Numerical Investigation of Jets in a Reacting Crossflow

by

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A thesis submitted in conformity with the requirements for the degree of Master of Applied Science
Graduate Department of Mechanical and Industrial Engineering
University of Toronto

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0-612-46088-6
Abstract

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The mixing of air jets into hot, fuel-rich mixture is an integral part of many staged combustion applications. This study concentrates on the exhaust system of an electric arc steelmelting furnace where high concentrations of carbon monoxide (CO) and hydrogen (H₂) are present. A three dimensional numerical code featuring two combustion models has been used to predict those emissions for various jet to cross-stream mass flow ratios and a comparison with experimental CO measurements was done. The results showed that both models were unable to predict CO and H₂ emissions for the conditions investigated. Thorough examination of the non-premixed flamelet revealed that the turbulent time scale was much faster than the chemical time scale, thus, collapsing one of the requirements of this model. With the eddy dissipation model, the CO and H₂ concentrations were severely underpredicted and convergence problems occurred when dissimilar chemical kinetic rates for CO and H₂ were incorporated.
Acknowledgements

I would like to thank my supervisors, Prof. Marilyn Lightstone and Prof. Murray Thomson. They provided me with outstanding support, guidance and patience throughout my Master's term. I would also like to thank Judy Cooper for her continuous technical assistance with the combustion models, especially with the flamelet library generation.

Special gratitude goes to my family, Karla and Joshua. They have been with me in bad and good times. Their encouragement and understanding is greatly appreciated.
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## Nomenclature

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<td>$\Gamma$</td>
<td>molecular thermal conductivity [W/m·K]</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>turbulent dissipation rate [W/kg]</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>thermal conductivity [W/m²·K]</td>
</tr>
<tr>
<td>$\mu$</td>
<td>molecular dynamic viscosity [Pa·s]</td>
</tr>
<tr>
<td>$\mu_t$</td>
<td>turbulent dynamic viscosity of momentum [Pa·s]</td>
</tr>
<tr>
<td>$\mu_t^H$</td>
<td>turbulent dynamic viscosity of heat [Pa·s]</td>
</tr>
<tr>
<td>$\nu$</td>
<td>molecular kinematic viscosity [m²/s]</td>
</tr>
<tr>
<td>$\rho_j$</td>
<td>jet density</td>
</tr>
<tr>
<td>$\rho_m$</td>
<td>mainstream density</td>
</tr>
<tr>
<td>$\phi$</td>
<td>equivalence ratio</td>
</tr>
<tr>
<td>$\theta$</td>
<td>normalized temperature</td>
</tr>
<tr>
<td>$\sigma_T$</td>
<td>mass-weighted standard deviation of temperature</td>
</tr>
<tr>
<td>$\tau_w$</td>
<td>wall shear [Pa]</td>
</tr>
<tr>
<td>$\chi$</td>
<td>instantaneous scalar dissipation rate [1/s]</td>
</tr>
<tr>
<td>$\chi_{st}$</td>
<td>stoichiometric scalar dissipation rate at [1/s]</td>
</tr>
<tr>
<td>$\chi_q$</td>
<td>scalar dissipation rate at quenching [1/s]</td>
</tr>
<tr>
<td>$A$</td>
<td>strain rate [1/s]</td>
</tr>
<tr>
<td>$A_c$</td>
<td>pre-exponential constant</td>
</tr>
<tr>
<td>$AMIX$</td>
<td>area-weighted standard deviation of mixture fraction</td>
</tr>
<tr>
<td>$C$</td>
<td>equation (2.6)</td>
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<tr>
<td>$C_p$</td>
<td>heat capacity at constant temperature [J/kg·K]</td>
</tr>
<tr>
<td>$C_l$</td>
<td>Craya-Curtet number</td>
</tr>
<tr>
<td>$D$</td>
<td>jet diameter [m]</td>
</tr>
<tr>
<td>$D$</td>
<td>diameter of cylindrical duct [m]</td>
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Da  Damkohler number
DR  jet-to-crossflow density ratio
$E_T$  activation energy [K]
$F$  mixture fraction
$F/A$  fuel to air ratio
$H$  total enthalpy
$H_o$  duct height (rectangular)
$J$  Momentum flux ratio
$K$  turbulent kinetic energy [$m^2/s^2$]
$Le$  Lewis number
$L_0$  half-radius of the jet [m]
$M$  molecular weight [kg/kmol]
$m$  mass flow ratio [kg/s]
$MR$  jet-to-crossflow mass flow ratio
$N$  number of orifices
$P$  pressure [Pa]
$Pr$  Prandtl number
$Pr_t$  turbulent Prandtl number
$R$  duct radius [m]
$\bar{R}$  universal gas constant
$R_{1/2}$  half-radius [m]
$R_{1/2}$  half area radius [m]
$Q''$  wall heat flux [W/m$^2$]
$S$  effective circumferential spacing between orifice centers
$T$  time [s]
$T$  temperature [K]
$T_j$ or $T_a$  jet or air temperature [K]
$T_m$ or $T_f$  mainstream or fuel temperature [K]
\[ U_i \quad \text{time-averaged velocity in } i \text{ direction [m/s]} \]
\[ U_m \quad \text{mainstream velocity [m/s]} \]
\[ V_j \quad \text{jet velocity [m/s]} \]
\[ x \quad \text{axial (streamwise) distance [m]} \]
\[ Y \quad \text{mass fraction of carbon} \]
\[ y^+ \quad \text{dimensionless distance from the wall} \]
\[ Z \quad \text{mixture fraction} \]
\[ Z' \quad \text{mixture fraction fluctuations} \]
\[ \bar{Z}^* \quad \text{mixture fraction variance} \]
1 Introduction

1.1 Motivation

The mixing of jets with a cross-stream is relevant to many engineering problems including combustion systems such as gas turbines, steelmelting furnaces and many others where staged combustion is involved. This project focuses on the exhaust system of an electric arc steelmelting furnace. The exhaust gases are a major environmental concern since they contain high concentrations of carbon monoxide (CO), hydrogen (H₂) and nitrogen oxides (NOₓ).

In electric arc furnaces (EAF) scrap steel is being recycled. Fumes generated as a result of melting the steel contain up to up to 40% combustibles, mainly carbon monoxide (CO) and hydrogen (H₂), at temperatures of up to 2000 K. A typical configuration of the fume extraction system is shown in Figure 1-1. In order to burn off the hot fuel rich mixture, air enters through a gap (circumferential slit) in the exhaust water-cooled duct walls. The air deflects the main flow.

Figure 1-1  Schematic of the EAF Fume Extraction System
and slowly mixes with the hot fuel producing a long turbulent diffusion flame. Further downstream, the combustion gases are cooled by a water spray prior to entering the gas filter systems. The purpose of the water-cooled ductwork and water spray coolers is to provide a suitable gas temperature at the particle removal facility.

The length of the water-cooled duct walls is large since the diffusion flame is long and heat exchange is poor. Therefore, there is an interest in reducing the length of the flame. This will reduce the cost and maintenance involved in the water-cooled ducts. In addition, optimizing the design of an EAF will result in lower CO and H\textsubscript{2} concentrations for minimal airflow over a wide range of operating conditions. Thus, alternate mixing mechanisms should be explored in order to develop a better pollution control device that will increase combustion efficiency. The use of computational fluid dynamics (CFD) modelling can aid in the development of such devices.

### 1.2 Objectives

The main objective of this work is to understand the physical behaviour of jets on the penetration and mixing performance in a mixing section. The key to this concept is rapid and uniform mixing. Hence, the fundamental mixing characteristics that govern the circumferential jets mixing in a cylindrical duct will be investigated.

The second objective is to study numerically the effectiveness and ability of an existing CFD code to predict various fluid flows ranging from a simple pipe flow to complex jet flow. This will be done by verifying the computational model to analytical and experimental results.

The last objective of this work is to assess the applicability of two combustion models in to predict combustion processes of jets in a reacting crossflow. In the numerical code, the non-premixed laminar flamelet and eddy dissipation models are available. Provided that their
predictions are reasonable, the code can then be used to model many jet mixing configurations so that an optimum mixer geometry can be designed. This will lead to the improvement of the combustion efficiency in exhaust gas combustors. Otherwise, detailed investigated of these models will be performed in order to determine the reasons for their inadequacy.
2 Literature Review

This chapter summarizes the experimental and numerical studies of jet enhanced mixing. In particular, this research looks at the interaction of jets in a crossflow. A cylindrical duct with circular orifices is the geometric configuration of interest. Non-reacting flows are considered first in order to gain insight into the mechanisms of fluid mixing. Reacting flows are then considered.

2.1 Non-Reacting Flows

Many researchers have investigated the characteristics of circumferential jets in a crossflowing fluid [1-22]. Since this flow mechanism occurs in numerous situations, it produced a large number of theoretical and experimental studies over many years. This section looks at specific studies that have been done on non-reacting jet mixing in cylindrical and rectangular duct configurations. All of the studies involve relatively cold jets of air that are being injected normally into the hot mainstream flow of air. The experimental studies examine the mixing performance for different flow configurations. They reveal that the key parameters affecting the fluid mixing are the momentum flux ratio, orifice shape, and the number of orifices employed. Since the conserved scalar for non-reacting flows is the temperature field, it is used to describe the mixing processes. To compare the mixing characteristics of different flow configurations, the scalar field is normalized as,

\[ \theta = \frac{T_m - T}{T_m - T_j} \]  

(2.1)
where \( m \) and \( j \) represent the mainstream and jet, respectively. Thus, \( \theta = 1 \) represents the jet fluid, and \( \theta = 0 \) represents the mainstream fluid. An alternate measure of mixing is the mixture fraction, \( f \), defined as:

\[
f = 1 - \theta = \frac{T - T_j}{T_m - T_j}
\]  

(2.2)

where \( f = 0 \) represent the jet flow and \( f = 1 \) represents the mainstream flow.

Detailed studies involving both the velocity and temperature measurements of jets in a crossflow reveal interesting structures of the jet as it progresses downstream [1]. Each jet creates a blockage in the crossflow, and as a consequence, the flow upstream of the jet decelerates causing an increase in pressure. This causes the deformation of the jet. Turbulent shear layers develop around the periphery of the jet due to high mixing between the crossflow and jet fluid. The lower momentum fluid in the shear layer at the sides of the jet will create a more curved trajectory than that of the higher velocity fluid in the core. This will form the characteristic kidney-shaped jet profile (Figure 2-1).
Downstream of the injection plane, the flow field is dominated by three vortex systems that mainly control the entrainment and mixing of the crossflow and jet fluid. A horseshoe vortex system is formed in the same way as in the flow around a cylinder mounted on a flat surface. Andreopoulos and Rodi [2] showed that the horseshoe vortex effect on fluid mixing is relatively small in comparison with the two other regions of high vorticity. The bound vortices are located at the lobes of each jet and therefore enhance the kidney-shaped profile of the jet as it continues downstream. For jets entering into a confined crossflow, two vortices, known as the crossflow vortices, are formed by crossflow fluid that passes between the jets into the low-pressure region located in their wake, beneath the core of the jet.

2.1.1 *Momentum-Flux Ratio, J*

This parameter is the most important flow variable influencing the jet mixing in a crossflow. The momentum flux ratio is the ratio of the momentum of the jet to the momentum of the mainstream, and it is defined as,

\[ J = \frac{\rho_j V_j^2}{\rho_m V_m^2} \]  

(2.3)

where \( \rho_j, \rho_m, V_j \) and \( V_m \) are the density and velocity of the jet and mainstream, respectively. Numerous experiments and numerical analysis were done to illustrate its effect in non-reacting flows in both rectangular and cylindrical ducts. Hatch et al. [3] performed a series of tests with eight orifices at three values of \( J \). The report compared mixture fraction variations and mixture non-uniformities from the leading edge of the jets to one radius downstream. Hatch et al. [3] found that the jet-to-mainstream momentum flux ratio significantly impacts the mixing characteristics of jets in a cylindrical geometry. The report has also shown that for a fixed configuration, the extent of jet penetration and circumferential mixing are determined by the
coupling between \( J \) and orifice geometry. A numerical comparison to the measured data by Hatch et al. [3] was also examined by Oechsle et al. [4] using a 3-D numerical analysis. Oechsle et al. [4] found similar behaviours in the mixing performance and temperature field. The report emphasized the importance of \( J \) and orifice geometry with regard to jet penetration and mixing. Talpallikar et al. [5] have conducted a 3-D numerical analysis in a non-reacting and reacting flows employing 12 circumferential slots. It was found that variations of \( J \) in a non-reacting flow, for a constant orifice geometry, orifice spacing and mass flow ratio, yield three types of jet penetrations: (1) under-penetration, (2) optimum penetration, and (3) over-penetration. Figure 2-2 illustrates three behaviour patterns of jet penetration in a non-reacting flow as a function of \( J \).

![Jet penetration behaviour as a function of J](image)

Vranos et al. [6] and Liscinsky et al. [7] performed experiments of non-reacting flows in cylindrical and rectangular ducts using planar digital imaging, in order to measure mixing rates. Similarly, they found that mixing is primarily a function of \( J \) and orifice spacing, and that jet penetration exhibits three distinct regions for a range of \( J \) values.
At low $J$ values the jets are located close to the wall. The crossflow fluid is unaffected by the entraining jets and forms a relatively unmixed core that continues downstream. This jet behaviour is known as under-penetrating. At optimum penetration the jets interact with the crossflow and better mixing is observed. Doerr et al. [8] investigated jet mixing with a confined crossflow in a rectangular duct. Temperature distribution, mixing rate and standard deviation were determined at discrete downstream locations. For all configurations examined, Doerr et al. [8] found that an optimum momentum flux ratio yielded a homogenous temperature distribution in the flow field downstream of the injection plane. As the optimum $J$ value is exceeded, a recirculation region starts to form upstream of the impinging jets that results in over-penetration and undesirable upstream mixing, and therefore blockage effects. The increased jet penetration to the center directs a larger portion of the jet flow towards the duct’s core, and therefore decreasing the circumferential mixing along the walls. To obtain a well-mixed flow field, it is important to have a good radial mixing.

### 2.1.2 Number of Orifices

The other contributing factor to jet penetration and mixing is the number of orifices used. The number of orifices is related to orifice spacing. By increasing the number of orifices in a cylindrical duct, while keeping the mass flow ratio constant, jet penetration is reduced. Hence, this creates the effect of decreasing $J$. Zhu et al. [9] studied numerically the effect of momentum flux ratio on the mass-weighted standard deviation of temperature, $\sigma_T$, at different straight slot aspect ratios and number of orifices. $\sigma_T$ is defined as mixture non-uniformity, in other words. low $\sigma_T$ values represent high mixing performance. Zhu et al. [9] found that the optimal configuration changes with the number of orifices. In addition, at a constant $J$ value, mixing
performance characterized by $\sigma_r$ is improved with an increase of number of orifices. This was also confirmed by Liscinsky et al. [7].

### 2.1.3 Effect of Orifice Shape

Liscinsky et al. [7] and Vranos et al. [6] have conducted experiments in cylindrical and rectangular ducts using planar digital imaging system. The Concentration distributions were measured in a plane normal to the duct axis at several downstream locations by planar digital imaging of the Mie-scattered light from an aerosol seed mixed the injectant. Spatial unmixedness of round holes and slanted slots injectors was compared as a function of $J$ at two axial downstream location, at 1.4 and 2.0 duct radii from the leading edge of the orifice ($x/R = 1.4$ and 2.0). It was observed that the mixing performance with the slot injectors was better.

![Figure 2-3](image)

Figure 2-3 Still movie frames of jet/jet and jet/mainstream interactions of round and slanted slot injectors at low speed flows (from Liscinsky et al. [7])

In addition, the unmixedness at $x/R = 2.0$ was lower than at $x/R = 1.4$. Hence, the fluid gets more mixed as it goes downstream. The reduction in unmixedness with downstream location
was also shown in other experiments [3, for example]. Holes were found to perform better than slots for $J < 20$, but worse as $J$ increased, since jet penetration was greater for low values of $J$. Thus, round holes provided better mixing right after injection, but the mixing slowed down with increasing downstream distance. On the other hand, the slanted slots continued to mix with downstream distance, hence, they required more downstream distance to obtain peak performance. Representative still frames from movies of low-speed flow are shown in Figure 2-3 where the jet flow is marked in dark colour. The black round dots indicate where the jets come from. This figure illustrates the difference in the jet/jet and jet/mainstream interactions between slanted slots and round injectors. The jet exiting a round hole forms two counter-rotating vortices of equal strength. The jet penetrates directly toward the center of the duct, and the jet cross section is stretched as $J$ increases. The connecting sheet moves closer to the duct axis, but the vortices tend to remain near the wall. However, the slanted slot jet forms a pair of counter-rotating vortices that are of unequal size and strength. The larger primary vortex forms at the leading edge of the slot and moves towards the duct wall, while the smaller vortex moves away from the wall. The jet interaction with the neighbouring jets occurs early in the injection process. This would explain why mixing performance was found to be better with slanted slots than with round holes, for a given $J$ value and downstream distance.

Hatch et al. [3] performed experiments for a fixed number of orifices with round hole, straight slot and slanted slot injectors. The findings indicate that initial mixing is better for the round holes, but slot orifices improve mixing downstream. Oechsle et al. [10] analyzed numerically three different sets of orifice shapes: Squares, elongated slots and equilateral triangles. Consequently, it was found that larger slanted slot angles and aspect ratios are generally the best mixing configurations at higher $J$ values. However, at lowest $J$ values
analyzed, the square and triangular orifices yielded better mixing. Therefore, the design of an optimum mixing section strongly depends on the operating conditions (i.e., \( J \)). From these conditions, it is possible to select the appropriate orifice configuration.

### 2.1.4 Effect of Density Ratio

Liscinsky et al. [7] showed the dependence of unmixedness on \( J \) for fixed orifice size and spacing for at two density ratios, \( DR = 1.0 \) and \( DR = 2.77 \). For non-reacting flows, the jet and mainstream fluids are gaseous consisting of air at atmospheric pressure. Air is treated as an ideal gas since the temperatures are relatively low (less than 1000 Kelvin). From the ideal-gas law,

\[
P = \rho RT
\]

where, \( P \) is the pressure, \( \rho \) is the density, \( R = \bar{R}/M \), \( \bar{R} \) is the universal gas constant (= 8.314 kJ/kmol·K), \( M \) is the molecular weight (for air \( M = 28.97 \) kg/kmol) and \( T \) is the absolute temperature. Assuming atmospheric pressure, the density ratio of the two streams, is therefore, a function of the temperature ratio. That is,

\[
DR = \frac{\rho_j}{\rho_m} = \frac{T_m}{T_j}
\]

where the subscripts \( m \) and \( j \) represent the mainstream and jet, respectively. In the experiment of Liscinsky et al. [7], it was shown that the mixing performance worsens as the density ratio increases above unity. It was concluded that \( J \) alone is not sufficient to characterize mixing. Holdeman [7] reported that the density ratio has a secondary effect based on the similarity in profile distributions. Hence, mixing rate decreases with increasing density ratio.
2.1.5 Optimization of Jet Mixing

Holdeman et al. [8], have conducted experiments in a rectangular ducts and determined a relationship on the basis of inspection of mean temperature profiles. They have shown that similar jet penetration, defined by the location of the centerline temperature of the jet, and similar mixing is obtained over a range of momentum flux ratios, \( J \), when the orifice spacing, \( S \), and the square root of the momentum flux ratio are inversely proportional, that is,

\[
C = \left( \frac{S}{H_o} \right) \sqrt{J}
\]  

(2.6)

where \( H_o \) is the duct height, independent of orifice size. For a constant jet to mainstream mass flow ratio, a similar jet penetration would be observed for widely-spaced orifices with low momentum flux ratio and for closely-spaced orifices with high momentum flux ratio.

Experimental data of non-reacting jets in a rectangular crossflow were correlated with respect to Equation (2.6) to obtain optimum penetration and mixing. Figure 2-4 shows values of \( C \) that yield optimum mixing. Holdeman [7] found that for single-sided injection, the centerplane profiles are approximately centered across the duct height and approach a uniform

![Figure 2-4](image-url)  

**Figure 2-4** Optimum \( C \) values for a single side injection, directly opposed injection and staggered injection jets in a rectangular duct
temperature distribution in the minimum downstream distance when \( C = 2.5 \). For two-sided directly opposed injection, optimum mixing is obtained at \( C = 1.25 \) because the effective mixing height is half of the duct height. For two-sided staggered injection, the effective orifice spacing would be half the actual spacing, and hence, \( C = 5 \) [7].

To extrapolate this expression to a cylindrical, or can, configuration, new definitions for \( H_o, S \) and \( C \) must be set. In a cylindrical duct, the radius, \( R \), corresponds to the rectangular duct height, \( H_o \). \( C = 2.5 \) is an appropriate choice because this is the optimum value for one-sided injection in a rectangular duct. Since the distance between the jets is a function of radial location, a radial location needs to be chosen. There are three options: (1) the outer wall, (2) the half-area radius, or (3) half of the physical radius. For a can, the optimum orifice spacing was chosen to be option number two: The radius that divides the can into equal areas, \( R_{1/2} \) (Figure 2-5). This would require the mean jet trajectory to intersect the point along the duct radius, which has equal amounts of mainstream and jet fluid on either side.

![Diagram](image)

**Figure 2-5** Rectangular and cylindrical duct - geometric considerations

The effective spacing relationship between the jet’s centerlines on the half area radius to the number of holes around the circumference of the can is,
\[ S = 2\pi \frac{R_{y^2}}{n} \]  \hspace{1cm} (2.7)

where,

\[ R_{y^2} = \frac{H_o}{\sqrt{2}} \]  \hspace{1cm} (2.8)

Substituting the above two equations into the relationship introduced in equation (2.6), results in the relationship between the number of orifices (for round holes), \( n \), and the momentum flux ratio, for a cylindrical duct, as,

\[ n = \frac{\pi\sqrt{2J}}{C} \]  \hspace{1cm} (2.9)

where \( C = 2.5 \), as defined above. Therefore, the above equation can determine the number of round holes for a specified design value of \( J \) that would give the optimum mixing.

Kroll et al. [9] conducted non-reacting mixing experiments in a cylindrical duct for momentum flux ratios of 25 and 52. Kroll et al. [9] examined the mixing both inside and downstream of the orifice by characterizing the mass addition performance, planar uniformity about a mean mixture fraction value and jet penetration. It was found that in order to yield the most uniform mixing at one duct radius downstream of the leading edge of the orifice, the mean jet trajectory needs to end up close to the duct's half-area radius. Sowa et al. [10] conducted experiments to describe the optimal mixer orifice geometry in a cylindrical duct. They looked at the relationship between the number of orifices, orifice aspect ratio and orifice angle at a constant mass flow ratio of 2.5 and a fixed \( J \) of 40. It was found that the optimum mixing occurred when the mean jet trajectories were in the range of \( 0.35 < r/R < 0.50 \) (where \( r = 0 \) is the mixer wall) at one radius downstream of the leading edge of the orifices. These findings agree with the assumption taken by Holdeman [7].
2.1.6 Effect of Jet and Mainstream Flow Coupling

Many jets-in-crossflow experiments are constructed such that the inlet profiles for both the mainstream and jets would produce a uniform velocity and turbulence profile. The reasons for this set-up are twofold. Firstly, uniform profiles could be reproduced by other experiments, allowing consistent data measurements. Secondly, uniform velocity profiles could be easily implemented in numerical analysis for mainstream and jet boundary conditions. How realistic the assumption of a uniform profile depends on the flow conditions between the jet and mainstream.

The study of Bain et al. [15] investigated jet boundary conditions in order to understand the effect of jet and mainstream flow coupling. To achieve this goal, the report used a numerical analysis using a code named CFD-ACE. The baseline configuration had an annular quick-mix zone with orifices located on both the inner and outer diameter liners. Plenum chambers supplied the initial flow to the orifices. The orifices were slots with semi-circular ends. For comparison purposes with the baseline configuration, a simple duct geometry was used with uniform velocity profiles at the orifices. The velocity magnitude was determined via three different methods. The first method used the velocity calculated from the plenum to mixer exit pressure drop, given as,

\[
V_j = \left[ \frac{2(P_i - P_{exit})}{\rho_j} \right]^{1/2}
\]  \hspace{1cm} (2.10)

The second method determined the pressure drop by using the total pressure in the plenum and the average static pressure across the duct, given as,
\[ V_j = \left[ \frac{2(p_i - p_{exit} + p_{inlet})}{\rho_j} \right] \]  

The third method calculated a velocity based on the mass flow through the geometric area of the orifice, given as,

\[ V_j = \frac{m_j}{\rho_j A_{orifice}} \]  

A constant mass flow through the jets was used for all three cases above.

From the analysis of the baseline configuration, a low normal velocity was seen at the leading edge of the orifice and a high normal velocity was seen at the trailing edge, yielding an inlet jet velocity that is highly non-uniform. Furthermore, the baseline configuration was validated with experimental measurements. The numerical results showed a good agreement with the experimental results at all downstream locations. Hence it was concluded that the plenum-supplied flow calculations captured the overall characteristics of the jets-in-crossflow.

When a comparison of the three uniform velocity methods was done with the baseline configuration, it was found that each method predicted jet over-penetration. Method three (equation (2.12)) produced the lowest jet velocity, although the jet was over-penetrating, but gave the closest overall agreement to the baseline case.

In addition, the effect of wall thickness was examined by Bain et al. [15]. By examining the temperature field, it was found that a thin-walled duct gave a higher jet penetration and a higher overall downstream mixing. The velocity field for both cases exhibited similar characteristics, however, the only difference was that the velocity profiles for the thin-walled case were pushed farther into the mainstream flow. This would result in a greater jet penetration towards the center of the duct.
Carotte and Stevens [1] investigated modifications to the dilution hole geometry that were designed to produce a more regular temperature pattern at the combustor exit. It was shown that there is a coupling between the annulus airflow and combustor interior flow.

Thus, the use of a uniform velocity profile at the jet’s inlet would result in jet over-penetration and mixing characteristics that are not representative of the actual flow. One approached that is used to capture the jet and mainstream coupling is to model an effective orifice flow area corresponding to the geometric area of the orifice multiplied by the an assumed discharge coefficient, $C_d$. A much better solution would be to have a flow entering the jet’s orifice from a plenum. However, this is difficult to implement due to lack of computational resources.

### 2.2 Reacting Flows

The studies of jets in a confined crossflow in a non-reacting flow were used as a starting point for a more practical combustion systems such as in gas turbine combustors. The advantage of the non-reacting environment is that they are less complicated and more accessible for the purposes of diagnostic examination. Recently, experimental and numerical analysis addressed the mixing of air jets into the hot, fuel-rich crossflow fluid in a cylindrical duct. To describe the mixing processes, the mixture fraction needs to be calculated based on a conserved quantity. For reacting flows, the temperature field is no longer conserved, hence, carbon species is chosen as a conserved scalar because it is not created nor destroyed. The definition of mixture fraction, $f$, is calculated based on carbon mass fraction and is given as,

$$ f = \frac{Y_m - Y}{Y_m - Y_i} \quad (2.13) $$
where $Y$ is the mass fraction of carbon species and the subscripts $m$ and $j$ represent the mainstream and jet flow, respectively. Since the carbon content in the air jets (approximately 21% O$_2$ and 79% N$_2$) is negligible, the mixture fraction reduces to,

$$f = \frac{Y_m - Y}{Y_m}$$

(2.14)

where $f = 0$ represents the mainstream flow and $f = 1$ represents the jet flow.

Talpallikar et al. [5] performed a numerical study of a jet mixing in a cylindrical quick-mix section employing 12 radial-inflow slots. The variations of $J$ and slot aspect ratio were investigated in both non-reacting (section 2.1.1) and reacting flows. For reacting flows, the report shows that $J$ influences jet mixing. At one diameter downstream of the leading edge of the orifices ($x/D = 1$), the temperature contours showed jet penetration patterns similar to the one discussed for non-reacting flows. That is, as $J$ increased the jet under-penetrated, reached an optimum penetration and with a further increase the jet over-penetrated. The mixing effectiveness (unmixedness) $\sigma_T$ at two axial locations ($x/D = 1$ and $x/D = 2$) illustrated an optimum mixing at the same $J$ value as in the temperature contour plots. This optimum $J$ value was slightly higher than the one predicted for non-reacting flow. At the optimum mixing, carbon monoxide (CO) concentrations were essentially eliminated by $x/D = 2$. The results suggested that importance of $J$ and orifice geometry in a reacting flow with regard to CO and NOx emissions. In addition, it was shown that the optimal mixing occurred when the jet penetrated to approximately mid-radius.

Leong et al. [16] conducted experiments at a constant mass flow of 2.5 and a fixed $J$ of 57. The experiment consisted of four round holes configurations, 8, 9, 10 and 12. Temperature and concentrations of O$_2$, CO$_2$, CO and HC were obtained upstream, downstream and within the orifice plane ($x/D = 1$). The reaction was assumed complete within one duct radius of the orifice
leading edge. It was found that as the number of round orifices increased, jet penetration decreased. The jet trajectory was considered to be the locus showing maximum $O_2$ concentrations. Of the four modules tested, the one that had the closely-spaced orifices (12-holes) exhibited jet penetration closest to the mixer half-radius and hence, appeared to produce the best uniform mixing. Leong et al. [17] performed similar experiments at the same mass flow and momentum flux conditions as in Leong et al. [16], however, the mixing module consisted of only 10 round holes. The experimental analysis for the 10 round holes revealed that the reaction was intense and that the bulk of the mixing occurred within $x/R = 1$. However, it was recognized that the reaction and mixing continued beyond this point, though, at a much lower rate.

Leong et al. [18] investigated radial jet mixing into a reacting crossflow confined to a cylindrical duct in order to determine the number of round holes that most effectively mixes the jets with the mainstream flow. By optimizing the mixing characteristics, the residence time of near-stoichiometric and unreacted packets are minimized, which in turn, reduces pollutant formation. The experiments were conducted at a constant $J$ of 57 and mass flow ratio of 2.5 with five round-hole configurations of 5, 10, 12, 14 and 18. Although Leong et al. [16, 17] previously examined the flow field in a reacting flow, this report continued their investigation by using the diagnostic and analysis techniques developed in their study to determine an optimum configuration. The parameters considered were the temperature, jet mixture fraction based on the carbon atom mass fraction (equation (2.14)) and equivalence ratio. Equivalence ratio is defined as,

$$\phi = \frac{(fuel/air)_{local}}{(fuel/air)_{stoichiometric}}$$  \hspace{1cm} (2.15)

These parameters were measured up to one diameter of the injection plane ($x/D = 1$). It was found that the bulk of the reaction and mixing occurred before $x/R = 1$. As found previously by
Leong et al. [16], as the number of round orifices increased, jet penetration decreased. The 8 round holes produced jet over-penetration, which caused the jet to accumulate in the central core of the mixer. In the 18 round holes configuration, the jet under-penetrated and caused the fuel-rich crossflow to pass unaffected by the jets through the central core of the mixer. Optimum penetration, with respect to both mixing and completeness of reaction, was observed for the 14 round holes. For this configuration, the jet penetrated before the mixer half-radius. The relationship proposed by Holdeman [7] for non-reacting flows, equation (2.9), yields an optimum number of round holes, \( n = 13 \), for \( J = 57 \). This shows that a possible correlation may exist between non-reacting and reacting jets in a crossflow.

Recently, Popovic et al. [19] conducted experiments to investigate the effects of variable mass flow ratio and orifice geometry on flame length and CO measurements of air jets in a cylindrical duct. Five geometric configurations were used and consisted of two gap configurations (two-dimensional slots) and three discrete opening configurations (4-round holes, 9-round holes and 4-streamlined slots with a 4:1 aspect ratio and rounded slot ends). The measurements were conducted at 48 diameters downstream from the injection plane \((x/D = 48)\), where it was assumed that all reactions were completed and the gases were fully mixed. It was found that the optimal \( J \) value for the discrete opening configurations follow Holdeman's [7] equation for optimum mixing in a non-reacting flow in a cylindrical duct, equation (2.9). In addition, discrete opening jets were shown to have shorter flame lengths and higher CO destruction efficiency compared to the gap configurations since in the gap configurations the mixing was limited to turbulent diffusion. Hence, the discrete openings exhibited better mixing characteristics. For the same number of orifices, that is, for 4-streamlined slots and 4-round holes, CO destruction efficiency was similar. The 9-round holes configuration, which has the
largest optimum $J$ value, was found to provide the best CO destruction efficiency for all mass flow (equivalence) ratios. In general, the flame lengths decreased with increasing $J$ value, and remained approximately constant at values above the optimum $J$.

In the study of Popovic et al. [19], the variations in the jet mass flow for all configurations have indicated an optimum CO destruction efficiency (maximum CO destruction). It was hypothesized that with an increase of jet mass flow to the optimum condition, that is at low jet mass flows, CO destruction improved since more air became available for the combustion process. Furthermore, with an increase of jet mass flow above the optimum condition, the CO concentration increased possibly due to an increased strain rate (velocity gradients) on the flame causing the flame to have locally extinct regions, and thus unstable. It was shown that by varying the orifice geometry, the rate of CO destruction changed with respect to the flow rate of the jet. The report stated that this was the result of jet mixing, jet penetration and turbulent diffusion.

Oechsle et al. [20] performed a numerical analysis on non-reacting and reacting flow fields of jet mixing in a cylindrical duct, for a fixed $J$ of 25. The report examined the effect of the variation in the number of orifices (8- and 12-round holes), mass flow ratio ($MR = 1.83, 2.67$) and the corresponding rich-zone equivalence ratio ($\phi = 1.35, 1.80$), from the leading edge of the orifices to one radius downstream, $0 < x/R < 1$. The equivalence ratio (equation (2.15)) is a conserved scalar that can also be used as an index of mixing, since it is directly associated with the jet mixture fraction, equation (2.14). For all the configurations, the results were compared by visual observation of the temperature and equivalence ratio field using the normalized parameter, so that a conserved scalar is compared in each case. This parameter, $f$, known as the mixture fraction, is given as,
non-reacting flow: \[ f = \frac{T - T_j}{T_m - T_j} \] (2.16)

reacting flow: \[ f = \frac{\phi - \phi_i}{\phi_m - \phi_i} \] (2.17)

where, for non-reaction flow, \( f = 0 \) represents the unmixed jet, and \( f = 1 \) represents the mainstream flow. For the reacting flow, \( f = 0 \) represents the jet equivalence ratio, and \( f = 1 \) represents the rich-zone equivalence ratio.

Oechsle et al. [20] have shown that the parameter \( f \) based on temperature (non-reacting) and equivalence ratio (reacting) distributions were similar. The results indicated that the core of the jet appeared to have less overall mixing and jet interactions became less significant in the reacting flows, as compared to the non-reacting cases. It was concluded that non-reacting temperature profiles could track the reacting flow mass flow (equivalence ratio) distribution reasonably well.

Oechsle and Holdeman [21] used a 3-D numerical model to predict the mixing flow field and NOx characteristics in a cylindrical duct. Eighteen configurations were examined consisting of round holes and slots with variable aspect ratios and slant angles. The parameters investigated were \( J \), orifice shape and slot slant angle. It was shown that the statistical mixing (mixing non-uniformity) parameters do not correlate with the NOx production at downstream axial locations from the leading edge of the orifices, that is, the planar variances lack the mixing history throughout the entire mixing region. It was also shown that jet penetration, and thus \( J \), plays an important role in the production of NOx. Over-penetrating and under-penetrating jet configurations resulted in an increased NOx production. In general, minimum NOx will be produced at optimum penetration, where optimum penetration is dependent on the axial location observed. Similar to the observations of Liscinsky et al. [7] with respect to orifice geometry.
low NO\textsubscript{x} production was found for round holes at low $J$ values, and for slanted slots for at high $J$ values.

### 2.3 Summary

This chapter deals with experimental and computational results on non-reacting and reacting jets with a confined crossflow in a cylindrical and a rectangular duct. Several flow variables were discussed that affect jet penetration and mixing. These variables include the momentum flux ratio, number of orifices, orifice shape, density ratio and jet-to-mainstream flow coupling. The adjustment of one or more of these variables will lead to optimal mixing, where uniform temperature distribution (non-reacting flows) and uniform mixture fraction (reacting flows) at the minimum downstream distance occurs. Generally for non-reacting flows, mixing is largely a function of momentum flux ratio and orifice spacing.

Reacting flows consist of both mixing and chemistry. Thus, it is difficult to deduce the primary variables that can influence the flow field. The optimal mixer design will therefore depend on the specific operating conditions. However, experiments of jets in a crossflow revealed that mixing dominates chemistry, since the $J$ value that minimizes CO emissions was found to follow the optimal mixing predicted in non-reacting flows.

Experiments in non-reacting and reacting flows are important because they provide the physical understanding of fluid mixing. This work will verify whether a modern CFD program is qualitatively and quantitatively able to predict these flows.
3 Mathematical Formulation

In order to use numerical models for fluid flow and heat transfer problems, it is necessary to solve and to understand the governing equations that describe the important physics of the problem. In this thesis, the governing equations for turbulent flow are needed and consist of the conservation of mass, conservation of momentum, conservation of energy, and other transport equations including the $k$-$\varepsilon$ turbulence model. The basic assumptions involved in this work listed as,

- The flow is steady, so that all derivatives with respect to time are zero ($d/dt = 0$);
- Incompressible flow, i.e., density fluctuations are negligible ($\rho' = 0$);
- The fluid used obeys the ideal gas law.

3.1 Governing Equations

The fundamental equations of fluid dynamics are the Navier-Stokes equations, which are based on the universal laws of mass, momentum and energy conservation. Using Einstein summation convention in a three-dimensional fluid flow ($i = 1, 2, 3$), the continuity equation for mass conservation is,

$$ \frac{\partial}{\partial x_i} (\rho u_i) = 0 $$

where $u_i = (u, v, w)$ and $x_j = (x, y, z)$. The Navier-Stokes equations for momentum transport are.

$$ \frac{\partial}{\partial x_j} (\rho u_j u_i) = - \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] + F_i $$

(3.2)
where \( \rho \) is the fluid density, \( u_i \) represents the velocities in the \( x_i \) direction, \( P \) is the pressure. \( \mu \) is the dynamic viscosity of the fluid and \( F_i \) represents all body forces. The energy equation is.

\[
c_p \frac{\partial}{\partial x_i} (\rho u_i T) = \frac{\partial}{\partial x_i} \left( \Gamma \frac{\partial T}{\partial x_i} \right) + q^e
\]  

(3.3)

where \( c_p \) represents the specific heat capacity, \( T \) is the temperature and \( \Gamma \) is the molecular conductivity of the fluid.

In order to solve turbulent flows, approximate modeling methods are used. One approach, which is the most frequently used for engineering flow problems, involves Reynolds averaging. With this approach, the mean turbulent flow fields are determined by means of the Reynolds-averaged form of the Navier-Stokes equations, in conjunction with a turbulence model for evaluating the statistical effects of the turbulence. The Reynolds-averaged form of the Navier-Stokes equations is derived by decomposing a given dependent variable into a mean, \( U \), and a fluctuating component, \( u'_j \), as shown,

\[
u_j = U_j + u'_j
\]  

(3.4)

and by time-averaging the Navier-Stokes equations.

By time-averaging the above three conservation equations, the Reynolds-averaged equations can be obtained for steady, incompressible flow. The continuity equations becomes.

\[
\frac{\partial}{\partial x_j} (\rho U_j) = 0
\]  

(3.5)

The momentum equations are,

\[
\frac{\partial}{\partial x_j} (\rho U_j U_i) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial U_j}{\partial x_j} + \frac{\partial U_i}{\partial x_i} \right) - \rho u'_j u'_j \right] + F_i
\]  

(3.6)

And the time-averaged energy equation is,
The averaging of the Navier-Stokes equations produces two new terms, \((-\rho \overline{u'u_j'})\) and \((-\rho \overline{u_j'T'})\), called the Reynolds stress and Reynolds heat flux, respectively.

In heated turbulent flows, the dominant contributions to momentum and heat transport are from the fluctuating motions of turbulence. The overall effects of these motions on the mean fields are represented by the turbulence stress and heat flux terms. Since these turbulence terms are estimated with a turbulence model, the accuracy of the numerical prediction basically depends on the turbulence model employed. In this thesis, a two-equation eddy viscosity model is used.

### 3.2 The Eddy Viscosity Model

The eddy viscosity model is based on the Boussinesq assumption that turbulent transport and laminar transport are analogous. This model, together with the \(k-\epsilon\) equations, is a commonly used turbulence model and is presented as,

\[
-\rho \overline{u'u_j'} = \mu_t \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \rho k \delta_{ij}
\]  
\quad (3.8)

where \(k\) represents the turbulent kinetic energy, \(\mu_t\) is the turbulent viscosity and \(\delta\) is the Kroenecker delta function, with respect to the momentum transport, and,

\[
-\rho \overline{u_j'T'} = \mu_t^h \frac{\partial T}{\partial x_j} 
\]  
\quad (3.9)

where \(\mu_t^h\) is the turbulent diffusivity of heat, with respect to the heat transport. The turbulent diffusivity of heat is defined as,
\[ \mu_t^H = \frac{\mu_t}{Pr_t} \]  \hspace{1cm} (3.10)

where \(Pr_t\) is the turbulent Prandtl number, assumed constant in this model with a value of 0.9.

The turbulent viscosity in equations (3.8) and (3.10) is determined from the parameters \(k\) and \(\varepsilon\) through this relationship,

\[ \mu_t = c_\mu \frac{\rho k^2}{\varepsilon} \]  \hspace{1cm} (3.11)

where the turbulent viscosity coefficient \(c_\mu\) is a constant with a value of 0.09 [23]. The quantities \(k\) and \(\varepsilon\) are the turbulent kinetic energy and its dissipation rate, respectively, and are defined as.

\[ k = \frac{1}{2} u_i' u_i' \]  \hspace{1cm} (3.12)

\[ \varepsilon = \mu \frac{\partial u_i'}{\partial x_j} \frac{\partial u_i'}{\partial x_j} \]  \hspace{1cm} (3.13)

These parameters are found by solving two transport equations,

\[ \rho \frac{\partial k}{\partial t} + \rho U_i \frac{\partial k}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_i} \right) + P - \rho \varepsilon \]  \hspace{1cm} (3.14)

and

\[ \rho \frac{\partial \varepsilon}{\partial t} + \rho U_i \frac{\partial \varepsilon}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\mu_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_i} \right) + \frac{\varepsilon}{k} (\varepsilon_1 P - \varepsilon_2 \rho \varepsilon) \]  \hspace{1cm} (3.15)

where \(P\) is the turbulent kinetic energy production due to the interaction of turbulent stresses and mean velocity gradients, as shown,

\[ P = -\rho u_i' u_j' \frac{\partial U_i}{\partial x_j} \]

\[ = \mu_t \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_j} \]  \hspace{1cm} (3.16)
The above transport equations include empirical constants whose values are given in Table 3.1. Note that the values of $c_1$, $c_2$, $\sigma_k$, $\sigma_\epsilon$, are based on the recommendation of Launder and Spalding [23].

<table>
<thead>
<tr>
<th>Constants</th>
<th>$c_1$</th>
<th>$c_2$</th>
<th>$\sigma_k$</th>
<th>$\sigma_\epsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Values</td>
<td>1.44</td>
<td>1.92</td>
<td>1.0</td>
<td>1.3</td>
</tr>
</tbody>
</table>

The main advantages of the eddy viscosity model are its relatively low computational time requirements, its reasonable success in predicting the mean field and turbulent shear stresses, its stability and its easy implementation into most turbulent CFD computer codes. However, this model has two major deficiencies. Firstly, it is subjected to the assumption that all Reynolds normal stresses are essentially equal, that is isotropic. And secondly, it is subjected to the local equilibrium assumption that the eddy viscosity coefficient, $c_\mu$, is a constant throughout the flow field. These deficiencies will affect problems involving recirculation and secondary flows.

3.3 Laminar Flamelet Model in a Turbulent Combustion

3.3.1 Overview

Turbulent combustion can be classified into two categories that identify different regimes defined by technical applications and time scales of turbulence and reaction (chemistry). Technical applications in turbulent combustion can be further divided, in general, into two sub-categories: Premixed and non-premixed. For example, combustion in a spark-ignition engine occurs under premixed conditions, while the combustion in a Diesel engine or in a gas-turbine engine takes place under non-premixed conditions. The second category is the ratio of the
turbulent to chemical time scales. A very intense turbulence will result in a short turbulent time scale. Chemical time scales become short if the temperature is high and they become long with decreasing temperature. This time scale ratio is the most fundamental property of a flamelet. Figure 3-1 shows a diagram where combustion applications are classified into different regimes. In real applications, different regimes may appear at the same time in different locations of the domain.

<table>
<thead>
<tr>
<th>Fast chemistry</th>
<th>Premixed</th>
<th>Partially and non-premixed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spark-ignition engines</td>
<td>Diesel engines</td>
<td></td>
</tr>
<tr>
<td>Gas turbine engines</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Combustion in furnaces</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Slow chemistry</td>
<td>(\text{NO}_x) formation in post-flame regions</td>
<td>Low (\text{NO}_x)-burners</td>
</tr>
</tbody>
</table>

Figure 3-1 Classification of turbulent combustion (from Peters [26])

The laminar flamelet concept covers the regime of premixed and non-premixed combustion with fast chemistry. This concept assumes that turbulent combustion occurs in thin sheets with an inner structure that is one-dimensional and time dependent. Hence, the turbulent flame is treated as an ensemble of thin laminar diffusion flamelets that are embedded within the turbulent flow field. Thin sheets will occur when the chemical time is short in comparison to the turbulent convection and diffusion time scales. The flamelet concept would become more accurate as the ratio of the turbulent to chemical time scale becomes larger. This ratio is known as the Damkohler number, and is defined as,
The condition for a flamelet to be thin is different for premixed and non-premixed combustion, and depends on the coordinate used in the flamelet structure. For premixed combustion the appropriate coordinate used is the spatial coordinate normal to the flamelet, while in non-premixed combustion the coordinate used is the mixture fraction.

The flamelet model gives a better insight into the flame structure and adds new details to the simulation of combustion processes compared to other common combustion models, such as the Eddy Dissipation Model (EDM). An arbitrary number of species with an arbitrary number of kinetic reactions may be used as long as their laminar chemical kinetic mechanism is known. The model solves for a scalar equation that is used to describe the location of the flame within the turbulent flow field. Furthermore, the flame front structure is a function of a few parameters in the turbulent field. The main advantage of the flamelet model is that the numerical resolution of small length and time scales is not necessary. Thus, the problem of solving highly non-linear kinetics in fluctuating flow fields is avoided, making the flamelet model extremely robust. Chemical compositions of laminar model flames are pre-calculated and stored in a library to reduce computational time. During the flow simulation, the stored values are used to determine the local species composition.

The coupling between non-equilibrium chemistry and fluctuating turbulence flow field is achieved by a statistical method. The statistical description of a turbulent reacting flow is included in the joint probability density function (pdf) of all dependent variables, that is, the three velocity components, the temperature and the species concentrations. This pdf used could be calculated at each location within the flow field by solving a pdf transport equation. A review on pdf methods for turbulent reactive flows has been given by Pope [25]. Pdf transport

\[ Da = \frac{t_{turbulent}}{t_{chemical}} \]
modelling has the advantage that the highly non-linear chemical source term does not need to be modelled. Although this approach avoids some of the modelling that is necessary in moment closure, important terms such as the fluctuating pressure gradient term and the molecular diffusion term still require modelling. However, if the reaction occurs in thin layers, as assumed in the flamelet concept, the molecular diffusion term would be closely coupled to the reaction term, and the problem of modelling the chemical source term is then shifted towards modelling the diffusion term. Since the required pdf transport equation is multidimensional, a Monte Carlo solution method could be applied. The fluctuations of all involved species can then calculated from the knowledge of the local pdf. However, there still exists an uncertainty about the modelling of the molecular diffusion term of the pdf transport equation, and a large computation effort is required.

An alternative and simpler approach that provides a more direct insight into the physics of the problem is to use a presumed pdf. A widely used and generally accepted presumed pdf is the beta function pdf. This method is easier to apply and provides a large number of measured pdf shapes in flames by evaluating of the assumed pdf parameters from the flow field. The flow field is predicted by solving a conserved scalar equation and its variance equation.

In summary, the general assumptions made in the derivation of the flamelet model are:

- Fast chemistry (large $Da$), i.e., combustion takes place in thin layers;
- Equal diffusivities: $Le = 1$;
- Combustion occurs in the limits of the flamelet regime;
- Two-feed flow consisting of fuel and oxidizer;
- No-flux boundary conditions on all other bounding surfaces (i.e., wall).
The next section will focus on the flamelet model for non-premixed turbulent combustion.

3.3.2 Non-Premixed Flamelet Model

Non-premixed combustion is generally associated with diffusion flames, where the mixing of fuel and oxidizer occurs simultaneously. Extensive studies of the flamelet concept for non-premixed combustion have been presented by Peters [24, 25, 27].

While the convective and diffusive time scales are in general of the same order of magnitude, the chemical time scale is very much smaller. For this reason, the assumption of local chemical equilibrium has often been used in modelling the diffusion flames, especially the mixtures of hydrogen or hydrogen/carbon-monoxide. Local equilibrium assumption is an important simplification since it eliminates many parameters from the analysis, such as the parameters associated with chemical kinetics. However, for hydrocarbon flames the assumption of local equilibrium results in an over-prediction of carbon monoxide and hydrogen on the rich side of the flamelet structure. Therefore, non-equilibrium effects are important for the prediction of carbon monoxide, hydrogen and also NOx. In addition, non-equilibrium effects are essential in predicting local flame extinction (quenching), lift-off and blow-out of jet diffusion flames.

3.3.2.1 Mixture Fraction

The mixture fraction, $Z$, is a very important quantity in the theory of non-premixed combustion. While reacting species are consumed or produced, chemical elements are conserved during chemical reactions. Therefore, the mass fraction of the chemical element $j$, is defined as.

$$Z_j = \sum_{i=1}^{n} \frac{a_i M_j}{M_i} Y_i$$

(3.18)
where subscript $i$ represents the reacting species, $M$ represents the molecular weight. $Y$ represents the mass fraction and $a_{ij}$ represents the number of elements $j$ in the species $i$. The definition of $Z_j$ can be further extended to introduce fuel and oxidizer element mass fractions as a linear combination of element mass fractions. For fuels containing carbon, hydrogen and oxygen as elements,

$$
Z_F = Z_{C,F} + Z_{H,F} + Z_{O,F}
$$

$$
Z_O = Z_{C,O} + Z_{H,O} + Z_{O,O}
$$

(3.19)

where $Z_{j,F}$ is the mass fraction of element $j$ in the fuel inlet, and $Z_{j,O}$ is the mass fraction of element $j$ in the oxidizer inlet. $Z_F$ and $Z_O$ are equal to the fuel and oxygen mass fractions in the non-reacting mixture. Both fuel and oxidizer stream may contain inerts such as nitrogen. In a two-feed non-premixed system consists of the fuel inlet (label 1) and oxidizer inlet (label 2), the mixture fraction is defined as,

$$
Z = \frac{Z_{F,1}}{Z_{F,1}} = 1 - \frac{Z_{O,2}}{Z_{O,2}}
$$

(3.20)

In addition, the stoichiometric mixture fraction for the following reaction,

$$
v_F F + v_O O_2 \rightarrow \text{products}
$$

(3.21)

is defined as,

$$
Z_{st} = \left[1 + \frac{Y_{F,1}v_O M_O}{Y_{O,2}v_F M_F}\right]^{-1}
$$

(3.22)

3.3.2.2 Scalar Dissipation Rate

The turbulent flow is influenced in the flamelet model by the instantaneous scalar dissipation rate, $\chi_{st}$, which represents non-equilibrium effects, and is defined as,
\[ \chi_{st} = 2D_T \left( \frac{\partial Z}{\partial x_t} \right)_{st}^2 \]  \hspace{1cm} (3.23)

The physical significance of \( \chi_{st} \) is discussed in Peters [26], which basically states that \( \chi_{st} \) decreases due to diffusion and increases due to straining by the flow field. It has the dimension of \((\text{time})^{-1}\) and may be interpreted as the inverse of a characteristic diffusion time.

The analysis of Peters [28] has shown that local extinction is essentially governed by the value of \( \chi_{st} \) at the flamelet. That is, local quenching of the flamelet occurs if \( \chi_{st} \) exceeds a critical value \( \chi_q \), the instantaneous scalar dissipation rate at quenching. At this condition, the rate of heat convection to both sides of the flamelets will not balance the heat production due to chemical reaction. Hence the maximum temperature will decrease until the flamelet is quenched. This behaviour is illustrated in Figure 3-2 by the S-shape for the steady-state flamelet equations. Here the maximum temperature is plotted as a function of the inverse of the scalar dissipation rate at stoichiometric conditions. The lower branch corresponds to the non-reacting flamelet prior to

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{s_shape_curve.png}
\caption{The S-shaped curve for diffusion flames. The points Q and I correspond to quenching and ignition, respectively (from Peters [26])}
\end{figure}
ignition. As $\chi_t$ is decreased, the ignition point $I$ is reached. For values smaller than $\chi_t$, a rapid unsteady transition to the upper burning branch occurs, which is accompanied by a large temperature increase. This unsteady transition is unlikely to occur in diffusion flames since the required large residence times (small values of $\chi_t$) will not be reached. Ignition of the initial mixture or re-ignition of quenched flamelets will require an ignition source. Burning of the flamelet corresponds to the upper branch of the curve. Subsequently, by increasing $\chi_t$, the point Q will be reached, where quenching occurs. The middle branch between the point I and Q is unstable and therefore has no physical significance.

Peters [26] stated that in order to uncouple chemical kinetics from turbulence, the scalar profiles from a laminar flow configuration should be evaluated, and consequently used in a turbulent flow. The appropriate choice for such a configuration is the laminar one-dimensional counter-flow geometry, as shown in Figure 3-3, since this configuration has a similar structure to

![Geometry of laminar counter-flow diffusion flame](image-url)

**Figure 3-3** Geometry of laminar counter-flow diffusion flame (from Bray and Peters [29])
the non-premixed flamelet model, and can be studied relatively easily both experimentally and numerically, which makes it the ideal choice for flamelet libraries. In a laminar one-dimensional counter-flow diffusion flame, fuel and oxidizer are issued from opposite sides towards each other and are reacting in the vicinity of a stagnation point boundary layer. From this configuration, the scalar dissipation rate, at the location where the mixture is stoichiometric, may be approximated, assuming constant density and diffusivity, by,

$$\chi_{\nu} = \frac{a}{\pi} \exp\left\{-2\left[\text{erf}^{-1}(2Z_{\nu})\right]^2\right\} = 4aZ_{\nu}^2\left[\text{erf}^{-1}(2Z_{\nu})\right]$$

(3.24)

where $a$ is the stagnation-point velocity gradient (also known as strain rate) and $\text{erf}^{-1}$ is the inverse of the complementary error function. The second expression in equation (3.24) is an approximation to the value of $\chi_{\nu}$ for small values of $Z_{\nu}$, which is appropriate for methane-air and hydrogen-air flames. At a strain rate value close to extinction, heat released by the reaction will just balance the heat loss by convection.

3.3.2.3 Regimes in Non-Premixed Turbulent Combustion

In a non-homogeneous mixture field, the reaction zone is attached to the high temperature region close to stoichiometric mixture and is advected and diffused with the mixture field. Consequently, there is no physical meaning to the velocity scale for diffusion flames. In order to determine how much physical space a diffusion flame occupies it is necessary to know how large the mixture fraction gradients are. Figure 3-4 illustrates two cases of a given mixture fraction flow field and the corresponding adiabatic temperature profiles. In both cases, the same mixture fraction gradient, $\partial Z/\partial x$, and therefore the same $\tilde{Z}_{\nu}$ (see equation (3.23)) is assumed, though, the mixture fraction variance around stoichiometric condition, $\tilde{Z}_{\nu}^2$, is different. In the left part Figure 3-4, the mixture fraction gradients are steep, the fluctuations are large and from the
corresponding flame temperature it can be seen that the reaction zones are separated and individual diffusion flamelets may exist. In this case, the flame is thin in physical space. In the

right part of Figure 3-4, the mixture fraction gradients and fluctuations are small and in the vicinity of stoichiometric value. The mixture is essentially premixed, the reaction zones are connected and combustion in such a situation corresponds to partially premixed. In this case, the flame is broad in physical space. Since the mixture fraction field fixes the flame position and the flame width, non-premixed combustion is best described by the mixture fraction, Z, rather than physical space.

To distinguish between partially premixed and the separated flamelet regimes, a criterion based on flame thickness in mixture fraction space and time scales has to be developed. The Kolmogorov time scale has the shortest characteristic time of turbulence, and is defined in terms of the kinematic viscosity, $v$, and the dissipation of turbulent kinetic energy, $\overline{\varepsilon}$,
The chemical time scale is related to the flamelet at extinction, where chemistry just balances heat loss by convection. The inverse of the strain rate represents the characteristic flow time \( t_F = a^{-1} \), and hence, the chemical time scale at extinction. The chemical time scale for diffusion flames is defined as,

\[
t_c = t_{F,q} = a_q^{-1}
\]  

The diffusion length scale is defined based on the strain rate, \( a \), and the diffusion coefficient, \( D \).

\[
l_d = \sqrt{\frac{D_{\text{ref}}}{a}}
\]  

where the diffusion coefficient is evaluated at a suitable reference condition, such as the maximum heat release rate. The mixture fraction profile across the diffusion flame is used to define the mixture fraction gradient normal to the reaction layer at stoichiometric condition, \((\frac{\partial \bar{Z}}{\partial x_n})_n\). The flame thickness in mixture fraction space is therefore,

\[
(\Delta Z)_F = \left(\frac{\partial \bar{Z}}{\partial x_n}\right)_n l_d = \sqrt{\frac{\chi_{\text{st}}}{2D_{\text{ref}}}} \sqrt{\frac{D_{\text{ref}}}{a}} = \sqrt{\frac{\chi_{\text{st}}}{2a}}
\]

where equations (3.23) and (3.27) have been combined. The flamelet thickness contains the reaction zone and the surrounding diffusive layers. Bray and Peters [29] have shown numerical calculations of \((\Delta Z)_F\) with \( \chi_{\text{ref}} \) taken at the maximum heat release rate for hydrogen-air and
methane-air diffusion flames. The results indicate that the flame thickness defined by equation (3.28) is nearly independent of the strain rate. This means that the flame thickness in mixture fraction space can be assumed to be constant.

Three Regimes of non-premixed combustion as function of mixture fraction fluctuations and characteristic time scales are shown in Figure 3-5. Fluctuations of the mixture fraction are defined as,

\[ Z' = \sqrt{\tilde{Z}^2} \]  

(3.29)

where \( \tilde{Z}^2 \) is the Favre-averaged mixture fraction variance. If the combustion is not fast compared to the turbulent processes, that is \((t_\eta / t_c) \ll 1\), turbulent mixing will influence the combustion before it is complete. The mixing eddies will create a broad region of partially premixed (and sometimes even totally premixed) mixture in which combustion takes place in distributed reaction zones. In this case, the flamelet model loses one of its requirements.

**Figure 3-5** Regimes in non-premixed turbulent combustion.
If the combustion process is fast, that is \((t_\eta/t_c) \gg 1\), the regime depends on the fluctuations in mixture fraction space, \(Z'\), with respect to flame thickness, \((\Delta Z)_F\). For small \(Z'\), the reaction zones are connected and the fluctuations around or near stoichiometry represent a partially premixed gas. This is the result of partial premixing or strong turbulent mixing. For large \(Z'\), the reaction zones are separated from each other and the combustion takes place in thin layers that are embedded within the turbulent flow field. In this region the flamelet concept is valid. However if \(Z'\) become too large, the flames in physical space will turn out to be very narrow and will extinguish because the heat loss due to the steep spatial gradients will not be balanced by heat production inside the flame structures. Therefore, if mixture fraction fluctuations are larger than flame thickness in mixture fraction space, separated flamelets will exist, otherwise connected reaction zones will exist.

3.4 Non-Premixed Flamelet Model Formulation

Basically, the non-premixed laminar flamelet concept occurs in a region of fast chemistry and the mixture fraction \(Z\) is its most important variable that describes flame structure. By assuming the mixture fraction to be given in the flow field as a function of space and time, the surface of the stoichiometric mixture, that fixes the location of the thin reaction zone, can be determined from,

\[
Z(\mathbf{x},t) = Z_{st}
\]  

To be able to describe the location of the flamelets anywhere in the flow field, a new coordinate system is introduced that is locally attached to the surface of stoichiometric mixture. The coordinate \(x_i\) is replaced by the mixture fraction \(Z\) such that it will not lie within this surface
(Figure 3-6). By definition, one of its coordinates, $x_i$, is locally perpendicular to the surface of stoichiometric mixture.

![Diagram of stoichiometric mixture](image)

**Figure 3-6** Surface of Stoichiometric mixture in a turbulent jet (from Peters [26])

The mixture fraction $Z$ is defined as the solution of a convective-diffusive equation.

$$\rho \frac{\partial Z}{\partial t} + \rho v \cdot \nabla Z = \nabla \cdot (\rho D \nabla Z)$$  \hspace{1cm} (3.31)

which has no chemical source term. The diffusion coefficient $D$ in the above equation is arbitrary since the assumption of equal diffusivities will be used later on. However, it is convenient to set it equal to the thermal diffusivity,

$$D = \frac{\lambda}{\rho c_p} = D_r$$  \hspace{1cm} (3.32)

where, $\lambda$ is the thermal conductivity, $\rho$ is the density and $c_p$ is the specific heat capacity at constant pressure.

The equations for mass fractions $Y_i$ and temperature are used to determine the structure of the flamelet. The species equations are defined as,

$$\rho \frac{\partial Y_i}{\partial t} + \rho v \cdot \nabla Y_i = \frac{1}{Le_i} \nabla \cdot (\rho D_i \nabla Y_i) + \dot{m}_i$$  \hspace{1cm} (i = 1,2,...,n)  \hspace{1cm} (3.33)

and the temperature equation (see (3.3)) is defined as,
In equations (3.33) and (3.34), $\dot{m}_i$ represents the chemical source term of species $i$. In equation (3.34), $\sum_{i=1}^{n} h_i \dot{m}_i$ represents the heat release rate due to chemical reactions, $q_R$ represents the heat loss due to radiation and $\frac{\partial p}{\partial t}$ represents the transient pressure gradient. The $\frac{\partial p}{\partial t}$ term is important for combustion involving fast changing pressure, for instance, the combustion process in closed burning chambers of a Diesel engine. The parameter $Le_i$ in equation (3.33) is the Lewis number for species $i$. Using the assumption of equal diffusivities will result in a constant Lewis number for all species as shown,

$$Le_i = \frac{\lambda}{\rho c_p D_i} = \frac{D_T}{D_i} = 1$$  \hspace{1cm} (3.35)

In order to transform the species and temperature equations into mixture fraction space, a coordinate transformation is used. By setting $Z = x_1$, $Z_2 = x_2$, $Z_3 = x_3$, and $\tau = t$ as independent variables (see Figure 3-6) the following transformation rules, as shown in Peters [26], can be applied,

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \frac{\partial Z}{\partial \tau} \frac{\partial}{\partial Z},$$

$$\frac{\partial}{\partial x_k} = \frac{\partial}{\partial Z_k} + \frac{\partial Z_k}{\partial x_k} \frac{\partial}{\partial Z}, \hspace{1cm} (k = 2, 3)$$  \hspace{1cm} (3.36)

$$\frac{\partial}{\partial x_i} = \frac{\partial Z}{\partial x_i} \frac{\partial}{\partial Z}$$

Hence, the temperature equation, equation (3.34) is transformed to,
\[ \begin{align*}
\rho c_p \left( \frac{\partial T}{\partial t} + u_2 \frac{\partial T}{\partial x_2} + u_3 \frac{\partial T}{\partial x_3} \right) - \sum_{k=2}^{3} \frac{\partial (\rho c_p D_T)}{\partial x_k} \frac{\partial T}{\partial Z_k} \\
- \rho c_p D_T \left[ (\nabla Z)^2 \frac{\partial^2 T}{\partial Z^2} + 2 \sum_{k=2}^{3} \frac{\partial Z}{\partial x_k} \frac{\partial^2 T}{\partial Z \partial x_k} + \sum_{k=2}^{3} \frac{\partial^2 T}{\partial Z^2} \right] \\
+ \left\{ \rho \frac{\partial Z}{\partial t} + \rho v \cdot \nabla Z - \nabla \cdot (\rho D_T \nabla Z) \right\} c_p \frac{\partial T}{\partial Z} = -\sum_{i=1}^{n} h_i \dot{m}_i + q_k + \frac{\partial p}{\partial t}
\end{align*} \quad (3.37) \\
\] 

Since the flamelet is assumed to be thin in the \( Z \) direction, only gradients normal to the surface of stoichiometric mixture are dominating. Therefore, all the terms involving derivatives with respect to \( Z_2 \) and \( Z_3 \) can be neglected. The term containing the time derivative is important if very rapid changes, such as ignition or extinction, occur, and when transient conditions are modelled. The simplified temperature equation becomes,

\[ \rho c_p \frac{\partial T}{\partial t} - \rho c_p \frac{\chi_{st}}{2} \frac{\partial^2 T}{\partial Z^2} = -\sum_{i=1}^{n} h_i \dot{m}_i + q_k + \frac{\partial p}{\partial t} \quad (3.38) \]

This equation is valid in the vicinity of stoichiometric mixture and is essentially one-dimensional. Similarly, the species equation, equation (3.33), can be transformed to,

\[ \frac{\rho}{\rho \chi_{st}} \frac{\partial Y_i}{\partial t} = \frac{\rho}{\rho \chi_{st}} \frac{\partial Y_i}{\partial Z} + \left\{ \rho \frac{\partial Z}{\partial t} + \rho v \cdot \nabla Z - \nabla \cdot (\rho D_T \nabla Z) \right\} \frac{\partial Y_i}{\partial Z} = \dot{m}_i \quad (3.39) \]

Pitsch and Peters [30] formulated flamelet equations for the chemical species that do not depend on the unity Lewis number assumption. This was accomplished by applying a new definition to the mixture fraction \( Z \). The new definition of \( Z \) does not determine the local species composition, but is defined from the solution of a conservation equation with an arbitrary diffusion coefficient and appropriate boundary conditions.

Equations (3.38) and (3.39) contain the instantaneous scalar dissipation rate at stoichiometric conditions \( \chi_{st} \) that is defined in equation (3.23). For turbulent non-premixed combustion \( \chi_{st} \) must be replaced by a conditional (Favre) average value \( \bar{\chi}_{st} \). Due to the
transformation shown above, it implicitly incorporates the influence of convection and diffusion normal to the surface of stoichiometric mixture. In the limit $\chi \to 0$, equation (3.38) indicates that the chemical source terms must sum to zero if the transient terms and radiative heat loss term are negligible, and hence, the local equilibrium model will be obtained.

In turbulent combustion the chemical reactions of interest are exothermic, with considerably higher temperature of the products than that of the reactants and with significant inhomogeneities in the density of the flow field. For this reason, it has become a common practice to use Favre-averaged equations in turbulent non-premixed combustion. In Favre averaging, all fluid mechanical quantities except the pressure are mass averaged. The fluctuations about the mass-averaged mean do not have zero mean but their mass-averaged value is zero. Thus, the Favre-averaged mixture fraction equation of equation (3.31) is.

$$\overline{\rho} \frac{\partial \overline{Z}}{\partial t} + \overline{\rho \nabla} \cdot \overline{\nabla Z} = \nabla \cdot (\overline{\rho D_i \nabla \overline{Z}})$$  \hspace{1cm} (3.40)

In addition to the Favre-averaged mixture fraction, the Favre-averaged mixture fraction variance, $\overline{Z^*}$, needs to be used. It is given as,

$$\overline{\rho} \frac{\partial \overline{Z^*}}{\partial t} + \overline{\rho \nabla} \cdot \overline{\nabla Z^*} = \nabla \cdot (\overline{\rho D_i \nabla \overline{Z^*}}) + 2 \overline{\rho D_i} (\nabla \overline{Z})^2 - \overline{\chi}$$  \hspace{1cm} (3.41)

where the last two terms in equation (3.41) describe the production and dissipation, respectively.

The variable $\overline{\chi}$ is the mean scalar dissipation rate, and is defined as,

$$\overline{\chi} = 2D (\nabla \overline{Z^*})^2$$  \hspace{1cm} (3.42)

In equations (3.40) and (3.41) diffusive terms containing molecular diffusivities, $D$, have been neglected as small compared to the turbulent transport terms, $D_i$, in the large Reynolds number
limit. Equation (3.42) indicates that diffusive effects are preserved in the mean scalar rate, which is modelled as,

$$\bar{\chi} = c_x \left( \frac{\bar{\varepsilon}}{k} \right) \bar{\chi}^*_2$$

(3.43)

with a modelling constant, \( c_x = 2.0 \).

Therefore, this model numerically solves the mean mixture fraction and the mixture fraction variance equations in addition to the continuity, momentum, energy and turbulence \((k-\epsilon)\) equations. The flamelet structure can then be calculated by solving the one-dimensional species and temperature equations in turbulent reacting flows. However, these solutions are available in the form of steady state flamelet libraries. The libraries contain all scalars as functions of the mixture fraction, mixture variance and scalar dissipation rate. Furthermore, the mean value of these scalars is obtained by using the presumed pdf approach (section 3.3.1). For the mixture fraction \( Z \), which varies between \( Z = 0 \) and \( Z = 1 \), the beta function pdf is widely used. It has the form,

$$\tilde{P}(Z, x, t) = \frac{Z^{\alpha-1}(1-Z)^{\beta-1}}{\Gamma(\alpha + \beta)} \Gamma(\alpha) \Gamma(\beta)$$

(3.44)

where \( \Gamma \) is the gamma function and \( \alpha \) and \( \beta \) are the parameters related to \( \bar{Z}(x, t) \) and \( \bar{Z}^*_2(x, t) \) by,

$$\gamma = \frac{\bar{Z}(1-\bar{Z})}{\bar{Z}^*_2} - 1 \geq 0$$

$$\alpha = \bar{Z} \gamma \quad , \quad \beta = (1-\bar{Z}) \gamma$$

(3.45)
3.5 Eddy Dissipation Model

3.5.1 Overview

As was shown in the previous section, turbulence and chemistry are the two fundamental phenomena involved in turbulent reacting flows. The eddy dissipation combustion model was developed for use in computational fluid dynamics (CFD) models to simulate the reactions occurring in flames. This model has been and still is widely used in predicting industrial reacting flows because of its simplicity and robust performance.

The eddy dissipation model is based on the eddy breakup concept from Spalding [31], which originally developed his model for premixed flames, and assumed that the chemical reaction is fast relative to the transport processes in the flow, that is, in the limits of large Damkohler number (equation (3.17)). Spalding [31] proposed a rate model related to the eddy lifetime, and thus mixing time in turbulent flows. Therefore, the rate is proportional to a mixing time defined by the turbulent kinetic energy, $k$, and its dissipation, $\varepsilon$, given by the ratio of $\varepsilon/k$. This means that the reaction is mixing limited and is as fast as the large eddies break up into small eddies through vortex stretching. However, this model required the fluctuations of mixture fraction as input variables, which was difficult to obtain and verify experimentally. Magnussen and Hjertager [32] generalized the eddy breakup by relating the dissipation of the eddies to the mean concentration of reacting species, instead of the concentration fluctuations. Magnussen’s model is known as the eddy dissipation model (EDM) and it applies to non-premixed, partially premixed and premixed flames.

In a reacting flow, the species and energy equations have source terms that represent the chemical source terms. Since these source terms are highly non-linear and strongly dependent
on temperature and species concentrations, a moment closure approach is inadequate. Therefore the modelling of the chemical source terms is approximated as a mean reaction rate. The rate of any reaction may be limited by kinetics or by physical mixing. Physical mixing describes the process of generating a homogeneous mixture of reactants at the molecular level. Chemical kinetics describes the rate at which molecules collide with sufficient energy to react. Both of these processes are essential for reaction to occur and either one may control the overall progress of the reaction. Hence, the rate of the reaction will be determined from the lowest rate.

3.5.2 EDM Formulation

Essentially, the eddy dissipation model (EDM) assumes that the combustion can be described using a single reaction where fuel and oxidant react together to form products and heat. The chemistry of the combustion may be represented on a molar basis as,

\[ v_F \text{Fuel} + v_O \text{Oxidant} \rightarrow v_P \text{Products} \tag{3.46} \]

where \( v_F, v_O \) and \( v_P \) represent moles of fuel, moles of oxidant required to combust \( v_F \) moles of fuel and moles of products generated in the reaction, respectively. The above reaction can be transformed into a general form on a mass fraction basis, given by,

\[ \text{Fuel} + r \text{Oxidant} \rightarrow (1 + r) \text{Products} \tag{3.47} \]

where \( r \) is the mass of oxidant required to combust a unit of mass of fuel, and is related to equation (3.46) by ,

\[ r = \frac{M_O v_O}{M_F v_F} \tag{3.48} \]

where \( M_F \) and \( M_O \) represent the molecular weight of fuel and oxidant, respectively. Note that the progress of the reaction is controlled by the rate in which fuel and oxidant mix.
The one equation model, equation (3.47), represents the simplest description of the reaction process. This model may be useful in obtaining the general heat generation in the reaction zone, but it is not useful in modelling staged combustion, flame lift-off, incomplete combustion or extinction. For these types of problems, it is necessary to account for some of the intermediate processes occurring in the flame. Consequently, more than one reaction is needed to be included. In a multi-reaction model, the challenge is to define the minimum number of reactions necessary to represent the important characteristics of a flame. Detailed reaction mechanisms are not practical in CFD because of the limitations in computational resources. Global reaction mechanisms, on the other hand, include the important elementary reaction and intermediate species, such as carbon monoxide and hydrogen, which would result in reasonable temperature predictions. For example, Hautmann et al. [33] determined an empirical four-reaction mechanism that is sufficient to represent the characteristics of aliphatic hydrocarbon in premixed flames. The structure of the reaction sequence described by Hautmann et al. [33] provides the basis for the design of the multiple reaction mechanism, where each reaction may contain up to two reactants and two products. The reaction in equation (3.47) is modified as.

\[ \text{Fuel}_k + r_k \text{Oxidant}_k \rightarrow f_k (1 + r_k) \text{Product}_1 + (1 - f_k)(1 + r_k) \text{Product}_2 \]  

(3.49)

where \( k \) is the reaction number, \( f \) represents the ratio of the mass of the first product to the total mass of the products and \( r \) is defined in equation (3.48).

The mass-averaged advection-diffusion equation for each mass fraction, \( Y_i \), is,

\[ \frac{\partial (\rho Y_i)}{\partial t} + \frac{\partial (\rho u_j Y_i)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( D_{i,\text{eff}} \frac{\partial Y_i}{\partial x_j} \right) + R_i \]  

(3.50)

This equation is similar to the species equation (3.33). The only differences are in the notations and in symbols. The source term \( R_i \) (\( \dot{n}_i \) in equation (3.33)) is calculated using the eddy
dissipation combustion model (EDM). The model requires that the fuel, oxidant and products will be available in a control volume before the reaction occurs. The fuel and oxidant are necessary components of the forward reaction. However, the products are not needed to be present as part of the reaction, although their presence will imply that heat will be produced due to combustion.

In the EDM, the conservation of energy equation is expressed in terms of a modified total enthalpy, $H^*$, which includes the enthalpy of formation of each species, $h_i^f$, and is given as.

$$H^* = H + \sum_i h_i^f Y_i$$  \hspace{1cm} (3.51)

In this form, the reaction does not add energy to the fluid, but it converts the energy stored chemically in the reactants into sensible heat. In other words, this form introduces an offset to the enthalpy curves for each of the species. Hence, the energy equation will not have an explicit heat source term which can be related to the scalar reaction rate, and temperature changes will only be due to the offset given by the heat of formation. The conservation of energy equation is.

$$\frac{\partial}{\partial t} \left[ \rho \left( H^* - \frac{P}{\rho} \right) \right] + \frac{\partial (\rho u_j H^*)}{\partial x_j} =$$

$$\frac{\partial}{\partial x_j} \left[ \lambda \frac{\partial T}{\partial x_j} + \frac{\mu_i}{\Pr_i} \frac{\partial h}{\partial x_j} + \frac{\mu_i}{\Pr_i} \frac{\partial (\sum_i h_i^f Y_i)}{\partial x_j} + \sum_i D_i \left( h_i + h_i^f \right) \frac{\partial Y_i}{\partial x_j} \right] + S_e$$  \hspace{1cm} (3.52)

where $\lambda$ is the thermal conductivity of the mixture, $D$ is the diffusion coefficient and $S_e$ is the source term due to potential energy and radiation. The above equation is then rearranged to separate the enthalpy of formation terms and express the energy equation in terms of the total enthalpy, $H$. It has the form,
By multiplying the species equation (3.50) by \( h'_i \) and summing over all the scalars \( i \), a new equation is created, which can then be subtracted from equation (3.52) to obtain the final form of the energy equation, with the assumption of a unity Lewis number (equation (3.35)). It is given as,

\[
\frac{\partial}{\partial t} \left[ \rho \left( H - \frac{P}{\rho} \right) \right] + \frac{\partial (\rho u_j H)}{\partial x_j} = \\
\frac{\partial}{\partial x_j} \left( \lambda \frac{\partial T}{\partial x_j} + \frac{\mu_i}{\text{Pr}_i} \frac{\partial h_i}{\partial x_j} + \sum_i D_i \frac{\partial Y_i}{\partial x_j} \right) + S_e - \sum_i h'_i R_i
\](3.53)

Therefore, the above energy equation has an added source term \( \sum_i h'_i R_i \) that accounts for the conversion of chemical energy into sensible heat.

The combustion source terms appearing in the species and energy equations, (3.50) and (3.54), consist of the parameter \( R_i \), which is the reaction rate (source term) of species \( i \). The reaction rate is determined from the minimum of the mixing and kinetic rate. It is essentially the sum of all sources in all participating reactions \( k \),

\[
R_i = \sum_k R_{i,k} = \sum_k \min(R_{i,k,edm}, R_{i,k,kin})
\](3.55)

The mixing rate accounts for turbulence-chemistry interactions. It is basically the rate of dissipation of the eddies, which depends on the turbulent kinetic energy, \( k \), and the rate of dissipation of this energy, \( \varepsilon \). Any of the reacting species - fuel \((f)\), oxidant \((o)\) or products \((p)\) -
may limit the combustion reaction. Thus, the minimum concentration of those species is used to calculate the rate. The eddy dissipation model (EDM) expresses this rate for the $k^{th}$ reaction as.

$$R_{k,edm} = -A_{ebu} \rho \epsilon \min\left\{ Y_f, \frac{Y_o}{r_k}, B_{ebu} \frac{Y_p}{1 + r_k}\right\}$$

(3.56)

where $A_{ebu}$ is a constant that may depend on the structure of the flame and the rate of reaction between fuel and oxidant, and its default value is set at 4.0. $B_{ebu}$ is a Magnussen constant for the products and its default value is 0.5. In addition, equation (3.48) determines the value for $r$. For a multi-reaction model, $k > 1$, the constant $B_{ebu}$ is not used.

The kinetic rate of change of any species in a reaction is described by an Arrhenius rate expression. The Arrhenius rate involves an exponential dependence on temperature and a power law dependence on the concentrations of the reacting chemical species. It is given in a general form as,

$$R_{k,kin} = -A_c T^\beta \exp\left(-\frac{E_r}{T}\right)[C_a]^n[C_b]^m$$

(3.57)

where $A_c$ is a pre-exponential factor, $\beta$ is the temperature exponent, $E_r$ is the activation energy of the reaction, $C_i$ is the molar concentration of reactant $i$, and $n$ and $m$ are the stoichiometric coefficients of the reactants.

Therefore, this model numerically solves the continuity, momentum, energy, species, and turbulence ($k$-$\epsilon$) equations. From the turbulence quantities and scalar concentrations, $R_{k,edm}$ is calculated, while $R_{k,kin}$ is calculated by the predicted the species concentrations. The minimum of the two will be used as a source term in the species and energy equations.


3.6 Solution Method

The governing equations are discretized and solved using a commercial finite volume program called CFX-TASCflow version 2.7.3 from AEA Technologies. The finite volume method uses the integral form of the conservation equations as the starting point. This form of the generic conservation equation is,

\[
\frac{\partial}{\partial t} \int_{\Omega} \rho \phi \, d\Omega + \int_{S} \rho \phi \mathbf{v} \cdot \mathbf{n} \, dS = \int_{S} \Gamma \nabla \phi \cdot \mathbf{n} \, dS + \int_{\Omega} q_{\phi} \, d\Omega
\]  

(3.58)

Where \( \Omega \) and \( S \) represent the volume and surface integrals, respectively. The solution method is subdivided into a finite number of small control volumes by a grid that defines the control volume boundaries. The variables are then defined at the centers of the control volumes, except at the boundaries where they are defined at the centers of the boundary faces. Equation (3.58) is discretized and one algebraic equation is obtained for each control volume. Details of the solution method are provided in the TASCflow theory manual [34].

Boundary conditions must be set for each variable at every boundary on the domain. The following boundary conditions are used in this thesis: Wall, inlet, outlet and symmetry. The velocity at the wall is given a no-slip condition. The velocity profile at the boundary layer is calculated by applying the law of the wall (also known as the log-law region). This region is determined by evaluating the high velocity gradients in the boundary layer region using an empirical correlation based on the shear stress at the wall. This allows a coarse mesh to be used and still include the behaviour in the boundary layer. The non-dimensional distance normal to the wall, \( y^+ \), is defined as,

\[
y^+ = \frac{\rho c_{\mu}^{1/4} \sqrt{k}}{\mu} \Delta y
\]  

(3.59)
where \( k \) is the turbulent kinetic energy, \( \rho \) is the density, \( c_\mu \) is the turbulent viscosity coefficient (given above), \( \mu \) is the dynamic viscosity and \( \Delta y \) is the distance from the wall to the nearest node in the flow. In order for the law of the wall to be applicable, \( y^+ \) must be in the range \( 30 < y^+ < 300 \).

At the inlet boundary, constant values for all variables except pressure are specified. For a specified inlet velocity, \( U_{i,\text{spec}} \), the inlet mass flow is calculated at integration points as:

\[
\dot{m}_{ip} = \rho_{ip} A_{ip} U_{i,\text{spec}}
\]

Inlet values for \( k \) and \( \varepsilon \) must also be entered, and are determined from specified turbulence intensity \( T_u \) and length scale, \( L_e \), by the following relationships,

\[
k = \frac{3}{2} T_u^2 U_b^2
\]

\[
\varepsilon = \frac{k^{3/2}}{L_e}
\]

At the outlet boundary, an average static pressure is applied, and zero normal gradients are set for all other variables. Lastly, at the planes of symmetry, the velocity component normal to the boundary is zero. In addition, all normal derivatives are set to zero. Further details are presented in [34].

The net convective flux through the control volume boundary is the sum of integrals over the six control volume faces in three-dimensional space. Since the surface integral is not known, an approximation is introduced. In TASCflow, A Mass Weighted Skewed (MWS) upstream differencing scheme [35] was used to solve the convective fluxes. The MWS provides a mass weighted average to the convective fluxes along a streamline upstream of the integration point.
The discretized algebraic equations are solved using a Gauss-Seidel solver. This solver is able to eliminate the high-frequency errors much faster than the low-frequency errors. In addition, low-frequency errors may stall the solver. TASCflow overcomes this problem by using an Additive Correction Multigrid (ACM) method, which translates the errors in a given solution iteration onto a coarser grid, and therefore increasing the frequency of the error. For further details regarding the multigrid method see [34].

3.6.1 Coupled Solver and Convergence

In the flamelet model, the coupling of laminar chemistry with the fluctuating turbulent flow field is done using a beta function pdf, which eliminates the difficulty with solving the chemical source terms. As a result, a normal fluid time step could be used to achieve solution convergence. However, the eddy dissipation model (EDM) adds one chemical time scale for every reaction used. If each of the reacting scalars is solved in a segregated way, the time step must be small enough to limit the change of each scalar in any given step. Hence, the smallest time scale may dominate the behaviour of the solution, and a large number of steps will be required to reach convergence of the fluid flow solution.

To minimize this problem, the solution of the scalar equations should be coupled. Coupling allows a larger time step to be used in order to solve the reacting flow and fluid flow. In this way, the reaction source is continually updated during convergence at the same rate for all species. This approach will help minimize species imbalances, which will reduce unphysical concentrations and temperatures in the solution domain. In TASCflow, the extra memory required to solve the coupled scalar equations limits the number of scalars to seven.

There is another way to improve convergence in chemically reacting turbulent flows. Since the chemical times are usually orders of magnitude smaller than the turbulent times and the
reaction rates depend strongly on other species and temperature, the solution might start to oscillate with no chance of convergence. In order to control the oscillations, a temperature damping parameter was set up in TASCflow, and it has the form,

\[
T^n = T^o + TDFAK \cdot T'
\]

(3.63)

where TDFAK is a temperature damping parameter that has a default of 0.25. In the above equation \( T^n, T^o \) and \( T' \) represent the new, old and the change in temperature, respectively. The solution iterations in TASCflow report the maximum relative amount of damping by the parameter \( T_{rel} \) as,

\[
T_{rel} = \frac{T' - TDFAK \cdot T'}{T^o}
\]

(3.64)

At convergence, \( T' \) should approach zero. Hence, temperature damping can effectively slow down the changes to a solution, and in TASCflow, it has a direct effect on the density through the equation of state. However, this technique may slow the convergence rate.

### 3.7 Summary

The mathematical representation of the governing equations has been introduced. The time-averaged form of the continuity, momentum and energy equation is shown together with the definition of the new Reynolds stress and heat flux terms. The turbulent eddy viscosity is used to model the Reynolds quantities with the aid of two transport equations, \( k \) and \( \epsilon \).

This chapter introduces two combustion models that will be used in this study - the laminar flamelet and the eddy dissipation model. The laminar flamelet model was described for non-premixed turbulent combustion. The most important parameter is the mixture fraction. The flow field is transformed into mixture fraction space and two transport equations are used to solve for this field. The flamelet model is related to the turbulent flow field by the scalar
dissipation rate. This parameter can determine non-equilibrium effects in flames such as flame stretch and extinguishing. In addition, non-premixed flamelet regimes are shown and explained. The specific flamelet regime depends on the chemical and turbulent time scales and on the fluctuations of the mixture fraction variance. A presumed beta pdf couples the information on the inner structure of the flamelets with the turbulent flow field. It is applied together with the species concentration obtained from the solution of a one-dimensional laminar counter-flow diffusion flame, which are given in a flamelet library, to form new scalar compositions.

The eddy dissipation model relates the rate of combustion to the rate of dissipation of eddies. Since mixing and chemistry are present in any combustion application, the rate of combustion is limited by the smaller of the two rates. If mixing time is slow and the chemistry is fast, the rate of reaction is expressed by the mean concentration of a reacting species, the turbulent kinetic energy and the rate of dissipation of this energy. If the chemistry is slow and the mixing time is fast, the rate of reaction is expressed by a chemical kinetic rate known as an Arrhenius rate. The reaction rates will then appear as source terms in the species and temperature equations.

The description of the solution method was given. The numerical solution is based on a finite volume approach. The boundary conditions as well as the solver type are briefly discussed. In addition, the coupled scalar solver is used in order to improve convergence while allowing for a larger time step. Temperature damping is applied to reduce solution oscillation.
4 Preliminary Validation Studies

The purpose of this chapter is to present the results from the validation of the numerical solutions given by TASCflow against those obtained analytically or experimentally. The validation studies discussed here were made in a logical manner, that is, simple flows were done first with subsequent studies adding increments of complexity. The following six validation cases will be shown:

- laminar pipe flow;
- turbulent pipe flow;
- jet in a quiescent flow;
- jet in a coflow;
- jet in a confined pipe flow, and
- non-reacting jets in a crossflow.

The first five cases will examine the numerical solution of velocity profile and pressure drop for different mesh types. The last validation case will lead into the next chapter which deals with reacting jets in a crossflow.

4.1 Laminar Pipe Flow

4.1.1 Description Of The Problem

The exact solution of the axial momentum equation for a laminar flow in a circular pipe is well known. The velocity profile for a steady state flow is parabolic which drops to zero at the walls and reaches a maximum at the pipe's centerline. For a pipe of radius \( R \) and length \( L \), the fully developed pipe flow has a velocity profile, \( U \), given as [36],
\[ U(r) = \frac{1}{4\mu} \frac{\Delta P}{\Delta x} (R^2 - r^2) \] (4.1)

Where \( r \) is the radial distance from the centerline to the wall, \( \mu \) is the dynamic viscosity and \( \Delta x \) is the length of the fully developed pipe flow. The pressure drop can be calculated by integrating the mass flow across the pipe from zero to \( R \), yielding the following expression,

\[ \Delta P = \frac{8\mu \dot{m}}{\pi \rho R^4} \] (4.2)

where \( \rho \) represents the fluid density and \( \dot{m} \) is the mass flow rate.

### 4.1.2 Description Of The Boundary Conditions and Simulation

A model of a simple pipe flow was created in TASCflow. The pipe length and its diameter were set to four meters and five centimetres, respectively. The pipe length was selected to allow the flow to fully develop, so that influences of the developing region will not be considered in the analysis. Three grid types were generated for this pipe: Rectangular, polar and butterfly. Those grids are shown in Figure 4-1. The polar grid can also be referred to as \( R-\theta \) or angular grid. There are two problems associated with this grid: (1) at centerline axis the volume collapses to zero and (2) nodal density increases towards the center. The rectangular grid has a problem associated with high skewness levels at the corners of the pipe where nodal density is high. The butterfly grid consists of rectangular and polar grids that are connected together, and hence, holds an advantage over the other two grids.

For all grids a 180-degree sector was used and a symmetrical boundary condition was imposed in order to represent a full pipe flow. In addition, each grid was run with a coarse and fine mesh. The coarse and fine mesh consisted of approximately 7500 and 22000 nodes.
respectively. Although, different grids were used, the number of nodes in a cross-section was approximately the same. This was also true for the number of nodal point in the flow direction.

Two fluids were tested. The first one was water, having properties at standard temperature and pressure, that is, \( \rho = 998.2 \text{ kg/m}^3 \) and \( \mu = 9.93\text{E}-4 \text{ kg/m/s} \). The second fluid was air, which also had properties at standard temperature and pressure, that is, \( \rho = 1.164 \text{ kg/m}^3 \) and \( \mu = 1.824\text{E}-5 \text{ kg/m/s} \).

Four boundary conditions were considered: Inlet, wall, symmetry and outlet. For the inlet boundary condition, a constant mass flow rate, \( \dot{m} \), was set normal to the boundary face, which had a value of \( 1.0\text{E}-02 \text{ kg/s} \) for water and \( 3.674\text{E}-04 \text{ kg/s} \) for air. This would produce a Reynolds number of approximately 513 for both water and air, which is in the range of laminar pipe flows. A no-slip wall condition was specified for the pipe wall, and symmetry was applied at the flat section of the grid (where the pipe divides into half). For the outlet boundary condition, a reference pressure of 101.325 kPa was specified at a single control volume.

The convergence criterion for each solution was set by specifying a maximum residual of \( 10^{-4} \) or less. In addition the equations were discretized using the upstream differencing scheme (UDS).

### 4.1.3 Results

The grids were compared by examining their flow solution behaviour in terms of errors in pressure drop and velocity profile. The best grid was the one that produced the lowest errors. In order to start the grid comparison, the fully developed flow length was checked by examining the pressure drop and velocity profiles. At a fully developed flow, the pressure drop varies linearly with downstream distance and the velocity profiles are identical. It was found that the fully
developed flow length was about two meters depending on the type of grid and mesh used. This length was acceptable for analysis purposes since the pipe length was four meters.

The first comparison was done using water. Figure 4-2 presents the coarse mesh velocity profile predicted by TASCflow for the different grid types compared to the theoretical solution. It can be seen that the velocity profile predicted by the three grids is very close to the solution given by equation (4.1). However, upon further examination of the percentage error between the theoretical and computational solutions, see Table 3.1, it was found that the butterfly grid yielded the least error: $0.73 \pm 0.245\%$ for coarse mesh and $0.31 \pm 0.039\%$ for fine mesh. The number following the '±' represent the 95% confidence level. The rectangular grid was found to have the greatest error with the coarse mesh, although, the fine mesh error was satisfactory.

The pressure drop along the developed region of the pipe was examined next. As can be seen from Table 3.1, the rectangular grid with fine mesh had the smallest percentage error between the predicted and theoretical solution. However, both the polar and butterfly grids predicted (with error of approximately 0.5%) the pressure drop quite well.

Next, the working fluid was changed from water to air in order to study more closely the influence of the working fluid on the grid type. Similar predictions of the velocity profile and pressure drop were obtained for the three grid types. The velocity profiles was plotted and the butterfly grid was found to have the least error, with $0.7 \pm 0.26\%$ for coarse mesh and $0.24 \pm 0.057\%$ for fine mesh. These errors are very close to the ones given in Table 3.1 for water. The pressure drop error was also the smallest in the butterfly grid, with 1.1% and 0.52% for coarse and fine mesh, respectively. Hence, there was no influence of the working fluid on the grid type.

The laminar flow validation study brings about two important points. Firstly, this study confirms that the numerical solution conserved both mass and momentum. And secondly, in
Figure 4-1  Representation of three coarse grid types: (a) Rectangular, (b) Polar, (c) Butterfly
Table 4.1: Comparison between the analytical and predicted velocity profile and pressure drop for various mesh and grid set-ups in a laminar water pipe flow

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Grid Type</th>
<th>% Error</th>
<th>Velocity</th>
<th>Pressure Drop</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse</td>
<td><em>Rectangular</em></td>
<td>1.4 ± 1.08</td>
<td>1.4</td>
<td>1.4</td>
</tr>
<tr>
<td></td>
<td>Polar</td>
<td>0.96 ± 0.577</td>
<td>0.52</td>
<td></td>
</tr>
<tr>
<td></td>
<td><em>Butterfly</em></td>
<td>0.73 ± 0.245</td>
<td>1.1</td>
<td></td>
</tr>
<tr>
<td>Fine</td>
<td><em>Rectangular</em></td>
<td>0.47 ± 0.332</td>
<td>0.26</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Polar</td>
<td>0.45 ± 0.186</td>
<td>0.49</td>
<td></td>
</tr>
<tr>
<td></td>
<td><em>Butterfly</em></td>
<td>0.31 ± 0.039</td>
<td>0.54</td>
<td></td>
</tr>
</tbody>
</table>
order to more accurately characterize a laminar flow or any other flow that will be shown later, a grid selection is relevant, especially where lack of computer resources are present. In this validation study, the butterfly grid was found to be the best grid characterizing this flow.

4.2 Turbulent Pipe Flow

4.2.1 Description Of The Problem

The next category of complexity deals with a turbulent pipe flow. Comparison of the predicted velocity profile and pressure drop to the analytical solutions were done for a pipe of radius \( R \) and length \( L \). In order to calculate the velocity distribution in a turbulent flow, one needs to understand the shear layer characteristics involved. In a typical velocity distribution in a turbulent flow, three regions are present near a wall. The first layer closest to the wall is known as the viscous wall layer, where laminar shear is dominant. The layer furthest away from the wall is the outer layer and turbulent shear dominates there. And the layer between the wall layer and the other layer is called the overlap layer. In this layer both laminar and turbulent shear are important. Also, the velocity in this layer was found by dimensional analysis to vary logarithmically with distance from the wall towards the center, and it is expressed as [36].

\[
\frac{u}{u^*} = \frac{1}{\kappa} \ln \frac{yu^*}{v} + B \tag{4.3}
\]

The equation representing this velocity is known as the logarithmic-overlap layer or log-law region. In the above equation, \( y \) is the distance from the wall, \( v \) in the kinematic viscosity. \( \kappa \) is the Von Karman constant equals to 0.41, \( B \) is an empirical constant equal to 5, and \( u^* \) represent the friction velocity and is defined as,
\[ u^* = \sqrt{\frac{\tau_w}{\rho}} \]  \hspace{1cm} (4.4)

where, \( \tau_w \) represents the wall shear stress. The logarithmic law starts at about \( y^+ = yu^*/\nu = 30 \) and ends at about \( y^+ = 500 \).

However, the logarithmic law, equation (4.3), can actually approximate nearly the entire velocity profile for turbulent flow in a pipe. An exception is for the outer layer when the pressure is increasing strongly downstream. The wall layer typically does not exceed two percent of the velocity profile and can be neglected. Therefore, equation (4.3) can be used as a good approximation to solve a turbulent pipe flow problem presented in this validation study.

By rearranging equation (4.3), the mean velocity, \( U \), can be expressed as a function of radial distance from the wall to the center of the pipe as follows,

\[ U(r) = U^* \left[ 2.44 \cdot \ln \left( \frac{U^*(R-r)\rho}{\mu} \right) + 5 \right] \]  \hspace{1cm} (4.5)

where, \( \nu = \mu/\rho \). The wall shear stress varies linearly from the centerline to the wall and is defined as,

\[ \tau_w = \frac{R \Delta P}{2 L} \]  \hspace{1cm} (4.6)

The pressure drop was approximated by Blasius [36], who presented the formulation for a horizontal pipe as,

\[ \Delta P = 0.158L \rho^{3/4} \mu^{1/4} D^{-5/4} V^{7/4} \]  \hspace{1cm} (4.7)

where, \( D \) is the pipe diameter and \( V \) is the inlet velocity. The above equation is valid for Reynolds number less than or equal to \( 10^5 \).
4.2.2 Description Of The Boundary Conditions and Simulation

The same pipe dimensions were used in this study as for the laminar flow study. Three grid types were generated for a ninety-degree sector and are shown in Figure 4-1. The same number of nodes and nodal distribution were used as in the previous study, that is, 7500 and 22000 nodes for coarse and fine mesh, respectively. The working fluid consisted of water and air at standard temperature and pressure, and the fluid properties were listed in the previous study.

Three boundary conditions were considered: Inlet, wall, symmetry and outlet. The $k$-$\varepsilon$ turbulence model used in this work required that the turbulence intensity $T_u$ and length scale $L_c$ be specified, in order to calculate the inlet turbulent kinetic energy its dissipation, respectively (see equations (3.61) and (3.62)). Thus, a turbulence intensity was given a value of 0.05 (5%) and the length scale was set at 0.01 meter, which was at the same order of magnitude as the pipe diameter. In addition, a uniform velocity profile normal to the boundary face was set equal to 10 m/s for water and 157.52 m/s for air, producing a Reynolds number of 5.03E+5, which is well into the turbulent region. For the wall boundary, a no-slip condition was set. The first node closest to the wall was calculated by the non-dimensional distance normal to the wall, equation (3.47), in order to account for the log-law region that was used in this model. Thus, the placement of first node was range of $30 < y^+ < 500$. A symmetry condition was set at the same boundary face as for the laminar flow study. For the outlet boundary condition, a reference pressure of 101.325 kPa was specified at a single control volume.

Similar to the previous study, the convergence criterion was set to $10^{-4}$ or less, and the same solver (UDS) was used for the numerical solution.
4.2.3 Results

The fully developed flow length was checked by considering the streamwise pressure distribution and velocity profiles. It was found that the fully developed flow length was about 1.5 meters upstream from the outlet depending on the type of grid and mesh used. Thus, the pipe length was sufficient for the current study.

A comparison similar to the one performed in the previous study was done. Figure 4-3 shows velocity profiles of the three grids and the analytical solution given in equation (4.5). Results obtained using water as the working fluid are presented in this figure. The velocity profile of a coarse mesh predicted well the analytical solution near the center of the pipe, but very poorly near the wall where gradient effects were dominant. However, the velocity profile in fine mesh improved the approximation of the wall gradient. Table 4.2 provides an overall percentage error between the different grid and mesh types to the analytical solution. The variation from coarse to fine mesh did not improve the percentage error in rectangular and polar grids, which are at 5% error. The butterfly grid, though, showed a big influence on the mesh type, contradictory to what was expected. That is, the butterfly grid increased its overall error with increasing nodal density. From these results, the polar grid provided the most accurate estimation of the velocity profile, while the butterfly grid provided the worst prediction.

By looking closely at Figure 4-3, one can see that the butterfly grid actually follows the velocity profile even better than the other grids. The contradiction between the graphical and tabular results is caused by the large percentage error near the wall, where the velocity profile is very steep. Since equation (4.5) is an approximation to the velocity distribution, the near wall profile might not be correct, and will influence the overall error. Due to the structure of each grid, the nodal locations would vary, and hence, would affect the overall error, especially near
Figure 4-3  Velocity profile in a turbulent pipe flow (coarse grid)

Table 4.2: Comparison between the analytical and predicted velocity profile and pressure drop for various mesh and grid set-ups in a turbulent water pipe flow

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Grid Type</th>
<th>% Error</th>
<th>Velocity</th>
<th>Pressure Drop</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse</td>
<td><em>Rectangular</em></td>
<td>4.9 ± 3.56</td>
<td>6.9</td>
<td></td>
</tr>
<tr>
<td></td>
<td><em>Polar</em></td>
<td>5.2 ± 3.16</td>
<td>10.7</td>
<td></td>
</tr>
<tr>
<td></td>
<td><em>Butterfly</em></td>
<td>7.3 ± 4.27</td>
<td>8.2</td>
<td></td>
</tr>
<tr>
<td>Fine</td>
<td><em>Rectangular</em></td>
<td>5.4 ± 2.84</td>
<td>9.5</td>
<td></td>
</tr>
<tr>
<td></td>
<td><em>Polar</em></td>
<td>5.4 ± 2.42</td>
<td>8.9</td>
<td></td>
</tr>
<tr>
<td></td>
<td><em>Butterfly</em></td>
<td>8.7 ± 3.77</td>
<td>7.5</td>
<td></td>
</tr>
</tbody>
</table>
the wall. This is why the butterfly grid did not have lower error with a finer mesh, but presented a better velocity profile around the centerline.

Table 4.2 also shows the overall error in pressure drop. The predicted pressure drop was compared to the analytical solution given in equation (4.7). A high percentage error in pressure drop was observed. This can be partially attributed to the fact the equation (4.7) is in itself an approximation, however, it is a good baseline for comparison purposes. As seen from the results, the rectangular grid had increased its percentage error with a change from coarse to fine mesh. This is believed to be due to the increase in skewness near the wall. On the other hand, varying the mesh from coarse to fine in polar and butterfly grid caused a reduction in error, as was anticipated. However, the butterfly grid provided the best estimate to the pressure drop, with 8.2% and 7.5% for coarse and fine mesh, respectively.

By changing the working fluid from water to air, similar conclusions were drawn. The velocity profile was predicted better in the butterfly grid, but had the worst overall velocity error. The only difference was that the change in mesh from coarse to fine has improved the overall error, with 9.2 ± 0.469% and 9.0 ± 0.369% for coarse and fine mesh, respectively. In addition, the pressure drop error was the lowest in the butterfly grid, with 8.3% and 7.4% for coarse and fine mesh, respectively. Those results indicate that the working fluid has no affect on the grid type, as was found in the previous study.

Therefore, the numerical model is able to predict the velocity profile and the pressure drop to approximately 5% and 8%, respectively. Also, the butterfly grid provides the best estimate to the pressure drop and velocity distribution.
4.3 Jet In A Quiescent Flow

4.3.1 Description Of The Problem

This validation study deals with free turbulent shear flows, where there is no rigid surface present in the region of interest. A jet in a quiescent flow consists of a circular jet of diameter $d$ that enters into a large stagnant mass of the same fluid with a uniform velocity $U_0$. Near the injection plane of the jet there is a core of flow with a uniform velocity, which equals the inlet jet velocity. Since the turbulence generated on the jet boundaries merges to the axis, the core is in the form of cone. This core is known as the potential core and the region that it occupies is called the flow development region. Following this region is a zone of fully developed flow, where the mean velocity on the jet’s axis decays linearly with downstream distance, that is, $U_{\text{max}} \propto x$. In addition, at every section the velocity decreases radially from a maximum on the axis to zero at large values of $r$. Hence, this region is also known as the similarity region since the normalized velocity profiles at every downstream section remain unchanged. Experimental observations [37] reveal that the length of the potential core for a jet in a quiescent flow is about 10 jet radii. This means that the normalized velocity profiles will be similar for $x/r > 10$.

The non-dimensional velocity profile in the fully developed region was estimated by Goertler [38] by the following expression,

$$\frac{U}{U_{cl}} = \left[ 1 + 57.76 \left( \frac{r}{x} \right)^2 \right]^{-2}$$  \hspace{1cm} (4.8)

where, $U_{cl}$ represents the centerline velocity. A characteristic width called the half-radius, $r_{1/2}$, is used to indicate the spread of the jet. The half-radius is the value of the $r$ at which the fluid
velocity is half the centerline value, that is, \( U/U_c = 0.5 \), and it varies linearly with downstream distance. Schlichting [39] presented an equation for the half-radius as,

\[ r_{1/2} = 0.0847x \]  

(4.9)

4.3.2 Description Of The Boundary Conditions and Simulation

A butterfly grid, Figure 4-4(b), was used to model the duct where the jet entrained into the surrounding fluid. This grid consisted of 23700 nodes in total. A jet diameter was chosen in such a way as to reduce the interaction between the jet boundary and the boundary of the duct, in order to accurately simulate jet flow in a stagnant fluid. The jet and the surrounding fluid were set to be air at standard temperature and pressure, and were modelled as a simple turbulent, incompressible flow. The properties for this fluid are listed in section 4.1.2.

Figure 4-4(a) shows a schematic representation of the duct with its boundary conditions. The hydraulic diameter of the jet was set at 7.5 mm and the diameter of the duct was set to 0.6 m, yielding a duct to jet diameter ratio of 80. The length of the duct was one meter, which provided an equivalent length of 133 jet diameters. The inlet section of the jet consisted of one grid embedding in a small section surrounding the jet, see Figure 4-4(b). Grid embedding was used in order to provide a better transition between the jet and the wall boundary faces. The actual inlet section of the jet had a square shape, although round jet was modelled, since a square shape was easier to employ. An assumption that a square jet would closely resemble the properties of a round jet was made. This assumption was later investigated, and its validity is examined in the next section.

The following four boundary conditions (Figure 4-4(a)) were used: Inlet, wall, opening and outlet. For the inlet condition, the jet was given a uniform velocity profile equals to 30 m/s.
Figure 4-4  (a) Schematic representation of boundary conditions, (b) cross-sectional mesh with one embedded grid
yielding a Reynolds number of about 14360 based on the jet's diameter. Since a $k-\varepsilon$ turbulence model was used, the turbulence intensity and length scale were specified as 0.05 and 0.007 m, respectively. In addition, a no-slip wall boundary was used at the inlet section of the duct (excluding the inlet section of the jet). For the outlet condition, a constant static pressure of 101.325 kPa was used. Furthermore, an opening boundary condition was used for the duct's walls by specifying a constant static pressure of 101.325 kPa for outflow and $T_u$ and $L_e$ equal to 0.05 and 0.007 m, respectively, for inflow with flow direction set normal to the boundary. An opening boundary condition allows the fluid flow to cross the boundary surface in either direction. This means that when the fluid is flowing out of the domain, the outlet boundary condition is applied, and where the fluid is flowing into the domain, the inlet boundary condition is applied.

Similar to the previous study, the convergence criterion was set to $10^{-4}$ or less, and the Linear Profile Scheme (LPS) solver was used for the numerical solution.

4.3.3 Results

In Figure 4-5 equation (4.8) was plotted together with the numerical predictions at three downstream, $x/d$, locations: 41.4, 87.4 and 133.3. This figure illustrates that all three locations are in the similarity region since they all fall on the same curve. The predicted half-radius (at $U/U_{cl} = 0.5$) equals to 0.096 while from equation (4.9) the half radius is 0.0847. From the above plot, the half-radius of the analytical solution is the exact value given by equation (4.9). Hence, the numerical predictions overestimate the half-radius by approximately 13.3%. Near the central axis, $-0.08 < r/x < 0.08$, the predictions are very close, from $r/x = \pm(0.08 - 0.17)$ they overestimate, and from $r/x = \pm(0.17 - 0.54)$ they underestimate. Thus, the numerical solution
overestimates the jet’s spreading. Overall, the numerical model is able to predict the velocity field well especially near the jet’s centerline.

The jet’s nozzle in the model was square and the analytical solution was for round jet. Since the numerical predictions indicate a similar solution to the round jet solution, the assumption taken was valid. Thus, a square nozzle would yield a similar velocity field as a round nozzle as long as the analysis is considered in the similarity region.

Figure 4-5  Normalized radial velocity profiles for three downstream locations and for Goertler’s solution
4.4 Jet In A Coflow

4.4.1 Description Of The Problem

In this section, the behaviour of a circular jet when the surrounding fluid is also in motion and in the direction of the jet will be investigated. In the previous study, the surrounding fluid was at rest, that is, \( U_{\text{coflow}} = 0 \), while in this study \( U_{\text{coflow}} > 0 \). As before, there are two distinct regions to be considered. The region nearest to the nozzle of the jet is called the flow development region, where the potential core is positioned and the jet has a constant uniform velocity. After this, the similarity region exists. In this region, the centerline velocity decays linearly with downstream distance in the initial stages, where the centerline velocity is much greater than the coflow velocity. However, the centerline velocity decays non-linearly as it approaches the coflow velocity. Therefore, a similarity in the normalized velocity profiles could not be achieved, unless the velocity ratio of the jet to the coflow becomes large. An ideal case was looked at in the previous study, where the velocity ratio was infinity, and hence, the velocity decayed linearly streamwise. Since the characteristic width of the jet is related to the velocity distribution, its value will depend on the conditions mentioned above.

Nickels and Perry [40] proposed a non-dimensional velocity profile in the form of.

\[
\frac{U - U_1}{U_{cl} - U_1} = \exp \left[-0.677 \left( \frac{r}{L_0(x)} \right)^2 + 0.364 \left( \frac{r}{L_0(x)} \right)^3 - 0.121 \left( \frac{r}{L_0(x)} \right)^4 \right]
\]

(4.10)

where \( U_1 \) represents a uniform constant velocity of the coflowing fluid, \( U_{cl} \) is the centerline jet velocity and \( L_0 \) is the half-radius of the jet at which the velocity \( (U - U_1)/(U_{cl} - U_1) = 0.5 \). The half-radius is a function of downstream distance and was approximated by Henbest and Yacoub [41] in the following expression,
\[
\frac{L_o}{d} = \frac{C_i \left( \frac{V}{d} \right)}{\sqrt{\frac{2.363 \, x}{\lambda_i} \frac{x}{d} + 30.95}}
\]

(4.11)

where, \( d \) is the diameter of the jet and \( \lambda_i \) is the velocity ratio defined by,

\[
\lambda_i = \frac{U_{jet} - U_1}{U_1}
\]

(4.12)

In equation (4.11), \( C_i \) is a constant that depends on the initial conditions at the nozzle exit plane and on \( \lambda_i \). Although the centerline velocity decay can be non-linear downstream of the jet nozzle, Henbest and Yacoub [41] collapsed the all the experimental data onto a single line and gave an estimations for the centerline velocity as,

\[
U_{ct} = U_1 + \left( U_{jet} - U_1 \right) A \left( \frac{x - x_0}{d} \right)^{-1}
\]

(4.13)

Where, \( A \) is a constant that depends on \( \lambda_i \) and \( x_0 \) is a virtual origin along the jet’s axis.

### 4.4.2 Description Of The Boundary Conditions and Simulation

The working fluid for both jet and coflow was air at standard temperature and pressure. Jet and duct diameters and the length of the duct were unchanged from the previous validation study. The jet’s nozzle was modelled with a square geometry, even though, circular jet was considered. The validity of this choice was discussed in the previous study.

A butterfly grid was generated like the one in Figure 4-4(b) with one grid embedding in the vicinity of the jet. However, three more grid refinements were performed, two of which are shown in Figure 4-6. Those grids were refined by embedding one extra grid in the vicinity of the nozzle. In the last refinement, the embedded grid of Figure 4-6(b) was generated with a larger nodal density. These grids were considered in order to study grid sensitivity. The total
Figure 4-6  Jet and coflow inlets with (a) 2 embedded, and (b) 3 embedded grids
number of nodes for each grid was 23700, 42450, 212400 and 334800, respectively.

Two cases were examined. The first case was for a jet velocity of 15 m/s and coflow velocity of 5 m/s. The second case was modelled with a jet velocity of 25 m/s and coflow velocity of 5 m/s. From the definition of equation (4.12), the two cases were for $\lambda_i = 2$ and $\lambda_i = 4$, respectively, and hence, from [41] $C_i = 0.352$ and 0.357, respectively. Substituting these constants into equation (4.11) yielded an expression for the jet's half-radius. In addition, the constants for equation (4.13) are given in [41] as, $A = 6.80$ and 6.48, $x_0 = -0.1$ and 0.2 for $\lambda_i = 2$ and 4, respectively.

Figure 4-4(a) shows the boundary conditions involved in the numerical model. Notice that for the coflow boundary condition, the wall condition from the previous study was replaced by an inlet condition. For the jet's inlet condition, a constant uniform velocity was set with a different value for each case. For the coflow's inlet condition, a constant uniform velocity of 5 m/s was set. For both inlet conditions, the turbulence intensity and length scale were given a value of 0.05 and 0.007, respectively. For the outflow condition, a constant static pressure of 101.325 kPa was set. Furthermore, an opening boundary condition was given to the duct's walls, in order to account for fluid flowing into or out of the domain. For this condition, a constant static pressure of 101.325 kPa was used for fluid coming out of the domain; the turbulence quantities $T_u$ and $L_e$ were specified equal to 0.05 and 0.03, respectively, for fluid flowing into the domain. For the two types of flow, the flow direction was determined implicitly as part of the numerical solution.
Figure 4-7  Grid sensitivity tests at $x/d = 87.4$ with respect to normalized radial velocity profiles having a velocity ratio $\lambda_i$ of (a) 3 and, (b) 5
Figure 4-8  Normalized radial velocity profiles at three downstream locations having a velocity ratio of (a) 3 and (b) 5
4.4.3 Results

For the two cases, \( \lambda_t = 2 \) and 4, the development length was estimated to be approximately 6 jet diameters downstream of the nozzle [37]. This length was far away from the region of analysis. Furthermore, grid sensitivity test was done to ensure that the numerical solution would be grid independent. Grid sensitivity was done at \( x/d = 87.4 \) for the two cases analyzed and are shown in Figure 4-7, together with the analytical solution of equation (4.10). Thus, for 3 embedded grids (see Figure 4-6(b)) the solution becomes independent.

The analysis of the first case, that is \( \lambda_t = 2 \), is shown in Figure 4-8(a). The numerical predictions at three downstream locations, \( x/d = 41.4, 87.4 \) and 133.3, were compared to the analytical solution of equation (4.10). It can be seen that the predictions overestimated the half-radius (where the normalized velocity \( (U-U_{cofflow})/(U_{cl}-U_{cofflow}) = 0.5 \)) at \( x/d = 41.4 \) and underestimated the half-radius at the outlet of the pipe, that is \( x/d = 133.3 \). However, the predictions at \( x/d = 87.4 \) yielded a very close approximation to the half-radius. According to the analytical solution, the half-radius of the jet was increasing with increasing streamwise distance \( x/d \), but the predictions showed that the half-radius reduced with increasing \( x/d \). Since this plot involves normalized quantities, it is unclear whether this is the result obtained by the numerical model. In order to further investigate this phenomenon, the radial velocity was plotted together with the analytical solution at the same \( x/d \) locations. This is shown in Figure 4-9(a), where the analytical solution was obtained from equation (4.10) with the centerline velocity of equation (4.13). From this plot, it is clear that both the numerical solution and the analytical solution showed that the half-radius increased and the centerline velocity decreased with \( x/d \). However, the numerical solution overestimated the centerline velocity, and hence, underestimated the jet’s
Figure 4-9  Radial velocity profiles at three downstream locations having a velocity ratio of (a) 3 and, (b) 5
spreading. This might be due to the isotropic nature of the \( k-\varepsilon \) model, which overpredicts the turbulent dissipation rate in high shear regions. In this study, a high shear region occurs in the boundary where the jet mixes with the coflow, and hence, the jet’s spreading is underpredicted.

The second case depicted a similar behaviour as discussed for the first case. The only difference between the first and second case was in the spread of the jet along the duct. This can be seen from Figure 4-8(b) and Figure 4-9(b). In this case, the jet exhibited a wider spread that was due to the larger velocity ratio between the jet coflow. This behaviour was anticipated since the half-radius is the largest in a jet with quiescent flow, that is, \( U_{coflow} = 0 \). This is illustrated in Figure 4-8(a) and (b) where Goertler solution for a jet in a quiescent flow was plotted. Henbest and Yacoub [41] and Smith and Hughes [42] conducted experiments to confirm this property.

Therefore, in the two cases analysed in this study, the centerline velocity and half-radius decayed non-linearly. Also, a comparison of the two cases revealed that the jet’s half-radius increased with increasing velocity ratio. The numerical solution underpredicted the jet’s spread and hence overpredicted its centerline velocity. Table 4.3 lists the errors in the half-radius predictions. Overall, the error are large, however, qualitative analysis shows that the numerical model is able to capture important properties of a jet in a coflow.

**Table 4.3: Jet’s half-radius errors**

<table>
<thead>
<tr>
<th>Velocity Ratio, ( \lambda_t )</th>
<th>Axial Location, x/d</th>
<th>Numerical Solution</th>
<th>Analytical Solution (4.10)</th>
<th>% Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>41.4</td>
<td>0.021</td>
<td>0.031</td>
<td>32.25</td>
</tr>
<tr>
<td></td>
<td>87.4</td>
<td>0.031</td>
<td>0.052</td>
<td>41.35</td>
</tr>
<tr>
<td></td>
<td>133.3</td>
<td>0.040</td>
<td>0.068</td>
<td>41.18</td>
</tr>
<tr>
<td>4</td>
<td>41.4</td>
<td>0.029</td>
<td>0.039</td>
<td>25.64</td>
</tr>
<tr>
<td></td>
<td>87.4</td>
<td>0.043</td>
<td>0.069</td>
<td>37.68</td>
</tr>
<tr>
<td></td>
<td>133.3</td>
<td>0.054</td>
<td>0.090</td>
<td>40.00</td>
</tr>
</tbody>
</table>
4.5 Jet In A Confined Pipe Flow

4.5.1 Description Of The Problem

In this validation study, the behaviour of a circular jet in a circular duct will be conducted. This problem is important in many engineering designs involving two flows of differing velocities, such as in the design of jet pumps and combustion chambers.

This study involves a circular jet of diameter $d_0$ with a constant velocity $U_j$, which enters coaxially into a duct of diameter $D_0$ having a uniform velocity $U_i$ that is smaller in magnitude than $U_0$. Depending on the velocity ratio of the jet to coflow $U_j/U_i$ at the entrance, two flow regimes occur along the duct. If the velocity ratio is small, the jet cannot consume the coflow before reaching the duct wall, and hence, the flow remains unseparated. If the velocity ratio is large, the jet consumes all the coflow and additional entrainment creates a reverse flow in order to conserve the total mass flow. Further downstream the flow completely loses its jet characteristics and degenerates eventually to fully developed pipe flow if the duct is long enough.

Barchilon and Curtet [43] conducted experiments of confined turbulent jets. Using hotwires and pitot tubes they measured mean velocities, variation of wall static pressure and size of the recirculation zone for water flow. They also used airflow to measure the RMS values of the axial velocity fluctuations. The flow was characterized by the Craya-Curtet number $Ct$. This parameter is the inverse square root of the total momentum, non-dimensionlized with the volume flux and the duct area and is given in the following expression,

$$
Ct = \frac{U_m}{\left[(U_j^2 - U_i^2)(d_0/D_0)^2 + 0.5(U_i^2 - U_m^2)\right]^{\frac{1}{2}}}
$$

(4.14)
where $U_m$ represents the mean velocity in the mixing duct and is defined as,

$$ U_m = (U_j - U_1)(d_o/D_o)^2 + U_1 \quad (4.15) $$

Barchilon and Curtet [43] showed that recirculation occurs when $Ct \leq 0.96$.

Physically, large or small values of $Ct$ correspond to small or large excess inlet momentum, respectively. In addition, in the limit of $Ct \to \infty$, a developing pipe flow occurs and in the limit of $Ct \to 0$, a free jet in quiescent surroundings occurs. Therefore, this study is a logical extension to the previous studies.

4.5.2 Description Of The Boundary Conditions and Simulation

The experimental conditions of Barchilon and Curtet [43] were modelled in this study. The jet and duct diameter were 0.16 and 0.012 meters, respectively. Table 4.4 shows three cases that were modelled with information on the $Ct$ number and mean velocity.

Table 4.4: Flow conditions

<table>
<thead>
<tr>
<th>Case</th>
<th>$U_j$ [m/s]</th>
<th>$U_1$ [m/s]</th>
<th>$U_m$ [m/s]</th>
<th>$Ct$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>12.936</td>
<td>0.8448</td>
<td>0.9128</td>
<td>0.976</td>
</tr>
<tr>
<td>2</td>
<td>12.538</td>
<td>0.3981</td>
<td>0.4664</td>
<td>0.506</td>
</tr>
<tr>
<td>3</td>
<td>12.962</td>
<td>0.0742</td>
<td>0.1467</td>
<td>0.152</td>
</tr>
</tbody>
</table>

Figure 4-10(a) illustrates the geometric configuration used in the numerical model. The duct’s length was set to 1.6 meters, which is at 10 duct diameters from the inlet. At this length, the flow was assumed to be fully developed. Furthermore, a two-dimensional flow was considered, thus, a 15-degree circular wedge was used with symmetry conditions at the two sides of this wedge. Three grids were generated and grid sensitivity test was done. The grids shown in Figure 4-10(b), (c) and (d) consisted of 8991, 12879 and 68781 nodes, respectively.

Four types of boundary conditions were used in the numerical model: Inlet, symmetry,
Figure 4-10  (a) Geometric representation of model and cross-sectional view of the mesh used in (b) coarse, (c) fine, and (d) embedded grids
wall and outlet. For the inlet condition, a uniform velocity profile was set for both the jet and coflow, depending on the case investigated. The turbulence quantities $T_u$ and $L_e$ were specified at values of 0.05 and 0.01 m, respectively, across the duct inlet. A no-slip wall condition was set at the walls of the ducts. The first node closest to the wall was positioned at an appropriate $y^+$, in agreement with the log-law region. Lastly, the outlet boundary condition was given a constant static pressure of 101.325 kPa.

Similar to the previous study, the convergence criterion was set to $10^{-4}$ or less, and the Mass Weighted Skewed (MWS) solver was used for the numerical solution.

4.5.3 Results

The grid dependence on the numerical solution was first examined. Figure 4-11 shows the radial velocity normalized with the mean velocity in the mixing section at a $C_l$ number of

![Figure 4-11 Grid sensitivity test at $C_l = 0.506$ at three $x/D_0$ locations](image-url)
0.506 and at three \( x/D_0 \) locations: 1.75, 2.25 and 4.0. The three grids used in this test are shown in Figure 4-10(b), (c) and (d). The average error between the second and third grid all \( x/D_0 \) locations is less than 2% for a nodal density increase of over five times. Hence, the second grid (Figure 4-10(c)) was used for validation purposes.

The Figure 4-12 shows the variation in the predicted and experimental [43] centerline velocity \( U_{cl} \) with respect to \( x/D_0 \) and \( C_t \) number. Near the entrance region, the numerical model is unable to predict well the existence of a potential core for all three cases. In the potential core the centerline velocity is constant, as was described in the two previous studies. Since the inlet boundary condition affects the overall predictions, a better specification would be needed. Zhu et al. [44] introduced the parabolic entrance region (PER) scheme, which allowed the fine resolution of the initial shear layer. This scheme was developed on the assumption that although the whole flow would be elliptic, a small region near the entrance would exist as a parabolic flow. Upon implementation, Zhu et al. [44] improved the prediction of confined jets with minimal computational effort. However, for the current validation study this scheme was not incorporated into the model.

Downstream of the potential core region, the predicted centerline velocity decayed quickly, especially at small values of \( C_t \), which was in agreement with the experimental data. For \( C_t = 0.976 \), the numerical solution underestimated the velocity up to \( x/D_0 \) of about 2. and overestimated the velocity at \( x/D_0 > 2 \). At this \( C_t \) value, no recirculation occurs [43]. For \( C_t = 0.506 \) and 0.152, the numerical solution underestimated the centerline velocity. At those \( C_t \) values, a recirculation zone is present [43].

In order to get a better understanding of the predicted velocity field, the velocity profiles for the three cases along with the experimental data points were plotted. Figure 4-13 shows the
Figure 4-12  Centerline velocity decay of a confined coflow jet
Figure 4-13  Axial mean velocity profiles of a confined coflow jet
radial velocity profiles at four $x/D_0$ locations: 0.375, 1.125, 1.875 and 2.50. At $x/D_0 = 0.375$, the numerical model gave very close predictions of the coflow and wall boundary layer for all $Ct$ values. Furthermore, the centerline velocity was underpredicted and the width of the jet was overpredicted. Thus, the half-radius of jet was overestimated. At $Ct$ values of 0.506 and 0.152, backflow was evident from the numerical predictions and experimental data. At $Ct = 0.506$, the numerical solution underpredicted the centerline velocity as well as the backflow region, however, at $Ct = 0.152$ it overpredicted the backflow region.

Overall, the numerical model underpredicted the centerline velocity and overpredicted the jet's half-radius. In addition, backflow is not predicted adequately. These discrepancies can be attributed to the isotropic nature of the $k$-$\varepsilon$ turbulence model, which cannot handle reverse flows appropriately.

4.6 Jets In A Crossflow

4.6.1 Description Of The Problem

This validation study focuses on non-reacting jet mixing in a cylindrical duct. A circular jet of diameter $D_j$ and velocity $V_j$ entering perpendicularly into a duct of diameter $D_m$ and velocity $U_m$ has a momentum flux ratio defined by (see Chapter 2),

$$ J = \frac{\rho_j V_j^2}{\rho_m V_m^2} $$

(4.16)

which is the ratio of the momentum of the jet to the momentum of the mainstream. In Chapter 2 it was shown that the key parameters affecting the fluid mixing are the momentum flux ratio, orifice shape and the number of orifices employed. For non-reacting flows, the conserved scalar
used to describe mixing is the temperature field or the normalized temperature field, which called the mixture fraction and is expressed as,

\[ f = \frac{T - T_j}{T_m - T_j} \]  

(4.17)

where, \( f = 1 \) represents the mainstream and \( f = 0 \) represents the jet flow.

In this study, the mixing effectiveness will be investigated. To quantify the mixing effectiveness, an area-weighted standard deviation of mixture fraction (AMIX) and a mass-weighted standard deviation of temperature (\( \sigma_T \)) will be calculated at every streamwise location in the cross-sectional plane of the duct. The former is known as the mixture non-uniformity and is defined as,

\[ AMIX = \sqrt{\frac{1}{A} \sum_{i=1}^{N} a_i (f_i - f_{equil})^2} \]  

(4.18)

where, \( A = \sum a_i \) is the cross-sectional area, \( f \) represents the mixture fraction calculated for each node \( i \), and \( f_{equil} \) is the equilibrium or fully-mixed value of the mixture fraction. The latter is defined as,

\[ \sigma_T = \sqrt{\frac{\sum_i \dot{m}_i (T_i - T_{avg})^2}{\sum_i \dot{m}_i / T_{avg}}} \]  

(4.19)

where, \( T_i \) and \( \dot{m}_i \) are the temperature and mass flow ratio in each computational node \( i \). Complete mixing would be achieved when the values of AMIX and \( \sigma_T \) across the plane would approach zero.

In addition, the mixing performance will be compared to Holdeman's [7] equation for the optimum momentum flux ratio \( J_{opt} \) as a function of number of orifices \( n \) that is expressed as,
where, \( C = 2.5 \). This equation was presented earlier in Chapter 2.

### 4.6.2 Description Of The Boundary Conditions and Simulation

The numerical model was validated against the experimental results of Hatch et al. [3]. The geometric configuration is shown in Figure 4-14(a). The mixing section was modelled as a constant diameter cylindrical duct with a single row of eight equally spaced circular orifices. The radius of the duct was set to 38.1 mm and the length of the duct was set to four jet radii downstream and 2.5 jet radii upstream from the leading edge of the jet and from the center of the orifice row, respectively. Note that in the experiment of Hatch et al. [3] the center of the orifice row was placed at one radius from the inlet edge of the mixing section. This dimensional change between the experiment and numerical model will be discussed in the following section.

The jet-to-mainstream mass flow ratio, mainstream flow rate, and jet and mainstream temperatures remained constant. Table 4.5 shows the operating conditions used in the numerical model. In the above table, \( DR \) represents the density ratio and \( MR \) is the mass ratio. Furthermore, nine cases were modelled with detailed dimensions and flow rates provided in Table 4.6.
Figure 4-14 (a) Geometric configuration of the mixing section, and (b) a streamwise and cross-sectional view of the computational grid.
Table 4.6: Flow conditions and dimensions

<table>
<thead>
<tr>
<th>Case</th>
<th>(V_{\text{jet}}) [m/s]</th>
<th>(D_{\text{jet}}) [mm]</th>
<th>Mom. Flux Ratio, (J)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>27.21</td>
<td>22.13</td>
<td>8.5</td>
</tr>
<tr>
<td>2</td>
<td>36.85</td>
<td>19.01</td>
<td>15.5</td>
</tr>
<tr>
<td>3</td>
<td>38.72</td>
<td>18.55</td>
<td>17.1</td>
</tr>
<tr>
<td>4</td>
<td>41.86</td>
<td>17.84</td>
<td>20.0</td>
</tr>
<tr>
<td>5</td>
<td>48.36</td>
<td>16.57</td>
<td>26.7</td>
</tr>
<tr>
<td>6</td>
<td>55.82</td>
<td>15.45</td>
<td>35.6</td>
</tr>
<tr>
<td>7</td>
<td>59.56</td>
<td>14.96</td>
<td>40.5</td>
</tr>
<tr>
<td>8</td>
<td>69.66</td>
<td>13.83</td>
<td>55.4</td>
</tr>
<tr>
<td>9</td>
<td>85.88</td>
<td>12.45</td>
<td>84.2</td>
</tr>
</tbody>
</table>

Since the overall mass flow ratio of jet to crossflow was kept constant, the orifice dimension also changed with the momentum flux ratio. Thus, for every case considered the grid system was changed.

Figure 4-14(b) shows the computational grid used in the numerical model. Note that the grid looks coarse at the axial location of the orifice. This was done in order to clearly illustrate the shape of the orifice, however, it does not represent the actual grid used for the analysis. Due to the symmetry of the radial jets, the computational domain covered only one-quarter of the cylindrical duct, that is a 90-degree sector. The grid density increased near the orifices and the wall in order to account for the high velocity and temperature gradients in these areas. In the cross-section of the duct a butterfly grid was generated, and grid sensitivity was tested using five meshes with a total of 87360, 172431, 260015, 332948 and 355320 nodes.

Four types of boundary conditions were used in the numerical model: Inlet, wall, symmetry and outlet. For the inlet condition, a uniform velocity profile was set at the inlets of the jet and mainstream with values listed in Table 4.6. The turbulence intensity and length scale were specified respectively as 0.05 and 0.01 m for the mainstream and 0.10 and 0.001 m for the jet flow. Smooth, no-slip and adiabatic boundary conditions were applied at the outer wall of the
duct and symmetry boundary conditions were applied in the radial direction along the duct. For the outlet condition, a constant static pressure of 101.325 kPa was specified.

Similar to the previous study, the convergence criterion was set to $10^{-4}$ or less, and the Mass Weighted Skewed (MWS) solver was used for the numerical solution.

4.6.3 Results

Grid sensitivity was first examined using a test case with $J = 84.2$. Figure 4-15 shows a sensitivity of $\sigma_T$ to grid density with respect to three streamwise locations. As can be seen, there is little change in $\sigma_T$ for the computational domain considered at all $x/R$ locations. However, the grid with the 332948 nodes was chosen since it had an average of less than 1% change in $\sigma_T$ compared with the grid that had the maximum number of nodes (355320). Since each case in this study needed a different grid system, the grid densities in all the cases were in the range of $332948 \pm 15000$.

![Figure 4-15 Grid sensitivity test at $J = 84.2$](image)
Two different methods were used to present the numerical results and compare them with the measured data. In the first method, qualitative analysis of the results was done by visual observation of the mixture fraction field. In the second method, the mixing performance was evaluated using statistical area- and mass-weighted deviations, that is, equations (4.18) and (4.19), respectively.

Figure 4-16 shows the variation in mixture fraction plots in the plane of the jet with respect to the momentum flux ratio. The three characteristics of jet penetration into a crossflow can be seen from this figure, as was described in Chapter 2. At $J = 8.5$, it can be seen that the jet underpenetrates since the jet flows nears the wall and a relatively unmixed mainstream core continues downstream. For $J = 15.5$ and 20.0, the mixture fraction field indicates that the jet approaches or is at optimum penetration since the jet mixes well with the mainstream flow. Although, at $J = 20$ the jet mixes with the mainstream in the shortest downstream distance. At $J = 26.7$ and 40.5, the jet overpenetrates since there is a recirculation region upstream of the impinging jets. Hence, this causes undesirable upstream mixing and mainstream blockage effects. As the momentum flux ratio increases the upstream mixing region increases as well. For this reason, the upstream distance from the centerline orifice row was increased to $x/R = 2.5$, in order to properly apply the inlet boundary condition for the numerical model at $J = 84.2$.

Figure 4-17 shows the numerically predicted mixture fraction field in various cross-sectional planes and with variations in the momentum flux ratio. From this figure it can be seen that the mixture fraction $f$ decreases at the central axis with increasing momentum flux ratio. which indicated an increase in jet penetration towards the center. At $J = 8.5$, jet underpenetration forms a relatively unmixed mainstream core that does not interact with the jets. At $J = 15.5$ and 20.0, the mixture fraction fields are similar and well mixed. From this figure, it is evident that $J$...
Figure 4-16  Mixture fraction plots in the plane to the jet in the range of $-1.67 < x/R < 2.0$ for various momentum flux ratios that given on the left side.
Figure 4-17  Mixture fraction plots in the cross-sectional plane of the duct for various \( x/R \) locations and momentum flux ratios.
= 20.0 approaches uniform and hence optimum mixing. Overpenetration is apparent for both $J = 26.7$ and 40.5 from the upstream mixing at $x/R = -0.06$ and from the large portion of jet flow in the vicinity of the central axis at $x/R = 1.0$, which causes a reduction in circumferential mixing along the walls. Furthermore, at $x/R = 1.0$ the radial mixture fraction distributions indicate an increase in $f$ from the central axis to the wall for the overpenetration cases. On the other hand, a decrease in $f$ from the central axis to the wall is shown for the underpenetration case at $x/R = 1.0$. This behaviour does not hold for the cases that approach optimum mixing, that is, at $J = 15.5$ and 20.0. This figure also shows that the numerical model is able to obtain the characteristic kidney-shaped jet profile.

The comparison of the experimentally measured data and numerically predicted results is shown in Figure 4-19. In this figure, equation (4.18) was used to calculate the area-weighted standard deviation of mixture fraction, where $f_{equil}$ was estimated to be 0.3125 [3]. It is important to note that the experimental data contained 50 points per 90-degree plane and an illustration of the measure points is provided in Figure 4-18.

![Figure 4-18 Experimental data points](image-url)
Figure 4-19  Mixing non-uniformity comparison between the numerical solution and experimental data using a (a) normal, and a (b) 50-point mesh
Figure 4-20 Mixing effectiveness predictions as a function of momentum flux ratio with respect to (a) mixture non-uniformity, and (b) $\sigma_T$. 
In Figure 4-19(a), all the computational nodes in the cross-sectional plane $x/R$ were used to calculate the mixture non-uniformity. The comparison indicates that the numerical model predicted less mixing for the same $x/R$ location and that mixing has improved with an increase in momentum flux ratio. The experimental results indicated that initially ($x/R < 0.3$) the high $J$ case was better mixed, but at $x/R > 0.3$ the low $J$ case was better mixed. This was anticipated experimentally and analytically since the optimum $J$ for eight right holes is 20.3 (see equation (4.20)) and $J = 26.7$ and 84.2 represent jet overpenetration. Thus, one would expect that as you increase $J$ the mixing would worsen. However, the numerical model is able to predict well the slopes of each curve along the duct.

The discrepancy between the predicted and measured results can be attributed to three factors. First, the upstream distance from the orifice centerline plays an important factor in initial mixing. Since in the experiment the upstream distance was fixed at $x/R = 1$, the jet was forced to mix completely with the mainstream, especially at $J = 84.2$. This explains why at $J = 84.2$ the mixture non-uniformity was lower than $J = 26.7$ starting from the leading edge of the jet. In the numerical model, the upstream distance was chosen so that the backflow would not influence the mainstream inlet condition. Secondly, the jet velocity entering the mixing section was non-uniform in the experiment. However, a uniform velocity at the jet inlet was assumed in the numerical model. This could greatly affect the jet penetration and mainstream flow and hence, change the temperature and velocity fields [1,15]. And thirdly, with only 50 measurement points per plane (see Figure 4-18), the experiment was unable to resolve the large gradients in the temperature distribution present in the vicinity of the jet entrance. Thus, the measured temperature distribution appeared more uniform, yielding lower mixture non-uniformity values. Figure 4-19(b) shows a comparison of the experimental data with the predicted results have only
50 nodes per plane, with the same node location as indicated in Figure 4-18. From this figure, it can be seen that the predicted mixture non-uniformity values are lower than those in Figure 4-19(a), as anticipated. Note that at $x/R = 0.34$, the two curves are almost in contact with each other. This is also seen in the experimentally measurement at $x/R = 0.30$, where the two curves intersect each other.

The mixing performance was also compared to Holdeman’s [7] correlation equation (4.20), where the optimum momentum flux ratio for eight round hold is 20.3. Figure 4-20 shows the numerical predictions of area- and mass-weighted standard deviations for all cases as a function of $J$. Both Figure 4-20(a) and (b) indicate an optimum $J$ value of 15.5 at four $x/R$ locations, where optimum mixing corresponds to the lowest deviation. Thus, the numerical predictions are close to the correlated value of $J_{opt} = 20.3$. At $J = 20$, the numerical model predicted a jet overpenetration, which would indicate that for the same momentum flux ratio the predicted temperature gradients would be greater than the measured results. This is caused by the assumption of uniform velocity profile.

In Figure 4-20(b), the minimum $\sigma_T$ occurs in the range $15.5 < J < 20.0$ at $x/R =1$. This indicates that it is relevant to investigate other downstream locations in order to get consistent mixing properties. In addition, a sensitivity test for downstream distance was performed in order to determine whether the predictions were influenced by the outlet condition, which was forced to behave as a fully developed flow. Hence, the downstream distance was increased by a factor of 2.5, that is to $x/R = 10$ from the orifice leading edge, and the test was ran at $J = 15.5$. It was found that the $AMIX$ and $\sigma_T$ varied by less than 2% at $x/R = 1$ to 4. Hence, the predictions were not influenced by the outlet distance.
4.7 Summary

The six validation studies examined the numerical model’s ability to predict simplest to complicated flows.

In the laminar validation study, the numerical model was able to predict with great accuracy the velocity profile and pressure drop. This confirmed that the model conserved both mass and momentum. In the turbulent validation study, the velocity profile and pressure drop were predicted with 5% and 8% errors respectively.

In both studies, the effect of grid type and working fluid were examined. The butterfly grid was found to yield the lowest errors for the same grid density. The accuracy of the results was found to be independent of the working fluid.

For a jet in quiescent surroundings, the numerical model was able to predict closely the jet’s half radius to about 13.3%. For a jet in a coflow, the numerical model was unable to predict well the jet’s centerline velocity and its half-radius. The prediction errors involved at all axial locations and at two velocity ratios ranged between 25 to 40%. Similar predictions were observed for a jet in a confine flow. In this flow a recirculation region was also present but was not correctly modelled. The discrepancies in all of these studies are mainly attributed to the lack of the $k$-$\varepsilon$ turbulence model to predict non-isotropic flows.

In the jet in a crossflow validation study, the numerical model provided good qualitative agreement with the experimental measurements. However, larger temperature gradients were predicted for the same momentum flux ratio. Thus, less mixing was predicted and the optimal mixing was slightly underpredicted.
5 Reacting Flow Studies

This chapter deals with the numerical modelling of jets in a confined reacting crossflow. The geometric configuration presented in the experiment by Popovic et al [19] was used in this study. In the numerical solution, two well-known combustion models, non-premixed flamelet model and eddy dissipation model, were used to assess flow field characteristics, such as mixture fraction, CO and H₂ concentrations and temperature. The purpose was to investigate whether existing models are able to predict emissions and combustion efficiency.

5.1 Description of Experiment

Popovic et al [19] conducted experiments of multiple jet mixing with a confined crossflow. The experimental facility shown in Figure 5-1 consists of four major parts: Fuel-air mixer, primary reactor, mixing module and exhaust tube. Methane and air were combined in the fuel-air mixer at a constant equivalence ratio, φ, of 1.5. At the primary reactor the fuel and air reacted and mixed well, yielding a hot fuel rich mixture to the mixing module. A thermocouple

Figure 5-1  Experimental facility (from Popovic et al. [19])
measuring the reactor exhaust temperature was placed two pipe diameters downstream of the reactor. From this point on, the pipe was insulated and this measured temperature represented the inlet boundary condition of the rich fuel mixture. In addition, the ceramic foam dissipated the flow and mixture non-uniformities before the mixture reached the mixing module.

The mixing module consisted of outer and inner glass (quartz) cylinders enclosed by two stainless steel plates. The length and diameter of the mixing module were 305 mm and 95 mm, respectively, and the diameter of the inner cylinder was 25.4 mm. Secondary air was supplied to the mixing module through a chamber filled with steel wool, which was used as a flow straightener. Within the outer cylinder, the temperature of the secondary air was measured at a position that was aligned with the center of the gap opening. This measured temperature represented the inlet boundary for the jets.

The exhaust tube was made of quartz and had a length of 1219.2 mm. The fluid temperature was measured at the centerline of the tube at 48 diameters downstream of the gap axis.

Four round orifices were modelled in this study. For this configuration, the inner glass cylinder in the mixing module was replaced by a combination of an insulated stainless steel module that was attached to the base plate and a quartz tube that slid thorough the groove in the steel module. Table 5.1 shows the geometric dimension and operating conditions in the mixing module for the case modelled.

<table>
<thead>
<tr>
<th>Number of jets</th>
<th>d_{jet} [mm]</th>
<th>\dot{m}_{fuel} [g/s]</th>
<th>T_{fuel} [K]</th>
<th>T_{air} [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>7</td>
<td>3.9</td>
<td>1370</td>
<td>438</td>
</tr>
</tbody>
</table>

**Table 5.1:** Experimental parameters used in this study
5.2 Laminar Flamelet Solution

5.2.1 Description Of The Boundary Conditions and Simulation

A grid was generated for a cylindrical duct of diameter \( D = 25.4 \) mm with four circumferential circular orifices having a diameter \( d = 7 \) mm. Figure 5-2 illustrates the geometric configuration and grid that were used to run the numerical simulation. According to the experiment, the initial length of the duct was set to four duct diameters upstream of the leading edge of the orifices. However, the duct's downstream length was shortened to 35 instead of 48 duct diameters from the leading edge of the orifices. This was done in order to reduce the number of computational nodes required to ensure that the grid meets the limitations on aspect ratio and skewness. Examining CO concentrations and temperature along the centerline axis for various air-to-fuel flow ratios confirmed that at \( x/D = 35 \) the flow was fully developed and the reaction completed. Thus, it was concluded that the numerical solution would yield the same predictions for \( x/D = 35 \) as it would if the duct was lengthened to \( x/D = 48 \), as in the experiment.

Figure 5-2(b) shows the computational grid used in the numerical model. Due to the symmetry of the radial jets, the computational domain covered only one-quarter of the cylindrical duct, that is a 90-degree sector. In the cross-sectional plane of the duct a butterfly grid was generated. Note that grid sensitivity test was not done for reasons that are discussed in section 0. For all the cases that were considered, the grid layout remained the same with a total of 133,875 nodes.

Four types of boundary conditions were used: Inlet, wall, symmetry and outlet. For the inlet condition, uniform velocity, temperature and scalar concentration profiles were specified for both the jets and crossflow boundaries. For the crossflow inlet, the turbulence intensity and
Figure 5-2  (a) Geometric configuration of the duct, and (b) a streamwise view of the duct with a cross-sectional view of the computational grid
length scale were set equal to 0.05 and 0.01 m, respectively, and for the jet inlet it was set to 0.10 and 0.007 m, respectively. Smooth, no-slip and adiabatic boundary conditions were applied at the outer wall of the duct and symmetry boundary conditions were applied radially along the duct. For the outlet condition, a constant static pressure of 101.325 kPa was specified.

Since the flamelet combustion model was used, three new parameters were added. Firstly, the crossflow inlet was specified as the fuel component, while the jet inlet was specified as the oxidizer component for the purpose of this model. Secondly, the mixture fraction scalar equation was set to a value of 1 and 0 at the fuel and oxidizer boundary conditions, respectively. Lastly, the mixture fraction variance was set equal to zero for both the fuel and oxidizer. The last two parameters were read automatically from the flamelet library information file that accompanied the flamelet library and the first parameter was a required input to the program.

Five cases with different air-to-fuel flow rates were investigated. For all cases, the fuel and air temperature and the fuel flow rate remained constant with values given in Table 5.1. The fuel flow rate value was changed into a velocity for the boundary condition specification using the duct's quarter area and a density based on the equation of state. Hence, the fuel velocity was found to be 29.7 m/s. In addition, the fuel entered the duct with an overall equivalence ratio of 1.5, which accounted for the upstream reaction of methane with air in the experiment. At this equivalence ratio, the equilibrium concentrations of all species involved were determined using a program called STANJAN [45], which calculates the equilibrium species concentrations at a given temperature and pressure. At a temperature of 1370 K and a pressure of 103.325 kPa, five major species come out from the reaction of methane-air: Carbon monoxide (CO), hydrogen (H₂), carbon dioxide (CO₂), water (H₂O) and nitrogen (N₂). The equilibrium mole and mass fractions of those species at the conditions mentioned above are shown in Table 5.2. Note that
those species make up the hot fuel mixture. The air jets consisted of 21% O₂ and 79% N₂ based on molar fraction or 23.3% O₂ and 76.7% N₂ based on mass fraction. In the numerical model, the species concentrations were entered in terms of mass fraction.

Table 5.2: Mole and mass fractions of the hot fuel mixture

<table>
<thead>
<tr>
<th></th>
<th>CO</th>
<th>H₂</th>
<th>CO₂</th>
<th>H₂O</th>
<th>N₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mole</td>
<td>0.070045</td>
<td>0.096344</td>
<td>0.054747</td>
<td>0.15324</td>
<td>0.62562</td>
</tr>
<tr>
<td>Mass</td>
<td>0.078946</td>
<td>0.0078152</td>
<td>0.096950</td>
<td>0.11109</td>
<td>0.70520</td>
</tr>
</tbody>
</table>

Table 4.6 summarizes the different flow conditions used in the numerical model. The overall equivalence ratio was calculated from the following expression [46],

\[
\phi = \frac{\dot{m}_{\text{Fuel}}}{M_{\text{Fuel}}} \frac{[4\text{CO} + 2\text{H}_2 + 4\text{CO}_2 + 2\text{H}_2\text{O}]}{2[\text{CO} + 4\text{CO}_2 + 2\text{H}_2\text{O}]}_{\text{Fuel}} + \frac{\dot{m}_{\text{Air}}}{M_{\text{Air}}} \frac{[4\text{O}_2]}{[4\text{CO} + 2\text{H}_2\text{O}]}_{\text{Air}}
\]  

(5.1)

where the subscripts of fuel and air represent the concentrations at the fuel and air inlets, respectively. In the above equation, \( M_{\text{Fuel}} \) and \( M_{\text{Air}} \) represent the molar mass of fuel and air, which are equal to 24.85 kg/kmol and 28.85 kg/kmol, respectively. For all cases, the numerical model used the equation of state to calculate the mean density of the fluid.

Table 5.3: Flow conditions and dimensions

<table>
<thead>
<tr>
<th>Case</th>
<th>( V_{\text{jet}} ) [m/s]</th>
<th>Mom. Flux Ratio, J</th>
<th>( \phi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>17.361</td>
<td>1.24</td>
<td>0.882</td>
</tr>
<tr>
<td>2</td>
<td>37.792</td>
<td>5.88</td>
<td>0.594</td>
</tr>
<tr>
<td>3</td>
<td>75.0</td>
<td>23.2</td>
<td>0.373</td>
</tr>
<tr>
<td>4</td>
<td>120.0</td>
<td>59.3</td>
<td>0.257</td>
</tr>
<tr>
<td>5</td>
<td>170.0</td>
<td>119.0</td>
<td>0.191</td>
</tr>
</tbody>
</table>

Note that \( J \) was calculated without taking into account the discharge coefficient \( C_d \) of the orifice since uniform velocity profiles were used (i.e., \( C_d = 1 \)). Consequently, the experiment and numerical model yielded the same \( \phi \) but different \( J \) since \( \phi \) is independent of \( C_d \) and \( J \) is
dependent on $C_d$. For example, for a fixed $\phi = 0.9$ the experimentally calculated $J$ was equal to about 2.5, while the numerical model yielded a value of 1.2. This difference is attributed to the experimental assumption used for $C_d$.

The convergence criterion was set to $10^{-4}$ or less for all the mass, momentum, energy and scalar equations. In addition, the Mass Weighted Skewed (MWS) discretization was used for the numerical solution.

The numerical model was run twice for each case. The first run converged the scalar, energy, U-momentum and mass equations with a time step of $1.0E-3$. The second run converged the V- and W-momentum equations with a time step of $1.0E-5$.

### 5.2.2 Flamelet Library

The laminar flamelet model provides species and temperature as a function of mixture fraction and its variance. It uses a flamelet library to determine species mass fractions instead of solving for them. The numerical model calculates a mean scalar dissipation rate (see Chapter 3) from the turbulent kinetic energy and its dissipation and then uses this value along with the mixture fraction value to interpolate the correct flamelet species concentrations from the flamelet library tables. The flamelet solution retrieved, therefore, depends on the fluid flow as well as mixture properties.

In this study, two libraries were generated that allowed for different temperature boundary conditions for the fuel.

#### 5.2.2.1 Generation of Base (Laminar) Libraries

A program to generate flamelet profiles was provided upon request by AEA Technology. This program simulated a diffusion flame by solving a detailed chemical kinetic mechanism. A
counterflow geometry is used with fuel at one end and air at the other. This results in a stagnation point flow. The chemical mechanism consists of ten species and 18 reactions. Table 5.4 lists the chemical reactions that were incorporated into the program.

### Table 5.4: Chemical mechanisms

<table>
<thead>
<tr>
<th>Reaction Type</th>
<th>Reactions</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2-O2 Mechanism</td>
<td>H2-O2 Chain Reactions</td>
</tr>
<tr>
<td></td>
<td>O2 + H ⇄ OH + O</td>
</tr>
<tr>
<td></td>
<td>H2 + O ⇄ OH + H</td>
</tr>
<tr>
<td></td>
<td>H2 + OH ⇄ H2O + H</td>
</tr>
<tr>
<td></td>
<td>OH + OH ⇄ H2O + O</td>
</tr>
<tr>
<td></td>
<td>HO2 Formation/Consumption</td>
</tr>
<tr>
<td></td>
<td>H + O2 + M' ⇄ HO2 + M'</td>
</tr>
<tr>
<td></td>
<td>HO2 + H → OH + OH</td>
</tr>
<tr>
<td></td>
<td>HO2 + H → H2 + O2</td>
</tr>
<tr>
<td></td>
<td>HO2 + OH → H2O + O2</td>
</tr>
<tr>
<td></td>
<td>HO2 + H → H2O + O</td>
</tr>
<tr>
<td></td>
<td>HO2 + O → OH + O2</td>
</tr>
<tr>
<td></td>
<td>H2O2 Formation/Consumption</td>
</tr>
<tr>
<td></td>
<td>HO2 + HO2 → H2O2 + O2</td>
</tr>
<tr>
<td></td>
<td>OH + OH + M' ⇄ H2O2 + M'</td>
</tr>
<tr>
<td></td>
<td>H2O2+ H → H2O + OH</td>
</tr>
<tr>
<td></td>
<td>H2O2+ OH ⇄ H2O + HO2</td>
</tr>
<tr>
<td></td>
<td>Radical Recombination</td>
</tr>
<tr>
<td></td>
<td>H +H +M' → H2 + M'</td>
</tr>
<tr>
<td></td>
<td>OH +H +M' → H2O + M'</td>
</tr>
<tr>
<td></td>
<td>O +O +M' → O2 + M'</td>
</tr>
<tr>
<td>CO/CO2 Mechanism</td>
<td>CO-CO2 Reaction</td>
</tr>
<tr>
<td></td>
<td>CO +OH ⇄ CO2 + H</td>
</tr>
</tbody>
</table>

where, M' = CO2, CO, N2, H2O and O2, respectively.

Fuel and air boundary conditions were the same as the one simulated in the numerical model. The species concentrations were entered in mole fraction with values listed in Table 5.2. The temperature was set to 1370 K for the first library and 1200 K for the second library. Air temperature was specified as 438 K. In addition, the input pressure was set to 101.325 kPa.
The base libraries contained all the species originally in the chemical mechanism at various strain rate steps up to flame extinction. Each library ensured a maximum temperature difference of no more than 30 degrees. This was confirmed by tabulating quantities that were given at the end of the program's execution, and consisted of the strain rate, maximum temperature and scalar dissipation rate. Near flame extinction, the relationship between strain rate and scalar dissipation rate becomes non-linear and it is usually accompanied by sharp drop in maximum temperature. The behaviour of scalar dissipation rate and maximum temperature is illustrated in Figure 5-3 for the two libraries. $T_{fuel} = 1370$ K is the actual inlet temperature of the fuel used in the numerical model, and $T_{fuel} = 1200$ K is the temperature of the fuel used in the flamelet generation for purposes that will be discussed in 0. As can be seen from this figure, at

![Figure 5-3](image-url)
$T_{\text{fuel}} = 1370 \text{ K}$, the fuel extinguishes at a strain rate of about 10000 l/s where the maximum temperature becomes the fuel temperature and the scalar dissipation experiences non-linear behaviour. At $T_{\text{fuel}} = 1200 \text{ K}$, the fuel extinguishes at a strain rate approximately 6000 l/s where the maximum temperature drops sharply. Notice that the high-temperature fuel extinguishes at a higher strain rate and scalar dissipation rate than the lower temperature fuel. Furthermore, the program was able to continue to run at much higher strain rates for the high-temperature fuel. However, the program did not converge beyond a strain rate of 6000 l/s for the low-temperature fuel and the last successful solution was taken to be the extinction point.

5.2.2.2 Reduction of Base Libraries

Some of the species in the base libraries turned out to exist in very small quantities. Those species could therefore be neglected. By manually looking through the libraries, H$_2$O$_2$ and HO$_2$ were found to have zero concentrations at all strain rates. Hence, the new reduced libraries consisted of eight species: CO, H$_2$, CO$_2$, H$_2$O, O$_2$, H, O and OH. The reduction in the number of species reduces execution time of the program for the final combined library. As a result, the computation time for the numerical model will also be shortened since fewer species will have to be looked up in the library.

5.2.2.3 Generation of Final Library

An extra base library that considered the equilibrium (also known as the Burke-Schumann) solution was added to the rest of the libraries. This base library provided the zero strain rate solution for the fuel mixture. A new program was executed which integrated the mixture fraction values for various strain rates over a beta-PDF and combined all the base libraries into one large file. This file was the final flamelet library. The purpose of the program
was to generate a mixture fraction field for each library that accounted for a Lewis number not equal to one, that is, unequal thermal and molecular diffusivities. This effect is not included when the numerical model solves for the mixture fraction equation, since the formulation of this equation assumes that $Le = 1$ (see Chapter 3).

Inside the library, flamelet tables were ordered by increasing mixture fraction, strain rate and mixture fraction variance. Figure 5-4 illustrates how the numerical model used this library to obtain species concentrations.

![Diagram](image)

**Figure 5-4** Connection between the numerical model and flamelet library
5.2.3 Results

The five cases in Table 4.6 were ran using a flamelet library with $T_{fuel} = 1370$ K. Carbon monoxide concentrations are normalized with the concentration of CO due to dilution, which is available at the inlet to the duct, and is defined as,

$$\frac{[CO]}{[CO]_d} = \frac{[CO]}{[CO]_i \cdot Z} \quad (5.2)$$

where, $Z$ represents the mixture (dilution) fraction and the subscript $i$ represent the inlet to the duct.

Figure 5-5 shows the normalized carbon monoxide (CO) plot of the numerical model and the experiment [19] at the outlet of the duct. An increase in equivalence ratio means that less air is available for the reaction, that is, the mass flow through the jet is reduced and vice versa. For

![Figure 5-5](image-url)  

**Figure 5-5**  Comparison of carbon monoxide concentrations at outlet
all cases, the reaction occurred at fuel lean conditions. As can be seen from the figure, the
numerical model predicts that CO increases with equivalence ratio, \( \phi \), for the entire range of \( \phi \) considered. This contradicts the experiment, which shows an optimum CO at an equivalence ratio of about 0.785. Above this value there is an increase in CO due to lack of air for the reaction. Below this value an increase in CO is thought to be due to the increased strain on the flame sheet which causes local extinguishing and thus instabilities in the body of the flame. The flamelet model is able to predict high CO concentrations from a \( \phi \geq 0.78 \) as in the experiment; however, at \( \phi \leq 0.78 \) the model predicts that even more CO is consumed by the chemical reaction. This result is non-physical since there will be a point where the flame will be extinguished by the large velocity gradients near and at the jets' entrance as the jet mass flow increases. This will result in high CO concentrations. Thus, the flamelet model is unable to predict flame extinguishing or blow-off.

CO destruction efficiencies were also calculated from the numerical solution and are shown in Table 5.5. The CO destruction efficiency is defined as,

\[
\eta = \left( 1 - \frac{[CO]}{[CO]_d} \right) \times 100\% 
\]

Table 5.5 shows that CO destruction improved with an increase of momentum flux ratio.

<table>
<thead>
<tr>
<th>Momentum Flux Ratio, J</th>
<th>CO Destruction Efficiency, ( \eta ) [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.24</td>
<td>99.34407</td>
</tr>
<tr>
<td>5.88</td>
<td>99.99520</td>
</tr>
<tr>
<td>23.16</td>
<td>99.99986</td>
</tr>
<tr>
<td>59.30</td>
<td>99.99995</td>
</tr>
<tr>
<td>119.0</td>
<td>99.99997</td>
</tr>
</tbody>
</table>
In order to further examine jets in a reacting crossflow characteristics, contour plots were created for six scalars: Mixture fraction, its variance, scalar dissipation rate, turbulent kinetic energy, normalized temperature and normalized CO concentrations. Figure 5-6 through Figure 5-9 show those scalars in the plane of the jet from \(-0.86 < x/D < 4.99\). These figures indicate jet penetration behaviours similar to those predicted for non-reacting flows. This can be seen from the mixture fraction and normalized temperature plots. At \(J = 1.2\), the jet underpenetrates and consequently the mainstream is influenced by the jet flow after a few duct diameters downstream of the jet. To get a well mixed flow at this condition will required a very long duct. At \(J = 5.9\), the jet reaches optimum penetration and the mixture is well mixed. At \(J = 23.2\), the jets penetrate deeper towards the center of the duct and backflow can be observed. At this condition the jet overpenetrate causing unmixed regions near the wall downstream of the jet. Further increase in \(J\) indicates a greater jet penetration and backflow. Notice that the normalized temperature plot follows the mixture fraction pattern very closely. Consequently, jet behaviour can be determined from either one, even though temperature is not a conserved scalar.

Figure 5-6 - Figure 5-9 also show that mixture fraction variance \(\tilde{Z}^*Z^2\) and scalar dissipation rate \(\tilde{\chi}\) exhibit similar patterns for all cases considered, where \(\tilde{\chi}\) was introduced in Chapter 3 as,

\[
\tilde{\chi} = 2.0 \left( \frac{\bar{e}}{k} \right) \tilde{Z}^*Z^2
\]

It can be seen that at the maximum \(\tilde{Z}^*Z^2\) location, \(\tilde{\chi}\) is also a maximum or near maximum. This is anticipated since the relationship between the two parameters is linear. However, the turbulent kinetic energy \(k\) contour plot does not seem to be inversely proportional to \(\tilde{\chi}\) as indicated by the above equation. One would expect that the increase in turbulence would act to reduce the \(\tilde{Z}^*Z^2\)
and thus smooth the mixture fraction field. This does not seem to occur in the numerical model. Thus, $\bar{\chi}$ is greatly influenced by the $\bar{Z}^{*2}$ field and only slightly by the turbulence field, especially at large $J$ values.

The normalized CO concentrations indicate similar jet behaviour as was described above. At $J = 1.2$, the jet is located close to the wall, and hence, at the centerline of the duct CO concentrations are high. At $J = 5.9$, the mixing between the fuel and air is improved and reaction occurs close to the wall. As a result, lower CO concentrations are predicted at the outlet. At $J = 23$, the reaction occurs closer to the jet and in the vicinity of the backflow region, yielding even lower CO concentrations at the outlet than at $J = 5.9$. At $J = 119$, the reaction mainly occurs upstream of the jet, where the backflow of the air meets the fuel. There is also a small reaction zone downstream and very close to the jet. It can be seen that within the reaction zones at least 90% of CO concentration is consumed. Other than those regions, the duct consists of air, which reduces even further CO concentrations. At this condition, it is believed that the reaction should be extremely unstable and the flame should extinguish by the large strain rates and the cooling effect of the airflow. This should cause minimal CO destruction. Therefore, the numerical model is unable to predict combustion for this type of flow.

Figure 5-10 - Figure 5-13 display contour plots of jets in a reacting crossflow parameters in the cross-sectional plane of the duct. Similar patterns can be observed when comparing the mixture fraction contour plot with the normalized temperature and normalized CO concentrations. The latter parameter, though, shows a closer resemblance to the mixture fraction pattern than the former. From these plots, jet underpenetration can be observed at $J = 1.2$ at all four $x/D$ locations. The fuel does not interact with the air by $x/D = 2$ in areas such as the central core and part of the wall of the duct. Downstream of this location at $x/D = 5$, mixing starts to
takes place in this plane, although, a much longer distance is required to achieve uniform mixing. At $J = 5.9$, the jet penetrates further towards the central axis and the air interacts well with the fuel by $x/D = 2$. At this location, a major portion of CO has been consumed by the reaction. However, large CO concentrations are present near the wall where the jet was injected. The reaction is nearly completed at $x/D = 5$ with the mixture fraction field approaching a uniform distribution. At $J = 23$ and 119, the jets penetrate deeper toward each other and backflow is evident from the low mixture fraction concentrations at the central core. At $J = 23$, uniform mixing is approached and the reaction is completed with at least 90% CO reduction by $x/D = 5$. At $J = 119$, the mixture fraction as well as the temperature plots indicate that the flow is fully mixed by $x/D = 5$, however, the reaction is completed by $x/D = 1.2$. This suggests that the reaction occurred upstream of this location, in the vicinity of the wall near the jets and in the backflow region upstream of the jets.

The quantities $\tilde{Z}^*^2$ and $\bar{\chi}$ exhibit similar patterns as was discussed for the contour plots in the plane of the jet. The turbulent kinetic energy seems to have a slight correlation to the $\tilde{Z}^*^2$ and $\bar{\chi}$ at $J = 1.2$ and 5.9 for $x/D = 1$ and 2. However, no correlation is observed for $J = 23$ and 119 at all cross-sectional planes. This suggests that at low $J$ the $\bar{\chi}$ is influenced by both the $\tilde{Z}^*^2$ and $k$, while at high $J$ values the $\bar{\chi}$ is only influenced by $\tilde{Z}^*^2$. Low $J$ values correspond to conditions where the jet underpenetrates or reaches optimum penetration, and high $J$ values correspond to conditions where the jet overpenetrates. Hence, the numerical predictions are able to predict qualitatively the decrease in CO concentrations with increase in jet mass flow up to approximately optimum conditions. However, as the jet mass flow is further increased the dependency of $\bar{\chi}$ on both $\tilde{Z}^*^2$ and $k$ breaks down and the numerical model is no longer able
Jets-in-crossflow characteristics at J = 1.2 in the plane of the jet from -0.96 < x/D < 4.99

Figure 5.6
Figure 5-7  Jets-in-crossflow characteristics at $J = 5.9$ in the plane of the jet from $-0.86 < x/D < 4.99$
Figure 5-8  Jets-in-crossflow characteristics at $J = 23.2$ in the plane of the jet from $-0.86 < x/D < 4.99$
Figure 5.9  Jets-in-crossflow characteristics at $J = 119$ in the plane of the jet from $-0.86 < x/D < 4.99$
Figure 5-10 Jets-in-crossflow characteristics for $J = 1.2$ in various cross-sectional planes
Figure 5-11  Jets-in-crossflow characteristics for $J = 5.9$ in various cross-sectional planes
Figure 5-12  Jets-in-crossflow characteristics for $J = 23.2$ in various cross-sectional planes
Figure 5-13  Jets-in-crossflow characteristics for J = 119 in various cross-sectional planes
to provide satisfactory predictions.

5.2.3.1 Verification of the Non-Premixed Flamelet Model

Two investigations were performed in order to determine the reasons for the failure of the flamelet model to predict jets in a reacting crossflow.

Regimes in non-premixed turbulent combustion were introduced in Chapter 3. Those regimes are based on the ratio of the Kolmogorov (turbulent) time scale to the chemical time scales and the fluctuations of the mixture fraction. The flamelet thickness \((\Delta Z)_F\) divides the flamelet region from the connected reaction zones and was calculated based on the stoichiometric mixture fraction \(Z_{st}\). The program that produced the flamelet library yielded a \(Z_{st} = 0.68493\), from which the \((\Delta Z)_F\) was found to equal to 0.3553. Thus, the time scales and the fluctuations of the mixture fraction were determined for \(J\) of 1.2, 5.9 and 23 at different \(x/D\) locations and were plotted as shown in Figure 5-14. Since grid sensitivity test was not performed in this study, the data point were obtained for a \(Z_{st} \pm 2\%\) or \(0.6712 < Z_{st} < 0.6986\) in order to allow for errors due to grid structure. As can be seen, all three \(J\) conditions at all \(x/D\) locations are in the distributed reaction zone. In this zone, the chemical reaction rate is not fast compared to turbulent processes. Hence, turbulent mixing effects influence the chemical reactions before they are complete. Therefore the flamelet model is unable to predict the flow distribution in this study since the flamelet model requires fast chemistry.

Figure 5-14 also shows that as the \(J\) values increase, the numerical model goes deeper into the distributed reaction zone, and hence, further away from the flamelet region. In addition, the distribution of the \(Z_{st}\) in the duct becomes more concentrated around a smaller range of mixture fraction fluctuations and time scales with an increase in \(J\). This indicates that the
reaction occurs in a smaller region and in the vicinity of the jets as more air is allowed to mix with fuel, as was observed in the contour plots.

Another test was performed which concerned the flamelet library used and not to the numerical model itself. Figure 5-15 shows the normalized CO concentrations as a function of mixture fraction for various strain rates, $a$, that were obtained from the flamelet library. Note that $Z = 1$ represents the fuel, $Z = 0$ represents the oxidizer and $a$ is the velocity gradient. At $a = 1$, reaction will occur where the amount of CO present in a control volume will depend on $Z$ and $\tilde{Z}^*$. From Figure 5-15, normalized CO concentrations will approach zero (for complete reaction) at approximately $Z = 0.55, 0.50$ and $0.33$ for a $\tilde{Z}^* = 0.01, 0.1$ and $0.4$, respectively, at $a = 1$. Thus, the increase in $\tilde{Z}^*$ causes an increase in CO concentrations for the same strain rate. At $a = 11500$, CO concentrations are linearly proportional to $Z$, and hence, the CO will be reduced due to dilution effects only. At this condition, no reaction will occur, the flame will extinguish and an increase in $\tilde{Z}^*$ will not influence the CO concentrations.

Furthermore, it can be seen that the difference between Figure 5-15(a) and (b) is negligible for a variance change from 0.01 to 0.1 at all strain rates. Since the maximum $\tilde{Z}^*$ did not exceed 0.09 for all cases considered in the numerical solution, there was no need to construct a flamelet library that had a variance greater than 0.1. However in this study, the flamelet library was generated for variances starting from 0.01 to 0.10 in steps of 0.01. Assuming that the predicted $\tilde{Z}^*$ field was correct, all those steps would actually become redundant and only one variance at a value of 0.1 will be required.

In the numerical model the maximum $\bar{x}$ was not greater than 2000 l/s, which from Figure 5-3, corresponds to $a = 4000$ l/s. At strain rate values not greater that 4000 l/s, the
Figure 5-14 Regimes in non-premixed turbulent combustion at $Z_{st} \pm 2\%$ for a $J$-value of (a) 1.2, (b) 5.9, and (c) 23
Figure 5-15  Normalized CO concentrations versus mixture fraction plot at various strain rates using and a variance of (a) 0.01, (b) 0.1, and (c) 0.4
flamelet library was unable to yield high CO concentrations that would correspond to flame extinguishing. The reason for the failure of the flamelet model in the numerical model was therefore due to either low variances and scalar dissipation rate predictions or to an incorrect flamelet library. Incorrect flamelet library would mean that the problem of predicting extinction is not related to the numerical model.

5.2.3.2 Sensitivity to Eddy Length Scale

The eddy (turbulence) length scale in the fuel boundary condition was reduced from $T_e = 0.01$ m to from $T_e = 0.001$ m for two reasons. First, it was assumed that the lower $T_e$ would better represent the fuel boundary condition of the experiment. The experiment used a ceramic foam with 10 pores per inch to dissipate mixture non-uniformities in the upstream flow, and hence, yielded a smaller length scale at the inlet to the duct. Secondly, in order to increase the $\tilde{\chi}$, the scalar $\varepsilon$ could be increased since it is linearly related to the $\tilde{\chi}$ (see equation (5.4)). The parameter $T_u$ was not changed in the boundary condition since a turbulence intensity of 5% for these types of flows was considered reasonable.

Three cases were modelled with a new $T_e$ value at the fuel inlet boundary condition. Table 5.6 shows the CO destruction efficiency as a function of $J$ at the outlet of the duct. The values in this table are identical to the values presented in Table 5.5. The results indicate that the numerical solution is independent to a change in $T_k$. From Table 5.8 it can be seen that the maximum $\tilde{Z}^{\infty 2}$ is slightly reduced and the maximum $\tilde{Y}$ value is smaller at $J = 5.9$ and bigger at $J = 23.2$, when compared with the original simulation. These changes are not significant and confirm that numerical model in unable to predict the reacting flow of this study.
Table 5.6: CO destruction efficiency for $T_{\text{fuel}} = 1370$ K with a smaller eddy length scale value

<table>
<thead>
<tr>
<th>Momentum Flux Ratio, $J$</th>
<th>CO Destruction Efficiency, $\eta$ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.88</td>
<td>99.99528</td>
</tr>
<tr>
<td>23.16</td>
<td>99.99986</td>
</tr>
<tr>
<td>119.0</td>
<td>99.99997</td>
</tr>
</tbody>
</table>

Table 5.7: CO destruction efficiency for $T_{\text{fuel}} = 1200$ K

<table>
<thead>
<tr>
<th>Momentum Flux Ratio, $J$</th>
<th>CO Destruction Efficiency, $\eta$ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.88</td>
<td>99.99742</td>
</tr>
<tr>
<td>23.16</td>
<td>99.99990</td>
</tr>
<tr>
<td>119.0</td>
<td>99.99997</td>
</tr>
</tbody>
</table>

Table 5.8: Comparison between different model conditions of maximum mixture fraction variance and scalar dissipation rate at two momentum flux ratios.

<table>
<thead>
<tr>
<th>$J$</th>
<th>$\tilde{Z}^{*2}_{\text{max}}$</th>
<th>$T_{\text{fuel}} = 1370$ K</th>
<th>$T_{\text{fuel}} = 1370$ K (smaller $T_e$)</th>
<th>$T_{\text{fuel}} = 1200$ K</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.88</td>
<td>value</td>
<td>0.076195</td>
<td>0.071989</td>
<td>0.076985</td>
</tr>
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<td>[46,12,14]:T</td>
<td>[47,12,14]:T</td>
<td>[47,12,14]:T</td>
</tr>
<tr>
<td></td>
<td>$Z$</td>
<td>0.51533</td>
<td>0.49381</td>
<td>0.49567</td>
</tr>
<tr>
<td></td>
<td>$[\text{CO}]/[\text{CO}]_{d}$</td>
<td>0.26801</td>
<td>0.24282</td>
<td>0.27043</td>
</tr>
<tr>
<td>23.16</td>
<td>value</td>
<td>878.7862</td>
<td>877.3899</td>
<td>882.9737</td>
</tr>
<tr>
<td></td>
<td>location</td>
<td>[34,7,1]:R</td>
<td>[34,7,1]:R</td>
<td>[34,7,1]:R</td>
</tr>
<tr>
<td></td>
<td>$Z$</td>
<td>0.74075</td>
<td>0.73924</td>
<td>0.73851</td>
</tr>
<tr>
<td></td>
<td>$[\text{CO}]/[\text{CO}]_{d}$</td>
<td>0.55789</td>
<td>0.55709</td>
<td>0.60228</td>
</tr>
<tr>
<td>119.0</td>
<td>value</td>
<td>0.065536</td>
<td>0.063481</td>
<td>0.065901</td>
</tr>
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<tr>
<td></td>
<td>$Z$</td>
<td>0.55556</td>
<td>0.60546</td>
<td>0.55221</td>
</tr>
<tr>
<td></td>
<td>$[\text{CO}]/[\text{CO}]_{d}$</td>
<td>0.28329</td>
<td>0.30638</td>
<td>0.28350</td>
</tr>
<tr>
<td>119.0</td>
<td>value</td>
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<td>1044.522</td>
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<td>location</td>
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<td>[34,7,1]:R</td>
</tr>
<tr>
<td></td>
<td>$Z$</td>
<td>0.84078</td>
<td>0.83960</td>
<td>0.84025</td>
</tr>
<tr>
<td></td>
<td>$[\text{CO}]/[\text{CO}]_{d}$</td>
<td>0.77006</td>
<td>0.76813</td>
<td>0.79841</td>
</tr>
</tbody>
</table>
5.2.3.3 Sensitivity to Flamelet Library

Sensitivity of the numerical solution to the flamelet library was performed in order to detect problems in the flamelet library. These problems could arise from the program's inability to generate a flamelet library for the specific fuel concentrations and temperature. If this would be the case, the flamelet model would only be partially responsible for its inability to predict the flow considered.

A new flamelet library was generated with a fuel temperature at 1200 K, and the numerical model was run for three $J$ conditions. Table 5.7 shows the results of CO destruction efficiency as a function of $J$. As can be seen, the numerical solution worsened for $J = 5.9$ and 23.2 since higher destruction efficiencies were predicted at the outlet of the duct, when compared with those from the original simulation. From Table 5.8, the maximum $\tilde{Z}^{*2}$ and the maximum $\tilde{\chi}$ slightly increased at both $J$ values. However, this effect might be significant since the $\tilde{\chi}$ at

![Figure 5-16 Normalized CO concentrations versus mixture fraction plot at various strain rates for $T_{\text{fuel}} = 1200$ K and a variance of 0.01](image-url)
extinction was approximately 2400 l/s, corresponding to $a = 6000$ l/s (see Figure 5-3). In order to find where the problem lay, the normalized CO concentrations were plotted as a function of mixture fraction with a $\tilde{Z}^*$ of 0.01. Figure 5-16 shows this relationship for various strain rates as obtained from the flamelet library. As can be seen, flame extinguishing will not be modelled since the numerical solution predicted a maximum $\tilde{\chi}$ of 1050 at $J = 23$, which is lower than the value of $\tilde{\chi}$ at extinguishing.

Further reduction of the fuel temperature in the flamelet library might achieve flame extinguishing, however, other problems would arise. If the fuel temperature in the flamelet library is much different from that at which the numerical model operates, strange temperature distributions would result since different species concentrations would develop in the duct, as with real temperature-dependent kinetics. Therefore, the flamelet library does not appear to be the source of error in the numerical model.

5.3 Eddy-Dissipation Model Solution

5.3.1 Description Of The Boundary Conditions and Simulation

The same geometric configuration and grid were used in this numerical model as was described in section 5.2.1 and shown in Figure 5-2. However, heat losses from the duct's wall were accounted in this model in order to simulate more closely the experiment. Heat losses were not implemented in the laminar flamelet model since the model is assumed to be adiabatic, which means that the system is given a fixed amount of energy (chemical or thermal).

In the experiment, there were many places along the duct's wall where heat was lost due to conduction, convection and radiation. Heat losses in the numerical model were simplified by
considering three places along the duct's wall where they were important. Figure 5-17 illustrates the heat losses inside and outside the mixing module. Since the temperature was measured above the orifice row (the grey area in the figure), it was assumed that this measurement represented the average temperature inside the mixing module. Thus, the fuel's flow heat loss within the mixing module ($Q''_1$ and $Q''_2$) was assumed equal to the heat gained by the air, which is expressed in terms of the total enthalpy $\Delta H$ as,

$$\Delta H = \dot{m}_{\text{air}} c_p (T_{\text{air}} - T_{\text{ambient}})$$

(5.5)

where, $c_p$ is the specific heat capacity of air at $T_{\text{ave}} = 0.5(T_{\text{air}} + T_{\text{ambient}}) = 365.5$ K and $T_{\text{ambient}}$ is the room temperature (approximately 293 K). The heat losses $Q_1$ and $Q_2$ were then assumed to be equal to half of the $\Delta H$. This assumption was reasonable since the temperature difference between fuel and air at a section up to $x/D = 4$ was larger than the temperature difference that occurred downstream of the orifices at a section up to $x/D = 12$. In the former section, combustion took place and caused a temperature increase of air inside the mixing module.

In the numerical model, three additional boundary conditions were implemented other than those described in section 5.2.1. Wall heat fluxes $Q''_1$, $Q''_2$ and $Q''_3$ were specified at three sections along the duct, respectively. Their values are shown in Table 5.9 together with the corresponding $J$ values. The third heat flux $Q''_3$ that occurred in a section of the duct from $x/D = 12$ to $x/D = 35$ was estimated by trial-and-error. The idea was to obtain a temperature at the
outlet of the duct, which corresponded to that of the experiment. Thus, the predicted outlet temperature was extrapolated to \( x/D = 48 \) using a parabolic regression. A good approximation to \( Q''_3 \) was made when the extrapolated temperature did not exceed the measured temperature by more than 150 degrees.

### Table 5.9: Heat loss along the duct's wall

<table>
<thead>
<tr>
<th>( J )</th>
<th>( Q''_1 ) [W/m²]</th>
<th>( Q''_2 ) [W/m²]</th>
<th>( Q''_3 ) [W/m²]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.24</td>
<td>18525.2</td>
<td>9262.62</td>
<td>29237.3</td>
</tr>
<tr>
<td>5.88</td>
<td>41417.0</td>
<td>20708.5</td>
<td>12425.9</td>
</tr>
<tr>
<td>23.2</td>
<td>82822.5</td>
<td>41411.3</td>
<td>3654.68</td>
</tr>
</tbody>
</table>

The Eddy Dissipation Model (EDM) involved a total of 5 species: CO, \( \text{H}_2 \), CO\(_2\), H\(_2\)O and \( \text{O}_2 \). The first four species were specified at the fuel boundary condition with mass fractions given in Table 5.2, and the last species was specified in the air jets boundary condition with a mass fraction of 23.3\%. In this study, two single-step reactions were considered to represent the characteristics of the flame. These reactions were described as shown.

\[
CO + \frac{1}{2} \text{O}_2 \rightarrow \text{CO}_2 
\]

\[
\text{H}_2 + \frac{1}{2} \text{O}_2 \rightarrow \text{H}_2\text{O}
\]

Kinetic reaction rates were incorporated into the numerical model through a user modifiable subroutine that was given in the source code directory of TASCflow. The kinetic rates of CO and \( \text{H}_2 \) were expressed in an Arrhenius form involving a pre-exponential factor, activation energy of the reaction and power law dependence on the concentration of four species that contribute to the reaction. The overall form of the reaction rate \( RR \) is expressed as,

\[
RR_f = A \cdot \exp \left[ -\frac{(E/R)}{T} \right] [F]^a [O_2]^b [H_2O]^c
\]
where, $F$ represents the fuel involved in the reaction rate, which can be either CO or H$_2$. In the above equation, the concentration of the species and the reaction rate were expressed in mol/cc and mol/cc/s, respectively. Since the species concentrations in the numerical model are expressed in term of mass fraction, the following equation was used in order to convert those concentrations into the appropriate form,

$$[X_{mol/vol}] = \frac{\rho[X_{mass/mass}]}{1000M_X}$$  \hspace{1cm} (5.9)

where, $X$ is any species, $\rho$ is the density of the mixture and $M_X$ is the molecular weight of species $X$. Furthermore, the numerical model requires that the reaction rate be defined in the unit of kg/m$^3$/s. Thus, equation (5.8) was changed to,

$$RR_F = 1000 \cdot M_F \cdot A \cdot \exp\left[\frac{-(E/R)}{T}\right] [F]^a [O_2]^b [H_2O]^c$$  \hspace{1cm} (5.10)

In addition, the mixture fraction field was calculated using the following expression.

$$Z = \frac{[CO]+[H_2]+[CO_2]+[H_2O]}{[CO],+[H_2],+[CO_2],+[H_2O],}$$  \hspace{1cm} (5.11)

where the species concentrations are in terms of molar fraction and the subscript $i$ represents the concentration at the fuel inlet.

The convergence criterion was set to $10^{-4}$ or less for all the mass, momentum, energy and scalar equations. In addition, the Mass Weighted Skewed (MWS) discretization was used for the numerical solution. As for the flamelet model, the numerical solution was run twice for each case. The first run converged the energy, U-momentum and mass equations with a time step of 1.0E-3. The second run converged the V- and W-momentum equations with a time step of 5.0E-6. Note that the rate of convergence for the species equations was fixed at 1.0, independent of the time step used. Their maximum residual decreased only when the time step was reduced.
Thus, the numerical model either had a problem coupling the scalar equations or it was unable to solve the scalar equations in a specific section of the grid where large gradients were located. The latter explanation is more reasonable since the grid was relatively coarse and was not able to capture accurately these gradients. In the former explanation, temperature damping was incorporated with no affect on convergence.

5.3.2 Results

Several cases were simulated where different reaction rates of CO and H₂ were incorporated into the numerical model. Table 5.10 shows the details of the reaction rates as specified in equation (5.10). In cases 1 and 2 the reaction rates of CO were obtained from Hautmann et al. [33], while the rest of the rates including those of H₂ were obtained using detailed chemical kinetics [47]. The cut-off temperature $T_{\text{cutoff}}$ is the maximum temperature for which the RR equals to zero, that is, the reaction freezes and flame extinction occurs. For all cases, the reaction rate of H₂ is faster than the reaction rate of CO by at least one order of magnitude [47]. This would mean that the molar concentration of H₂ should be lower than that of CO at the outlet of the duct. However, the numerical solution was unable to predict that for five out of seven cases. For these cases, the H₂ concentrations at the outlet were larger than CO concentrations by at least six orders of magnitude. The failure of the numerical model is attributed to the convergence problem discussed in the previous section.

Cases 4 and 5 yielded a reasonable solution. Notice that for case 4, the reaction rate coefficients of CO were used in the reaction rate H₂, and for case 5, the reaction rate coefficients of H₂ were used in the reaction rate of CO. The purpose was to investigate the reason for the strange CO and H₂ concentrations. Thus, it was found that the numerical model converged if the reaction rate coefficients were made equal for both CO and H₂.
Table 5.10: List of reaction rates for CO and H₂

<table>
<thead>
<tr>
<th>Case</th>
<th>Reaction Rate</th>
<th>A</th>
<th>E/R</th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>T_{cutoff}</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>RR_{CO}</td>
<td>8.620×10^{13}</td>
<td>20143</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>-</td>
<td>didn't converge</td>
</tr>
<tr>
<td></td>
<td>RR_{H₂}</td>
<td>1.0×10^{12}</td>
<td>18000</td>
<td>1</td>
<td>0.5</td>
<td>-</td>
<td>-</td>
<td>didn't converge</td>
</tr>
<tr>
<td>2</td>
<td>RR_{CO}</td>
<td>8.620×10^{13}</td>
<td>20143</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>-</td>
<td>didn't converge</td>
</tr>
<tr>
<td></td>
<td>RR_{H₂}</td>
<td>1.0×10^{11}</td>
<td>15000</td>
<td>1</td>
<td>0.5</td>
<td>-</td>
<td>-</td>
<td>didn't converge</td>
</tr>
<tr>
<td>3</td>
<td>RR_{CO}</td>
<td>2.167×10^{13}</td>
<td>20000</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>950</td>
<td>didn't converge</td>
</tr>
<tr>
<td></td>
<td>RR_{H₂}</td>
<td>5.0×10^{10}</td>
<td>13000</td>
<td>1</td>
<td>0.5</td>
<td>-</td>
<td>950</td>
<td>converged</td>
</tr>
<tr>
<td>4</td>
<td>RR_{CO}</td>
<td>2.167×10^{13}</td>
<td>20000</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>950</td>
<td>converged</td>
</tr>
<tr>
<td></td>
<td>RR_{H₂}</td>
<td>2.167×10^{13}</td>
<td>20000</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>950</td>
<td>converged</td>
</tr>
<tr>
<td>5</td>
<td>RR_{CO}</td>
<td>5.0×10^{10}</td>
<td>13000</td>
<td>1</td>
<td>0.5</td>
<td>-</td>
<td>950</td>
<td>converged</td>
</tr>
<tr>
<td></td>
<td>RR_{H₂}</td>
<td>5.0×10^{10}</td>
<td>13000</td>
<td>1</td>
<td>0.5</td>
<td>-</td>
<td>950</td>
<td>converged</td>
</tr>
<tr>
<td>6</td>
<td>RR_{CO}</td>
<td>4.0×10^{8}</td>
<td>5000</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>1100</td>
<td>didn’t converge</td>
</tr>
<tr>
<td></td>
<td>RR_{H₂}</td>
<td>7.0×10^{11}</td>
<td>6000</td>
<td>1</td>
<td>1</td>
<td>-</td>
<td>1100</td>
<td>didn’t converge</td>
</tr>
<tr>
<td>7</td>
<td>RR_{CO}</td>
<td>2.0×10^{6}</td>
<td>0</td>
<td>1</td>
<td>0.5</td>
<td>-</td>
<td>1100</td>
<td>didn’t converge</td>
</tr>
<tr>
<td></td>
<td>RR_{H₂}</td>
<td>7.0×10^{11}</td>
<td>6000</td>
<td>1</td>
<td>1</td>
<td>-</td>
<td>1100</td>
<td>didn’t converge</td>
</tr>
</tbody>
</table>

Consequently, a decision was made to use case 4 in order to analyze CO and H₂ emissions at the outlet of the duct for three flow conditions. This is a conservative choice since the reaction rate of H₂ is smaller than the its actual rate, hence, resulting in an overprediction of H₂ concentrations. Figure 5-18 shows the normalized diluted emissions compared to the experiment of [19] as a function of equivalence ratio φ. This figure illustrates that the CO emissions are underpredicted by approximately seven orders of magnitude. Further analysis into the behaviour of both CO and H₂ for the range of φ considered will not be given for two reasons. Firstly, those concentrations are greatly underpredicted. Secondly, H₂ concentrations are incorrect since the reaction rate of H₂ was used for the purpose of testing convergence and did not represent the actual rate (see Table 5.10, case 4).
Thus, Figure 5-18 confirms that there are two problems with the EDM when reaction rates are incorporated. There is a convergence problem when the reaction rates of CO and H₂ have different coefficients. This might be the result of different chemical time scales that are associated with those reaction rates. In addition, when convergence is achieved by using similar CO and H₂ reaction rate coefficients, the numerical solution underpredicts their concentrations. These problems are attributed to the mathematical model.

### 5.4 Summary

The non-premixed flamelet model was unable to predict the combustion process that occurred when circular air jets reacted with the crossflowing rich fuel mixture. CO concentrations were reduced with an increase in airflow, and hence no optimum flow condition
was reached. However, jet penetration characteristics were observed as was found for non-reacting flows.

For all cases considered the mixture fraction variance was below 0.1, which indicated that turbulent mixing affected combustion. Furthermore, it was shown that the mixture variance was a major influence on the scalar dissipation rate especially when jet overpenetration occurred. Hence, the low scalar dissipation rates were not able to predict flame extinguishing.

Several tests were done to determine the reason for the flamelet model behaviour. The flamelet regime indicated that the combustion in the numerical solution took place in distributed reaction zones, and thus, the mixture consisted of partially or totally premixed regions. The flamelet library indicated that the predicted scalar dissipation rate was far away from flame extinguishing. The decrease in turbulent length scale did not affect combustion at all. In addition, the numerical predictions were found to be independent of the flamelet library used, under the condition that the flamelet library was generated with sensible boundary conditions that were not very different from the numerical simulation. These tests proved that the non-premixed flamelet model could not be used to predict jets in a reacting crossflow under these conditions.

The EDM was also unable predict the combustion process in this study. The reason for its failure was due to convergence or numerical problems as opposed to its concept as in the flamelet model. The difference in the definition of the reaction rates of CO and H₂ appeared to be the source of the problem since different chemical time scales lead to convergence problems.
6 Closure

6.1 Summary and Conclusions

Mixing characteristics that govern circumferential jets in a cylindrical duct were examined. It was found that for non-reacting flows mixing is largely a function of momentum flux ratio and orifice spacing. Optimal mixing could be achieved by adjusting those parameters. However, in reacting flows turbulent and chemical time scales are the important quantities. Optimal mixer design is dependent on specific operating conditions since either one may dominate, and hence, influence the overall system.

The preliminary validations revealed that the numerical model was able to conserve the continuity, momentum and energy equations. The jet velocity was underpredicted where shear affects were large since the $k$-$\varepsilon$ turbulence model is isotropic. The numerical solution for non-reacting jets in a crossflow yielded good qualitative agreement with the experimental measurements. However, mixing in the duct was overpredicted for the flow conditions examined due to overprediction of the temperature field. As a result, optimal mixing was underpredicted.

This study examined the applicability of two widely used combustion models for jet mixing in a reacting crossflow. Those models consisted of the non-premixed laminar flamelet and eddy dissipation. The numerical model was validated with the experimental data of Popovic et al. [19] by comparing the concentrations of CO and H$_2$ at the exhaust.

The non-premixed flamelet model works under the assumption of fast chemistry and its flame structure is described by the mixture fraction $Z$. Turbulence field is coupled with the combustion process by a parameter known as the scalar dissipation rate, which decreases due to
turbulent mixing and increases due to straining by the flow field. Flame extinguishing will occur when the scalar dissipation rate approaches a critical value, which depends on the type of fuel and its temperature. In this model, species concentrations were stored in a flamelet library as a function of mixture fraction, strain rate and mixture fraction variance.

The eddy dissipation model determines the rate of reaction from the minimum of either the mixing rate or kinetic rate. The mixing rate relates the dissipation of turbulent eddies to the concentration of reacting species, while the kinetic rate describes the rate of change of reacting species with respect to time. This model is applicable for non-premixed, partially and fully premixed flames.

The flamelet model was unable to capture the characteristics of CO concentrations for different air-to-fuel flow conditions. CO concentrations were reduced with increasing airflow since flame extinction was never approached. A detailed analysis of this model revealed that the turbulence time scale was faster than the chemical time scale and that the mixture fraction fluctuations were small due to intense mixing. Thus, the numerical solution was outside of the flamelet regime and inside a regime of distributed reaction zones where partially or fully premixed flames occur. These predictions were independent of turbulence length scale specification in the fuel inlet boundary condition and the flamelet library was ruled out as another factor involving in the model’s failure.

The eddy dissipation model was also unable to describe the combustion process. The predicted CO and H₂ concentrations were much lower than the experimental measurements, even though, wall heat losses and kinetic rates were accounted for. These predictions were obtained when the kinetic rates of CO and H₂ had the same coefficients. However, the model did not
converge when the kinetic rates were structured differently. Therefore, the numerical predictions are not reliable and the use of the EDM to predict emissions is not advisable.

For the two combustion models, the influence of the turbulence model was not believed to be significant to the outcome of the numerical solution.

6.2 Recommendations for Future Work

In order to validate the experiment [19], a more advanced combustion model should be used. Peters [24] and Bray and Peters [29] discuss the concept of fully premixed flamelet model where a \( G \)-equation replaces the \( Z \)-equation. Basically, the \( G \)-equation is distance function from the flame front, which is described by either burned or unburned fuel. In addition, Peters [24] reviews the concept of partially premixed flamelet model. This model uses both the \( Z \)-equation and the \( G \)-equation to describe the flame structure. Thus, it represents a better combustion model and should be explored in the future to predict CO and \( \text{H}_2 \) concentrations.

The eddy dissipation model should not be used to predict emissions for a jet mixing in a reacting crossflow. However, this model may be used for the purpose of temperature predictions with satisfactory results.

Once a new combustion model is implemented in the numerical code, the work of validating the experiment [19] should continue. Furthermore, the numerical model should be used to predict emissions and flame length with respect to momentum flux ratio with various orifice geometry and spacing.
7 References


