selected from Chen et al. (1993) and Rogg (1995), except for $\text{H}_2$. The value of the Lewis number for $\text{H}_2$ is arbitrarily chosen so that the variable Lewis number flamelet accurately predicts the $\text{CH}_4$ vs. $\text{H}_2$ profiles as shown in Figs. 7.4 and 7.5. The numerical values used of the Lewis numbers are 0.97, 1.10, 0.83, 1.39, 1.11, 0.45, 0.18, 0.73, 0.70, 1.10, 1.0, 1.27, 1.28, 1.12, 1.10, 1.0, 1.0, 1.0, 1.0 for $\text{CH}_4, \text{O}_2, \text{H}_2\text{O}, \text{CO}_2, \text{CO}, \text{H}_2, \text{H}, \text{OH}, \text{O}, \text{HO}_2, \text{CH}_3, \text{CHO}, \text{CH}_2\text{O}, \text{H}_2\text{O}_2, \text{CH}, \text{CH}_2$ and $\text{N}_2$ respectively. The variable Lewis number flamelet remarkably improves the prediction of NO especially inside the recirculation zone as shown in Figs. 7.2 and 7.3.
Figure 7.2: Radial profiles of NO in the HM1 flame. O measurements, — full molecular transport, —— Le=1.0, —— variable Lewis number
Figure 7.3: Radial profiles of NO in the HM3 flame. O measurements, —— full molecular transport, --- $Le=1.0$, ••• variable Lewis number
Figure 7.4: CH₄ vs. H₂ profiles at different axial locations in the HM1 flame.
- measurements, —— full molecular transport, —— Le=1.0, - - - variable Lewis number
Figure 7.5: CH$_4$ vs. H$_2$ profiles at different axial locations in the HM3 flame.

○ measurements, --- full molecular transport, --- Le=1.0, - - - variable Lewis number.
7.5 Discussion

The results of the present calculations are very encouraging and the level of agreement is better than those of Sanders et al. (1997) and Chen and Chang (1996). Sanders et al. (1997) reported an overprediction by a factor of 10 with the full molecular transport and a factor of 3 with $Le=1.0$ flamelets. Chen and Chang (1996) also reported an overprediction by a factor of 3-10 depending on the locations of the flame. With the inclusion of radiation effect in their calculations, the NO level was still overpredicted by a factor of 2.

The results presented here show that the formation of NO is very sensitive to differential diffusion effects. Neither the full molecular transport of the species nor the equal diffusivity and unity Lewis number assumptions accurately predict the extent of the differential diffusion of the species in the turbulent flames. An improved prediction by the ad-hoc variable Lewis number flamelet calculation implies that the correct handling of the differential diffusion effects is very important to improve the agreement. However, the correct handling of the extent of the differential diffusion effects in the turbulent flames is lacking in the present modelling concept and it is essential to develop a model to include this effect.

The NO formed through the thermal route is considered here. Chen and Chang (1996) have shown that the Zeldovich mechanism is the dominant pathways for the production of NO in a turbulent CH$_4$/H$_2$ jet flame except in the rich parts of the flame. In the rich part of the flame, they have shown that the NO is consumed mainly through the reaction step $HCCO+NO=CO+HCNO$. The importance of NO reburning through the HCN and CN intermediates in the rich system is described by a number of researchers (Miller and Bowman 1989; Dupont et al. 1995). Thus, the overprediction of NO in the fuel rich side can be attributed to the non inclusion of the NO reburn mechanism.

Some more general remarks can be made on the formation of NO from predicted contour plots. Figures 7.6 and 7.7 show the predicted contours of the mean reaction rate, mean mass fraction of NO and mean temperature for the HM1 and HM2 flames respectively. The effects of residence time on the NO formation rate is clearly evident from these figures. For the HM1 flame, the stoichiometric mixture fraction lies on the outer edge of the outer vortex (see, section 6.6). The gas mixtures have more time to react inside the recirculation bubble and the mean NO formation rate is high. At the high jet momentum of the HM3 flame, the stoichiometric mixture fraction lies in the inner
vortex zone. In the HM3 flame, the outer vortex is shorter and the inner vortex loses its recirculation pattern due to jet expansion. The residence time in the inner vortex zone is much shorter than that in the outer vortex and hence the NO-formation rate is much less in the HM3 flame. The mean reaction rate contours resemble the mean temperature contours. However, NO-formation is only confined to the high temperature region along the flame front. For both the flames, the mean NO-formation rate is low in the neck zone and increases further downstream. Though the mean NO-formation is confined along the stoichiometric mixture fraction, the contour plots show that the mean NO exists in a wide area of the flames due to the convection and diffusion processes.
Figure 7.6: Contours of (a) mean reaction rate $\dot{\omega}_{NO}$, (b) mean mass fraction of NO and (c) temperature of the HM1 flame
Figure 7.7: Contours of (a) mean reaction rate $\dot{\omega}_{NO}$, (b) mean mass fraction of NO and (c) temperature of the HM3 flame
7.6 Summary

1. The performance of the flamelet based NO modelling technique is appraised against the single point measurements in the bluff body configuration.

2. The flamelet based model yielded reasonable predictions of NO with the thermal NO mechanism. The prediction in the fuel rich zone is somewhat poor and the full NO mechanism involving all the pathways and the NO reburn may produce good results.

3. The calculations have raised novel issues about the differential diffusion effects. It is shown that neither the full molecular transport nor the unity Lewis number accurately represents the transport of the species in the turbulent flame. An arbitrary variable Lewis number flamelet model implemented in the present study shows considerable improvements in the predictions.
The laminar flamelet model is further employed to study the effect of radiation heat transfer effect on the bluff body flames presented in chapters 5 and 6. No reported radiation data is available for these flames to compare the radiative properties such as, the radiative intensities and the corresponding wall heat flux. However, the results presented here show that the predictive capability of the laminar flamelet model can be improved by incorporating the radiation heat transfer.

8.1 Flamelet based radiation model

The radiation heat losses are often neglected in the turbulent combustion modelling. Marracino and Lentini (1997) stated that out of 30 modelling or theoretical papers on turbulent combustion presented at the twenty-sixth Symposium (International) on Combustion, as few as three papers considered the radiation heat transfer. Even when the radiation heat transfer is accounted for, the simplified assumptions introduced to avoid the direct coupling between the radiation and the combustion, as in Chen and Chang (1996), can invalidate the quantitative analysis. Uncertainties in the predicted gas temperatures of $>100$ K due to radiation heat exchange can undermine the investigations in extended and improved reaction schemes, for example, for emissions prediction.

The influence of radiation heat loss on the structure of laminar flamelet has been investigated by a number of researchers by including the radiation source term in the enthalpy equation of the counterflow diffusion flame or in the flamelet equations on the mixture fraction space (Chen et al. 1993; Chan et al. 1995; Balthasar et al. 1996).
However, Bray and Peters (1994) argue that when the radiation heat loss term is retained in the flamelet equations, it implies that the radiation heat exchange occurs as thin gas radiative emissions to the surroundings within a thin region of high temperature. Radiation heat exchange is a global phenomenon and therefore radiation from practical flames does not correspond to the radiation from laminar flamelets. In order to include the radiation heat exchange in turbulent flame calculations, emission and re-absorption over a whole range of length scales of the turbulent flame must be taken into consideration by solving a transport equation of enthalpy containing the radiation source term. In the context of the flamelet modelling strategy, the coupling between the flamelet library and the mean scalar variable in the turbulent flame can be achieved by introducing an additional parameter, enthalpy defect. The flamelet library with enthalpy defects corresponding to situations in turbulent flames can be generated by modifying the source term of the flamelet equations or by modifying the available enthalpy (Bray and Peters 1994). This approach has been successfully implemented by Marracino and Lentini (1997). A similar model for the inclusion of radiation heat transfer in the flamelet modelling has been reported by Young and Moss (1995) and Brookes and Moss (1999), which further accounts for soot radiation. However, the model in the present form can not account for the finite rate chemistry. The method proposed by Bray and Peters (1994) and implemented by Marracino and Lentini (1997) accounts for the finite rate chemistry effects and hence, is implemented in the present study. The prediction of Marracino and Lentini (1997) suffers from the crude treatment of the radiation heat transfer by the thin gas approximations. The present study gives a further insight into the coupled radiation/flamelet modelling by employing the ray tracing based discrete transfer method (DTM) of Lockwood and Shah (1981).
8.2 Incorporation of radiation heat transfer in the flamelet model

In addition to the mixture fraction and the scalar dissipation rate, a third parameter is required to incorporate radiation heat loss. Enthalpy defect, defined as the difference between actual and adiabatic enthalpy, is found to be the suitable parameter to account for the radiation loss (Marracino and Lentini 1997; Bray and Peters 1994). The enthalpy defect, $\zeta$ is given by:

$$\zeta = h - [h_o + Z(h_f - h_o)]$$  \hspace{1cm} (8.1)

The scalar variables now depend on the mixture fraction, the scalar dissipation rate and the enthalpy defect as:

$$\phi = \phi(Z, \chi_{st}, \zeta)$$  \hspace{1cm} (8.2)

The average values of the scalar variables in the turbulent field can be recovered by introducing the joint pdf of $Z$ and $\chi_{st}$, as:

$$\overline{\phi} = \int_0^{\infty} \int_0^1 \phi(Z, \chi_{st}, \zeta)P(Z, \chi_{st})dZd\chi_{st}$$  \hspace{1cm} (8.3)

where the effect of turbulent fluctuations of the enthalpy are neglected according to Bray and Peters (1994) and Marracino and Lentini (1997).

This model requires as an input a set of flamelet profiles with enthalpy defects. The flamelet profiles are organised as 'shelves' (Marracino and Lentini 1997). Each shelf contains entries for the flamelet profiles referring to the values of the scalar dissipation rate ranging from very low to the extinction limit plus the inert state and each shelf represents a different value of $\zeta$.

Once the required flamelet profiles are generated, the incorporation of the radiation heat transfer in the calculation procedure is straightforward. In the CFD code the mean enthalpy is calculated from its conservation equation with the radiation source term:

$$\frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_j \bar{h}) = \frac{\partial}{\partial x_j} \left( \mu_{eff} \frac{\partial \bar{h}}{\partial x_j} \right) + S_h$$  \hspace{1cm} (8.4)

With the value of mean enthalpy, the enthalpy defect is calculated at each grid node and with this value of the enthalpy defect, the flamelet entries for the enthalpy defect
is bracketed using the pre-calculated library. The mean value of the scalar variable is calculated from integration over the joint probability density function of mixture fraction and scalar dissipation rate and interpolation between the two bracketed enthalpy defects entries. If \( m \) denotes the library shelf index, such that the enthalpy defect at a node lies between \( \zeta_m \) and \( \zeta_{m-1} \), then the interpolation is carried out as,

\[
\bar{\phi} = \frac{\zeta - \zeta_m}{\zeta_{m-1} - \zeta_m} \bar{\phi}_{m-1} + \frac{\zeta_{m-1} - \bar{\phi}}{\zeta_{m-1} - \zeta_m} \bar{\phi}_m
\]

(8.5)

where \( \bar{\phi}_m \) stands for,

\[
\bar{\phi} = \int_0^\infty \int_0^1 \phi(Z, \chi_{st}, \zeta_m) P(Z, \chi_{st}) dZ d\chi_{st}
\]

(8.6)

and similarly, for \( \bar{\phi}_{m-1} \).

### 8.3 Generation of flamelet library with enthalpy defect

The flamelet library with the required enthalpy defect can be generated by modifying the source term in the flamelet equations or by modifying the available enthalpy (Bray and Peters 1994). Marracino and Lentini (1997) have given a procedure for the generation of flamelet library with the enthalpy defect. They have solved the flamelet equations on the mixture fraction space with the reduced temperature at the boundaries. However, to keep the boundary temperature at a realistic level for the case of higher enthalpy defects, they reduced the solution domain from the usual domain of \( Z = 0 \) to \( Z = 1 \) to a smaller range (say \( Z = 0.1 \) to \( Z = 0.95 \)).

In the present study, a different method is implemented for the generation of the flamelet library. The method is based on a suggestion by Lentini (1998). In this method, the flamelet profiles are generated by the counterflow diffusion flame method with the unity Lewis number assumption. The flamelet profiles with the required enthalpy defect are obtained by reducing the available enthalpy (more precisely the temperature) at both the boundaries. The assumption of unity Lewis number is very important as it forces the enthalpy defect to be of the same value across the flamelet thickness (Marracino and Lentini 1997). To achieve higher enthalpy defects, the temperature at the boundary has to be unrealistically low. This is avoided by feeding slightly rich air (corresponding
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Figure 8.1: Schematic drawing of the flamelet profile for temperature showing adiabatic flamelet and flamelet with enthalpy defect.

to mixture fraction, say $Z_1$) and slightly lean fuel (corresponding to mixture fraction, say $Z_2$). The temperatures at $Z_1$ and $Z_2$ are then reduced from the adiabatic values to achieve the required enthalpy defect. This concept is shown schematically in Fig. 8.1. The compositions at $Z_1$ and $Z_2$ have to be specified, which are in principle unknown. As a first approximation, the compositions are taken from the already computed shelf immediately above at the relevant $Z$. In fact, the compositions depend predominantly on the mixture fraction and more weakly on the enthalpy in the fuel rich and lean zone; this concept is substantiated by Faeth et al. (1989). Still, there exists local error, which is expected to have minimal impact on the turbulent flame computations.

8.4 Radiation model

The radiation heat exchange in the flame is modelled by the the general radiation calculation technique the discrete transfer method (DTM) (Lockwood and Shah 1981). The method is based on the direct solution of radiation transport equation:

$$\frac{dI}{ds} = k_s \left( \frac{E_s}{\pi} - I \right)$$

(8.7)
where $I$ is the intensity of radiation in the direction of $\Omega$, $k$ is the gas absorption coefficient, and $E_\Omega$ is the black body emissive power, $\sigma T^4$. This equation may be integrated to yield the recurrence relation:

$$I_{n+1} = E_\Omega \left( 1.0 - e^{-k\delta s} \right) + I_n e^{-k\delta s} \tag{8.8}$$

where $n$ and $n+1$ denote successive locations separated by $\delta s$. The recurrence relation is applied along an arbitrarily chosen 'representative direction' $\Omega$'s, normally of equal angular spacing, emanating from arbitrarily chosen wall locations, usually the center points of grid cell surfaces coincident with a wall and terminating at the impingement locations on opposite walls.

The heat balance at the wall is given by:

$$q_{w,+} = (1.0 - \varepsilon_w)q_{w,-} + \varepsilon_w E_w \tag{8.9}$$

The radiation intensity leaving the wall is:

$$I_o = \frac{q_{w,+}}{\pi} \tag{8.10}$$

The incident flux is obtained from:

$$q_{w,-} = \sum_{all} I_j(\Omega_j, n) \delta \Omega_j \tag{8.11}$$

where $I_j$ is the calculated intensity in the discretised angle $\delta \Omega_j$ and $n$ is the unit vector normal to the wall.

The radiation source term for the cell for each representative direction is given by:

$$S_h = (I_{n+1} - I_n) \delta \Delta \delta \Omega \tag{8.12}$$

At a wall location, usually the centrepoint of a grid cell surface coinciding with the wall, the representative direction is selected. Each representative direction is then traced through the cells until the far wall is reached. There, the intensity $I_o$ leaving the surface is taken to be the intensity of the adjacent centre point of the cell, where it is known. This process is repeated until the difference between the old negative flux and the new one is within some prescribed error.

The weighted sum of the gray gases (WSGG) approach is used in the calculation of
the emissivities and the absorption coefficients. The global emissivity of the participating non-gray gas mixture is represented by (Hottel and Sarofim 1967):

\[ \varepsilon_g = \sum_n a_{g,n}(T)[1 - \exp(k_{g,n}(p_w + p_c)L)] \]  

(8.13)

where the summation \( n \) is over the gases of the assumed mixture; \( p_w \) and \( p_c \) is the partial pressure of water vapour and carbon dioxide and \( L \) is the mean radiation path length. The influence of temperature is introduced by the weighting coefficient:

\[ a_{g,n} = b_{1,n} + b_{2,n}T \]  

(8.14)

These coefficients have been fitted to the gas mixture total emittance evaluated from the spectral data by Truelove (1976). The value of \( k_g \) required for the calculations is then obtained from the 'pseudo gray' approximation:

\[ \varepsilon_g = 1 - \exp(-k_gL) \]  

(8.15)

8.5 Radiation in Correa and Gulati bluff body flame

The flamelet model with the radiation heat transfer is tested in the bluff body stabilised flame of Correa and Gulati (see chapter 5 for details of the flame). Six shelves of flamelet profiles are generated corresponding to enthalpy defects of 0.0, -15.0, -30.0, -40.0, -50.0 and -60.0 kJ/kg and each shelf contains six flamelet profiles. The value of the extinction limit is different for different shelves and the extinction limit is reduced at higher enthalpy defects. This is quite obvious because the lesser amount of energy is available to sustain the flame at higher enthalpy defects and as a result the flamelet will be extinguished at a lower scalar dissipation rate. The flamelet library of temperature profiles for different enthalpy defects are shown in Fig. 8.2. The flamelet library also includes similar profiles for density and mass fraction of species. As expected, the temperature is reduced by both the scalar dissipation rate and the enthalpy defect. Another important feature is that the temperature profiles do not span the \( Z = 0 \) to \( Z = 1.0 \) range at higher enthalpy defects. This is because, slightly rich air and lean fuel are fed at the boundaries and the temperatures are reduced from the adiabatic condition to achieve
the required enthalpy defects. The generation of flamelet library with enthalpy defects is explained in section 8.3.

The predicted contours of temperature and enthalpy defect are shown in Fig. 8.3. The enthalpy defect is very small until $x/D=20$, indicating that the effect of radiation heat transfer is negligible in the near field of the flame. The peak temperature is confined between $x/D=38$ and $x/D=46$. However, the maximum enthalpy defect is confined between $x/D=50$ and $x/D=60$. Though the temperatures are slightly less than the peak temperature in this region, the size of the zone is larger than the peak temperature region. That is the reason for the peak radiation heat exchange occurring not at the peak temperature region, but further downstream. The axial temperature profile is shown in Fig. 8.4. The effect of radiation is negligible until $x/D=30$. The effect of radiation becomes important at the far field location of the flame where the temperature is high. The temperature with radiation model is about 15 K less than the temperature without the radiation effect.
Figure 8.2: Flamelet profiles for temperature with (a) $\zeta = 0.0 \, \text{kJ/kg}$, (b) $\zeta = -15.0 \, \text{kJ/kg}$, (c) $\zeta = -30.0 \, \text{kJ/kg}$, (d) $\zeta = -40.0 \, \text{kJ/kg}$, (e) $\zeta = -50.0 \, \text{kJ/kg}$, (f) $\zeta = -60.0 \, \text{kJ/kg}$ for CO/H$_2$/N$_2$ fuel.
Figure 8.3: Contours of (a) temperature and (b) enthalpy defect considering radiation heat transfer in the CO/H₂/N₂ flame
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8.6 Radiation in Sydney bluff body flame HM1

The predictions of the HM1 flame by different combustion models are presented in section 6.3.2. There, it was shown that the laminar flamelet model with \( Le=1.0 \) has produced better predictions than other combustion models. Here, the effects of radiation heat transfer on temperature and mass fraction of OH, H2O and CO2 are presented.

Five shelves of flamelet profiles are generated corresponding to enthalpy defects of 0.0, -30.0, -60.0, -90.0, -120.0 kJ/kg. Each shelf contains a single flamelet profile corresponding to the strain rate of \( a=100.0 \) s\(^{-1} \). The results presented in section 6.3.2 show that the effect of flame stretching is not significant in this flame and thus the flamelet model with a single flamelet will be sufficient to reproduce the main features of this flame. The use of a single flamelet in each shelf has considerably reduced the computational time.

The predicted temperature with and without radiation is shown in Fig. 8.5. The effect of radiation heat transfer is observed inside the recirculation zone, specially at \( x/D=0.26 \) and \( x/D=0.6 \). At \( x/D=0.26 \), the peak temperature is reduced by about 40 K
due to radiation. The difference in temperature with and without radiation is reduced to about 30 K at $x/D=0.6$. Further downstream, the effect of radiation gradually decreases. At the neck zone, the radiation heat transfer reduces the temperature by about 15 K compared to the adiabatic calculation.

Radial mass fraction of OH profiles are shown in Fig. 8.6. The inclusion of radiation heat transfer remarkably improves the agreement between the predictions and the measurements. The prediction with radiation heat transfer is particularly good at $x/D=0.6$ and $x/D=0.9$. The OH profiles at $x/D=0.26$ show discontinuity when the radiation is included in the calculation. Similar discontinuities are also observed by Marracino and Lentini (1997). As explained in Marracino and Lentini (1997), this discontinuity occurs where the enthalpy defect crosses the value corresponding to a particular shelf, say $m$. On one side of the location, the mean quantities are obtained from interpolation between shelves $m$ and $m-1$ and the other side, between shelves $m$ and $m+1$, and since a limited number of shelves are used in the calculation, the interpolation results in the observed discontinuity.

The effect of radiation heat transfer on $\text{H}_2\text{O}$ and $\text{CO}_2$ mass fraction is very small as shown in Figs. 8.7 and 8.8.
Figure 8.5: Radial profiles of temperature in the HM1 flame. —— without radiation, ——— with radiation
Figure 8.6: Radial profiles of mass fraction of OH in the HM1 flame. —— without radiation, ———— with radiation
Figure 8.7: Radial profiles of mass fraction of H$_2$O in the HMI flame. —— without radiation, —— with radiation
Figure 8.8: Radial profiles of mass fraction of CO₂ in the HM1 flame. —— without radiation, —— with radiation
8.7 Discussion

The incorporation of radiation heat transfer in the laminar flamelet modelling is shown to improve the prediction of the radical species OH. Since experimental measurements of O are not available, the prediction of OH radical can be treated as an indication of O prediction. The radiation heat transfer also influences the temperature field. Thus the present calculation method will be very helpful for improving the prediction of NO emission. However, the method for incorporating the radiation heat transfer implemented here is valid for the assumption of unity Lewis number of the flamelet. The flamelet with unity Lewis number on the other hand has yielded severe underprediction of NO. The flamelet with the differential diffusion effect has resulted in a better prediction of NO as discussed in chapter 7. The current calculation method, therefore, has to be modified before the influence of radiation heat transfer on the emission of NO can be studied. The incorporation of radiation heat transfer with the differential diffusion flamelet is however very complex. The main problem arises in the generation of flamelet libraries with enthalpy defects. With the differential diffusion effect of the species, the enthalpy defect across the flamelet will not remain constant at those values imposed on the boundaries. Therefore, a single shelf can not be specified by a fixed enthalpy defect and the Eq. 8.1 will no longer be valid. If each self $m$ is computed by enforcing the enthalpy defect $\zeta$ at the boundaries, the enthalpy defect across the flamelet will be a function of both $Z$ and $\chi_{st}$ (Marracino and Lentini 1997):

$$\left[\zeta(Z, \chi_{st})\right]_m = \left[h(Z, \chi_{st})\right]_m - \left[h(Z, \chi_{st})\right]_o$$

(8.16)

where index $O$ refers to the self in adiabatic condition. This equation replaces the definition 8.1. The incorporation then requires a very complex integration and interpolation than those given by Eqs. (8.5) and (8.6).

Some more general features of the radiation heat exchange in the HM1 flame can be revealed from the contour plots of enthalpy defects and radiation source term, Fig. 8.9. The maximum radiation source term is confined at the high temperature zone inside the recirculation region. The enthalpy in the flow field is also influenced by the convection and diffusion processes. As a result, the contours of the enthalpy defect do no follow the source term contours. The maximum enthalpy defect is confined near the bluff body face. Further downstream the value of the enthalpy defect gradually decreases.
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The effect of the radiation heat transfer on the chemical reaction is included through the enthalpy defect. Therefore the combustion inside the recirculation zone will be more influenced by radiation heat transfer and the influence will gradually decrease further downstream.

The calculations reported here was carried out using 16x16 rays per cell. Further increase of the rays did not change the mean values. Therefore it is concluded that the radiation calculation using 16x16 is accurate enough to present predictions without imposing severe overheads on the overall calculation procedure.

Finally, the convergence speed of the coupled radiation-combustion calculation algorithm somewhat depends on the frequency at which the radiation algorithm is called relative to the main CFD routine. Earlier in the calculation, a low frequency can be detrimental to the convergence as large perturbations are inflicted on the enthalpy equa-

Figure 8.9: Contour plots of (a) enthalpy defect, (b) radiation source term for the HM1 flame
tion (Bressloff et al. 1996). It is not essential to update the radiation field with every CFD iteration; rather such an approach is very demanding. As a compromise, the radiation routine is called after every 5 CFD iterations for the present analysis. However, it should be noted that no sensitivity analysis was carried out to determine the optimum frequency.

8.8 Summary

1. A coupled flamelet/radiation modelling strategy is presented that combines the prediction of finite rate chemistry effects with a detailed solution of the radiative heat exchange.

2. The effect of the radiation heat transfer on temperature and mass fraction of OH, H₂O and CO₂ is studied. It is shown that for the geometries presented here, the effect of radiation is important at regions where the temperatures are > 2000 K.

3. The effect of the radiation is found very important for OH prediction. The radiation heat transfer remarkably improves the prediction of OH mass fraction. This has further implications for the prediction of NO emission.

4. The coupled flamelet/radiation modeling strategy presented here has potential for further improvement.
Concluding Remarks

In the previous chapters, various aspects of the turbulent non-premixed combustion modelling of bluff body flames are investigated and discussed. This last chapter is devoted to the discussion of the main conclusions of this study. The main focal points of the study, the assessment of combustion models and flamelet based NO modelling and flamelet based radiation modelling are discussed below.

An in-house CFD code is developed for the assessment of different combustion models. The eddy break-up, flame sheet, equilibrium and laminar flamelet models are incorporated in the CFD code. The influence of the numerical error associated with the discretisation scheme is assessed by comparing the results obtained by the hybrid, power law and TVD schemes. The configurations used for the validation and assessment of the combustion models are bluff body burners. The high quality experimental database available from the University of Sydney and other reported measurements are used for the purpose of evaluating the combustion models. The bluff body burner configuration is selected because the burner provides a suitable model problem for industrial flows. The flow in the bluff body burner shows one or two complex recirculation zones similar to many industrial flows, but the initial and boundary conditions are more simple and well-defined than for industrial burners. The bluff body burner also provides a controlled environment for the study of turbulence-chemistry interaction at the neck zone. The combustion of different fuels ranging from simple H$_2$/CO and CO/H$_2$/N$_2$ to complex CH$_4$/H$_2$ is investigated for different inlet fuel velocities. The predicted results display the effects of turbulent mixing and the effects of chemical reactions on the modelling capabilities.
9.1 Assessment of combustion models

The performance of the flame sheet, eddy break-up, chemical equilibrium and laminar flamelet models are analysed for predicting temperature, major and minor species for a number of bluff body flames. The comparison of the predictions and the measurements in the HC1 and HM1 flames provides insight into the behaviour of the near equilibrium chemistry regime. The temperature and H$_2$O mass fraction are well predicted by the flame sheet, equilibrium (constrained equilibrium for CH$_4$/H$_2$ fuel) and laminar flamelet models. The prediction of CO$_2$ mass fraction by the equilibrium (constrained equilibrium) and the laminar flamelet models is good, while that of the flame sheet model is poor. The correct prediction of CO in the HM1 flame is very difficult to obtain by the flamelet model. The constrained equilibrium model, however, shows limited success. Only the laminar flamelet model is found to be capable of predicting the correct level of OH mass fraction. Thus it is concluded that even for the near equilibrium flames, an advanced chemistry model like the laminar flamelet model is required for the complete description of thermo-chemical behaviour of the flames.

The predictions of the flames which are far away from the chemical equilibrium condition, such as the syngas (CO/H$_2$/N$_2$), HC2, HM2 and HM3 flames, are difficult. Fast chemistry based combustion models such as the flame sheet, eddy break-up, equilibrium (and constrained equilibrium) models failed to predict the temperature and product mass fractions for the flames mentioned above. The overall predictions of temperature and major and minor species by the flamelet model are good for the HC2 and syngas flames. The flamelet model, on the other hand, failed to yield good predictions for the HM2 and HM3 flames. The main reason behind this discrepancy is the difference in chemical reactions of CO/H$_2$/N$_2$, H$_2$/CO and CH$_4$/H$_2$ fuels and their interactions with the turbulence. The CO/H$_2$/N$_2$ and H$_2$/CO fuels have high stoichiometric mixture fractions, $Z_{sr} = 0.323$ and $Z_{sr} = 0.135$ respectively. The reaction zone for these fuels lies inside the turbulent shear layer, where the stretching of the flame is high. The stretching in these fuels reduce the temperature and mass fraction of products considerably from the equilibrium values. Laminar flamelet calculations for these fuels also show the reduction in peak temperature of approximately 800 K and considerable reductions in the mass fraction of combustion products when the flame is stretched to the extinction limit. The reductions in temperature and mass fractions of products in the syngas and HC2 flames from the equilibrium condition are comparable to the reductions in the
flamelet temperature and mass fraction of products at the higher scalar dissipation rates. Another notable feature of the syngas and HC2 flames is the absence of the localised extinction. The laminar flamelet model can handle this type of finite-rate chemistry effect through the scalar dissipation rate. The finite-rate chemistry effect in CH4/H2 flame is quite different. The CH4/H2 fuel has a low stoichiometric mixture fraction $Z_{st} = 0.05$. As a result, the flame fronts of the HM2 and MH3 flames lie outside the shear layer. The turbulence intensity along the flame front is relatively low, which is expected to be dominated by the large structures. The reaction zones are stretched by the large scales of turbulence, which will not interfere with the inner structure of flames. Large structures also quench the flame locally. The computations show that the mean scalar dissipation rates along the flame fronts in the HM2 and HM3 flames are far below the extinction limit. Therefore, the laminar flamelet model, where the finite-rate chemistry effect is incorporated through the mean scalar dissipation rate failed to predict the local extinction in the HM2 and HM3 flames. The use of other stretching parameters e.g. a modified scalar dissipation rate and the strain rate also was also unable to predict the local extinction. Instead, the use of the strain rate as the stretching parameter has produced unrealistic behaviours in the HM3 flame. The present study concludes that the laminar flamelet model is capable of predicting flames which are far away from the equilibrium condition, provided the localised extinction is absent in the flames.

Based on the performance of the combustion models in a number of flames with different types of fuel and turbulent mixing rate, a number of recommendations can be made for other turbulent flame calculations. The flame-sheet, eddy break-up and equilibrium models are found to be inadequate even for the near equilibrium flames. Therefore, more advanced models, such as the laminar flamelet model, have to be used to provide a complete description of the flame. In situations, where finite rate chemistry effects are important the laminar flamelet model is a good choice. In this context, it is important to distinguish between two types of finite-rate chemistry effects. The first type of the finite-rate chemistry effect that are caused by the interaction of the turbulent mixing and chemical kinetics, but which do not lead to local extinction. The laminar flamelet model is capable of predicting this type of finite-rate chemistry effect. In the second type, where the turbulent mixing leads to considerable local extinction even though the mean stretching rate is below the extinction limit. The laminar flamelet model is not capable of predicting the flames where local extinction is observed. The transient effects are very important when localised extinction occurs. The prediction of
localised extinction requires a detailed analysis of the time scales involving reaction, convection and diffusion processes and it is envisaged that a transient laminar flamelet model will be able to predict the localised extinction phenomenon.

9.2 Flamelet based NO modelling

The detailed analysis of the predicted results under different fuels and flow conditions has indicated that the laminar flamelet model is the best choice for predicting temperature and major and minor species concentrations. The laminar flamelet model is also found to be suitable for the prediction of NO. However, the predicted results are shown to be very sensitive to the differential diffusion effects. The flamelet with differential diffusion effects has yielded better predictions than the flamelet with the unity Lewis number. This is contrary to the findings of the predictions of temperature and species concentrations. The flamelet with unity Lewis number has provided better predictions for temperature and species concentrations. A closer scrutiny of the differential diffusion effect has revealed that neither the full molecular transport nor the unity Lewis number can represent the true extent of the diffusion effects in the turbulent flames. An arbitrary variable Lewis number flamelet model is utilised to demonstrate that great improvements can be achieved by incorporating the actual differential diffusion effects. The current understanding of differential diffusion effect is still very limited. From the modelling point of view, it is in principle, possible to account for the differential diffusion effects. For this to happen, a large quantity of experimental data is required to identify and correlate the differential diffusion parameter with the Reynolds number, chemical reaction e.g. the stoichiometric mixture fraction and the reaction zone thickness, and types of parent fuel. Based on the observed correlation, the model for the differential diffusion can be developed, which in turn can be utilised in the laminar flamelet method of turbulent combustion calculation.

The emission of NO is adequately represented by the Zeldovick mechanism. However, it has been shown that the prediction in the fuel rich zone is not adequate and the reaction mechanism involving NO reburn may provide better predictions in the fuel rich zone.

Finally, it can be concluded that the laminar flamelet model can be employed for the prediction of pollutant emissions with a sufficient degree of accuracy.
9.3 Flamelet based radiation modelling

The effect of radiation heat transfer on the predictive capability of the laminar flamelet model is investigated. The coupling between the radiation and combustion is achieved through an additional parameter, the enthalpy defect. The flamelet library with the required enthalpy defect is generated by modifying the available enthalpy at the boundaries. The overall computational strategy combines the modelling of finite rate chemistry effects with the detailed solution of the accompanying coupled equation of radiative exchange.

The radiative heat exchange is computed by the discrete transfer model and the gas radiation properties are established from the concentrations of CO\textsubscript{2} and H\textsubscript{2}O available from the combustion calculations. A weighted sum of gray gases (WSGG) method is employed for the radiation properties calculations. Radiation properties, emissivities and intensities have been computed from the mean values of the scalar variables. The influence of turbulence fluctuations on these properties (turbulence/radiation interactions) is not included in the radiation exchange calculation.

The coupled flamelet/radiation calculations of the bluff body flames reveal that the influence of radiation is important in the high temperature zones of around 2000 K. Though no experimental data is available to ascertain the accuracy of the radiation intensities and related heat fluxes, the incorporation of radiation has improved the predictive capabilities of the laminar flamelet model. The improved agreement for the OH radical is remarkable and may be fortuitous, but, it can be safely concluded that the present coupled radiation/flamelet model will result in better prediction of temperature and major and minor species which in turn will improve the prediction of pollutant emissions such as NO.

There exist much scopes for the improvement of the predictive capabilities of the current radiation/flamelet model. The current method is applicable only for the unity Lewis number flamelets, but it can be extended for the differential diffusion flamelet. The use of advanced radiative properties algorithms such as the wide band and the narrow band models will be more realistic and accurate than the WSGG model. The implications of the turbulence/radiation interactions for these flames remains to be established.
9.4 Present contribution

The main contributions of the thesis are:

1. The flame sheet, equilibrium, eddy break up and laminar flamelet models have been implemented in an in-house code for the study of turbulence-combustion interaction and for the assessment of different submodels.

2. Errors associated with the discretisation schemes have been systematically assessed. This establishes a firm basis for evaluating the mathematical models studied.

3. The flamelet based NO modelling strategy has been presented. The thermal NO mechanism has been shown to provide reasonably good predictions.

4. The coupled flamelet/radiation model has been implemented. The model combines the finite rate chemistry effects with a detailed solution of the radiative heat exchange.

5. It has been shown that the laminar flamelet model is well capable of predicting temperature and concentrations of major and minor species for flames at near equilibrium as well as away from equilibrium but without the local extinction.

6. The effects of differential diffusion on temperature and species concentrations have been studied. It has been shown that the unity Lewis number flamelet gives a better representation of the transport of the species in turbulent flames.

7. The prediction of NO has been shown to be very sensitive to the differential diffusion effect. An arbitrary variable flamelet has been shown to produce a better prediction of NO.

8. It has been shown that only the scalar dissipation rate as the non-equilibrium parameter can reproduce the correct trend of the flame structure.
9.5 Recommendations for future work

The present study has raised many novel issues that need further investigation. Some of these are:

1. The laminar flamelet model should be modified to include the actual differential diffusion effects instead of the current approach of either setting full molecular transport or setting the equal mass diffusivities and unity Lewis number.

2. The sensitivity of the different reaction mechanisms on the prediction capability of the laminar flamelet model should be studied.

3. Different pathways of NO formation should be implemented in the laminar flamelet model.

4. The flamelet/radiation model has a lot of potential for further development. The advanced property calculation algorithms should be utilised and effects of turbulence/radiation interactions should be investigated.

5. The transient effects in the laminar flamelet modelling should be investigated, specially for the prediction of CO and local extinction in hydrocarbon flames.
### Appendix A

**Table A.1: Detailed Mechanism and rate data in units of mol, cm, s, kJ**


<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>( B_\beta )</th>
<th>( a_\beta )</th>
<th>( E_\beta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1f</td>
<td>( \text{O}_2 + H \rightarrow \text{OH} + \text{O} )</td>
<td>2.000E+14</td>
<td>0.00</td>
<td>70.30</td>
</tr>
<tr>
<td>1b</td>
<td>( \text{OH} + \text{O} \rightarrow \text{O}_2 + \text{H} )</td>
<td>1.568E+13</td>
<td>0.00</td>
<td>3.52</td>
</tr>
<tr>
<td>2f</td>
<td>( \text{H}_2 + \text{O} \rightarrow \text{OH} + \text{H} )</td>
<td>5.060E+04</td>
<td>2.67</td>
<td>26.30</td>
</tr>
<tr>
<td>2b</td>
<td>( \text{OH} + \text{H} \rightarrow \text{H}_2 + \text{O} )</td>
<td>2.222E+04</td>
<td>2.67</td>
<td>18.29</td>
</tr>
<tr>
<td>3f</td>
<td>( \text{H}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{H} )</td>
<td>1.000E+08</td>
<td>1.60</td>
<td>13.80</td>
</tr>
<tr>
<td>3b</td>
<td>( \text{H}_2\text{O} + \text{H} \rightarrow \text{OH} + \text{O} )</td>
<td>4.312E+08</td>
<td>1.60</td>
<td>76.46</td>
</tr>
<tr>
<td>4f</td>
<td>( \text{OH} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O} )</td>
<td>1.500E+09</td>
<td>1.14</td>
<td>0.42</td>
</tr>
<tr>
<td>4b</td>
<td>( \text{H}_2\text{O} + \text{O} \rightarrow \text{OH} + \text{OH} )</td>
<td>1.473E+10</td>
<td>1.14</td>
<td>71.09</td>
</tr>
</tbody>
</table>

|  | \( \text{H}_2/\text{O}_2 \) Chain Reactions |
| | **HO\(_2\)** Formation and Consumption |
| 5f  | \( \text{O}_2 + \text{H} + \text{M}' \rightarrow \text{HO}_2 + \text{M}' \) | 2.300E+18 | -0.80 | 0.00 |
| 5b  | \( \text{HO}_2 + \text{M}' \rightarrow \text{O}_2 + \text{H} + \text{M}' \) | 3.190E+18 | -0.80 | 195.39 |
| 6   | \( \text{HO}_2 + \text{H} \rightarrow \text{OH} + \text{OH} \) | 1.500E+14 | 0.00 | 4.20 |
| 7   | \( \text{HO}_2 + \text{H} \rightarrow \text{H}_2 + \text{O}_2 \) | 2.500E+13 | 0.00 | 2.90 |
| 8   | \( \text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2 \) | 6.000E+13 | 0.00 | 0.00 |
| 9   | \( \text{HO}_2 + \text{H} \rightarrow \text{H}_2\text{O} + \text{O} \) | 3.000E+13 | 0.00 | 7.20 |
| 10  | \( \text{HO}_2 + \text{O} \rightarrow \text{OH} + \text{O}_2 \) | 1.800E+13 | 0.00 | -1.70 |

|  | \( \text{H}_2\text{O}_2 \) Formation and Consumption |
| | continued in next page |

continued in next page
<table>
<thead>
<tr>
<th>No.</th>
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<th>$a_\beta$</th>
<th>$E_\beta$</th>
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<tr>
<td>12b</td>
<td>H$_2$O$_2$ + M$'$ → OH + OH + M$'$</td>
<td>1.692E+24</td>
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<td>202.29</td>
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<tr>
<td>13</td>
<td>H$_2$O$_2$ + H → H$_2$O + OH</td>
<td>1.000E+13</td>
<td>0.00</td>
<td>15.00</td>
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<tr>
<td>14f</td>
<td>H$_2$O$_2$ + OH → H$_2$O + HO$_2$</td>
<td>5.400E+12</td>
<td>0.00</td>
<td>4.20</td>
</tr>
<tr>
<td>14b</td>
<td>HO$_2$ + HO$_2$ → H$_2$O$_2$ + OH</td>
<td>1.802E+13</td>
<td>0.00</td>
<td>134.75</td>
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</table>

**Recombination Reactions**

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<th>$E_\beta$</th>
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<tr>
<td>15</td>
<td>H + H + M$'$ → H$_2$ + M$'$</td>
<td>1.800E+18</td>
<td>-1.00</td>
<td>0.00</td>
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<tr>
<td>16</td>
<td>OH + H + M$'$ → H$_2$O + M$'$</td>
<td>2.200E+22</td>
<td>-2.00</td>
<td>0.00</td>
</tr>
<tr>
<td>17</td>
<td>O + O + M$'$ → O$_2$ + M$'$</td>
<td>2.900E+17</td>
<td>-1.00</td>
<td>0.00</td>
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</tbody>
</table>

**CO/CO$_2$ Mechanism**

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<th>$a_\beta$</th>
<th>$E_\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>18f</td>
<td>CO + OH → CO$_2$ + H</td>
<td>4.400E+06</td>
<td>1.50</td>
<td>-3.10</td>
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<tr>
<td>18b</td>
<td>CO$_2$ + H → CO + OH</td>
<td>4.956E+08</td>
<td>1.50</td>
<td>89.76</td>
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**CH Consumption**

<table>
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<th>$a_\beta$</th>
<th>$E_\beta$</th>
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</thead>
<tbody>
<tr>
<td>19</td>
<td>CH + O$_2$ → HCO + O</td>
<td>3.000E+13</td>
<td>0.00</td>
<td>0.00</td>
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<tr>
<td>20</td>
<td>CO$_2$ + CH → HCO + CO</td>
<td>3.400E+12</td>
<td>0.00</td>
<td>2.90</td>
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**HCO Consumption**

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<td>21</td>
<td>HCO + H → CO + H$_2$</td>
<td>2.000E+14</td>
<td>0.00</td>
<td>0.00</td>
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<tr>
<td>22</td>
<td>HCO + OH → CO + H$_2$O</td>
<td>1.000E+14</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>23</td>
<td>HCO + O$_2$ → CO + HO$_2$</td>
<td>3.000E+12</td>
<td>0.00</td>
<td>0.00</td>
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<tr>
<td>24f</td>
<td>HCO + M$'$ → CO + H + M$'$</td>
<td>7.100E+14</td>
<td>0.00</td>
<td>70.30</td>
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<tr>
<td>24b</td>
<td>CO + H + M$'$ → HCO + M$'$</td>
<td>1.136E+15</td>
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<td>9.97</td>
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**CH$_2$ Consumption**

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<th>$a_\beta$</th>
<th>$E_\beta$</th>
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<tr>
<td>25f</td>
<td>CH$_2$ + H → CH$_2$ + H</td>
<td>8.400E+09</td>
<td>1.50</td>
<td>1.40</td>
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<tr>
<td>25b</td>
<td>CH + H$_2$ → CH$_2$ + H</td>
<td>5.830E+09</td>
<td>1.50</td>
<td>13.08</td>
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<tr>
<td>26</td>
<td>CH$_2$ + O → CO + H + H</td>
<td>8.000E+13</td>
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<td>0.00</td>
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<tr>
<td>27</td>
<td>CH$_2$ + O$_2$ → CO + OH + O</td>
<td>6.500E+12</td>
<td>0.00</td>
<td>6.30</td>
</tr>
<tr>
<td>28</td>
<td>CH$_2$ + O$_2$ → CO$_2$ + H + H</td>
<td>6.500E+12</td>
<td>0.00</td>
<td>6.30</td>
</tr>
</tbody>
</table>

**CH$_2$O Consumption**

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<th>$a_\beta$</th>
<th>$E_\beta$</th>
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<tr>
<td>29</td>
<td>CH$_2$O + H → HCO + H$_2$</td>
<td>2.500E+13</td>
<td>0.00</td>
<td>16.70</td>
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<tr>
<td>30</td>
<td>CH$_2$O + O → HCO + OH</td>
<td>3.500E+13</td>
<td>0.00</td>
<td>14.60</td>
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<tr>
<td>31</td>
<td>CH$_2$O + OH → HCO + H$_2$O</td>
<td>3.000E+13</td>
<td>0.00</td>
<td>5.00</td>
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<tr>
<td>32</td>
<td>CH$_2$O + M$'$ → HCO + H + M$'$</td>
<td>1.400E+17</td>
<td>0.00</td>
<td>320.00</td>
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<th>$a_{\beta}$</th>
<th>$E_{\beta}$</th>
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<tr>
<td>33f</td>
<td>$\text{CH}_3 + \text{H} \rightarrow \text{CH}_2 + \text{H}_2$</td>
<td>$1.800\text{E+14}$</td>
<td>0.00</td>
<td>63.00</td>
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<tr>
<td>33b</td>
<td>$\text{CH}_2 + \text{H}_2 \rightarrow \text{CH}_3 + \text{H}$</td>
<td>$3.680\text{E+13}$</td>
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<td>44.30</td>
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<tr>
<td>34</td>
<td>$\text{CH}_3 + \text{H} \rightarrow \text{CH}<em>4$ \quad $k</em>\infty$</td>
<td>$2.108\text{E+14}$</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>\qquad \quad $k_0$</td>
<td>$6.257\text{E+23}$</td>
<td>-1.80</td>
<td>0.00</td>
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<tr>
<td>35</td>
<td>$\text{CH}_3 + \text{O} \rightarrow \text{CH}_2\text{O} + \text{H}$</td>
<td>$7.000\text{E+13}$</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>37</td>
<td>$\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{OH}$</td>
<td>$3.400\text{E+11}$</td>
<td>0.00</td>
<td>37.40</td>
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<tr>
<td>38f</td>
<td>$\text{CH}_4 + \text{H} \rightarrow \text{CH}_3 + \text{H}_2$</td>
<td>$2.200\text{E+04}$</td>
<td>3.00</td>
<td>36.60</td>
</tr>
<tr>
<td>38b</td>
<td>$\text{CH}_3 + \text{H}_2 \rightarrow \text{CH}_4 + \text{H}$</td>
<td>$8.391\text{E+02}$</td>
<td>3.00</td>
<td>34.56</td>
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<td>39</td>
<td>$\text{CH}_4 + \text{O} \rightarrow \text{CH}_3 + \text{OH}$</td>
<td>$1.200\text{E+07}$</td>
<td>2.10</td>
<td>31.90</td>
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<tr>
<td>40f</td>
<td>$\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3 + \text{H}_2\text{O}$</td>
<td>$1.600\text{E+06}$</td>
<td>2.10</td>
<td>10.30</td>
</tr>
<tr>
<td>40f</td>
<td>$\text{CH}_3 + \text{H}_2\text{O} \rightarrow \text{CH}_4 + \text{OH}$</td>
<td>$2.631\text{E+05}$</td>
<td>2.10</td>
<td>70.92</td>
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</table>

The third body coefficients with respect to molecular hydrogen are 6.5 for CH$_4$, 6.5 for H$_2$, 1.5 for CO$_2$, 0.75 for CO, 0.4 for O$_2$, 0.4 for N$_2$ and 1.0 for all other species.
Computational results from the third TNF workshop

Computations presented in the third TNF workshop (TNF3 1998) for the HM1 flame were carried out by four research groups. The names of the contributing groups are listed below. All flowfield calculations were carried out by using either k-ε or Reynolds stress (RS) models of turbulence. A brief summary of different combustion and turbulence model as well as computational domain and grid size used by different research groups are tabulated in Table B.1. The predicted results of the HM1 flame is reproduced in Figs. B.1-B.4. These figures are obtained from Masri (1997). The following terminology was used to describe different turbulence models (TNF3 1998):

- RS-S: Standard Reynolds Stress Model with $C_{\varepsilon_1} = 1.44$
- RS-M: Modified Reynolds Stress Model with $C_{\varepsilon_1} = 1.60$
- k-ε-S: Standard k-ε model with $C_{\varepsilon_1} = 1.44$
- k-ε-M: Modified k-ε model with $C_{\varepsilon_1} = 1.60$

Contributing groups:

- Department of Fuel and Energy
  Leeds University, UK
  Contact person: Dr Graham Spence

- Department of Mechanical Engineering
  The University of Sydney
  Contact person: Dr Bassam Dally
Appendix B

• Department of Mechanical Engineering
  Pohang University of Science and Technology
  Pohang, Korea
  Contact person: Prof. Kang, Y. Huh

• Technische Universiteit Delft
  Department of Applied Physics
  Delft, The Netherlands
  Contact person: Dr Tim Peeters
## Table B.1: Summary of computations. Reference: (TNF3 1998)

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Figure B.1: Radial profiles of mean mixture fraction ($\bar{\xi}$) in the reacting jet (case HM1) (CH$_4$/H$_2$ fuel, bulk jet velocity = 118m/s, coflow air velocity = 40m/s). Green solid dots: Experimental data; blue-dashed line: Korea, k-ε-S (K-NKES); red-dashed line: Sydney, k-ε-M (S-NKEM); green-solid line: Delft, Rs-M (D-RRSM); black-solid line: Leeds, Rs-S (L-NRSS); purple-solid line: Sydney, Rs-M (S-RRSM). Note: Red solid triangles shown for x=13 and 30mm are for flame HM2 which has a bulk jet velocity of 178m/s)
Figure B.2: Radial profiles of the rms fluctuations of mixture fraction ($\xi'$) in the reacting jet (case HM1) (CH$_4$/H$_2$ fuel, bulk jet velocity = 118 m/s, coflow air velocity = 40 m/s). Legend as in figure B.1.
Figure B.3: Radial profiles of mean temperature in the reacting jet (case HM1) (CH$_4$/H$_2$ fuel, bulk jet velocity = 118m/s, coflow air velocity = 40m/s). Legend as in figure B.1. Note: Red solid triangles shown for x=13 and 30mm are for flame HM2 which has a bulk jet velocity of 178m/s)
Figure B.4: Radial profiles of mean mass fraction of OH in the reacting jet (case HM1) (CH$_4$/H$_2$ fuel, bulk jet velocity = 118m/s, coflow air velocity = 40m/s). Legend as in figure B.1. Note: Red solid triangles shown for x=13 and 30 mm are for flame HM2 which has a bulk jet velocity of 178 m/s)
References


