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Numerical Studies of Reacting and Non-Reacting
Underexpanded Sonic Jets

by

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Submitted for the Degree of Doctor of Philosophy

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Abstract

The objective of this work was to model underexpanded turbulent sonic jets and the lifted diffusion flames which result should ignition occur. This relates to the accidental release of combustible gases from high pressure pipelines. A pressure-based CFD methodology has been employed, incorporating extensions to handle high speed, shock containing flows. The methodology extended previous studies of high speed flow employing pressure based methods to unlimited Mach Numbers. This has been achieved by developing a Mach number dependent differencing scheme for the pressure correction equation. This allowed high pressure ratio jets containing strong normal shocks to be computed. Numerical accuracy was improved by applying a second order accurate total variation diminishing scheme to the convective differencing. A standard two-equation turbulence model was used, with an optional compressibility correction. Predictions are presented over a large range of pressure ratios and extensive comparison to the available experimental data showed the correct shock cell wavelength, but a too rapid decay of the shock cell structure. The compressibility correction had no effect on the shock cell decay, but increased the potential core length, improving the agreement with the experimental data. Far field velocities and mixture fraction profiles also show a good agreement with experimental data when employing the compressibility correction.

Following ignition, the resulting underexpanded jet diffusion flames are lifted from the nozzle rim by several diameters due to flame quenching processes. A quenching mechanism based on the strain rate of the largest eddies and applied either in a local manner or using a lift-off threshold was initially calibrated and validated for subsonic lifted diffusion flames, showing excellent agreement to experimental measurements. The mechanism was subsequently applied to underexpanded jet diffusion flames and showed good agreement to experimental data. Predictions of the lift-off height based on cold flow computations showed a reduced accuracy. The eddy dissipation concept, fast chemical reacting system and presumed β-pdf combustion models were applied and compared using the two quenching mechanisms. The various models predicted significantly different temperature fields close to the nozzle, but were similar further downstream. More experimental data is required in order to determine the accuracy of the models. A pseudo nozzle approximation has also been developed which replaced underexpanded jets with perfectly expanded supersonic jets and removed the need to compute the shock containing region. The approximation was successfully validated for both reacting and non-reacting underexpanded jets.
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Contents

Chapter 1. Introduction

1.1 Preamble 1

1.2 Review of Non-Reacting Underexpanded Jet Literature 6
   1.2.1 Experimental Studies 6
   1.2.2 Analytical Methods 11
   1.2.3 Numerical Studies 12
   1.2.4 Unsteady Features 20

1.3 Review of Lifted Diffusion Flame Literature 23
   1.3.1 Attached Diffusion Flames 23
   1.3.2 Lifted-Diffusion Flames 25
   1.3.3 Underexpanded Jet Diffusion Flames 27

1.4 Objectives 29

Chapter 2. Non-Reacting Methodology 31

2.1 Introduction 31
   2.1.1 Requirements of the Methodology 31
   2.1.2 Numerical Methods for Shock Containing Flows 31
   2.1.3 Review of Density Based Methods for High Speed Flows 33
   2.1.4 Flow at all Speeds 36
   2.1.5 Review of Pressure Based Methods 37
   2.1.6 Outline of Methodology 40

2.2 Governing Equations 41
   2.2.1 Navier-Stokes Equations 41
   2.2.2 Treatment of Turbulence 42
      2.2.2.1 Continuity 44
      2.2.2.2 Momentum 45
      2.2.2.3 Total Enthalpy 45
      2.2.2.4 Scalar Transport 45
   2.2.3 Constant Enthalpy Assumption 46

2.3 Closure: Turbulence Modelling 47
   2.3.1 Review of Available Turbulence models 47
      2.3.1.1 First Order Models 47
      2.3.1.2 Reynolds Stress Models 48
      2.3.1.3 Algebraic Stress Models 49
   2.3.2 The k-ε Turbulence Model 49
2.3.3 Turbulence in Compressible flow
2.3.4 Compressibility Corrected k-e Model

2.4 Summary of Governing Equations
2.4.1 Axisymmetric Co-ordinate System

2.5 Discretisation
2.5.1 Finite Volume Technique
2.5.2 Convective differencing
2.5.2.1 Hybrid Differencing Scheme
2.5.2.2 TVD
2.5.3 Form of Equations

2.6 Pressure Correction Scheme
2.6.1 Correction Equation
2.6.2 Transformation to Pressure Based Equation
2.6.3 Flux Construction
2.6.4 Retarded Pressure Scheme
2.6.5 TVD Differencing

2.7 Solution Details
2.7.1 Time Step Definition
2.7.2 k-e Limits
2.7.3 Equation of State
2.7.4 Boundary Conditions
2.7.4.1 Jet
2.7.4.2 Symmetry
2.7.4.3 Constant pressure

2.8 Closure

Chapter 3. Non-Reacting Results

3.1 Introduction
3.2 Computational Setup and Grid Generation
3.3 Predicted Flow Features
3.3.1 Moderately Underexpanded Jets
3.3.2 Highly Underexpanded Jets

3.4 Numerical Issues
3.4.1 Convective Differencing Scheme
3.4.1.1 Subsonic Jet Calculation
3.4.1.2 Numerical Dissipation - the Effect of Momentum Upwinding
3.4.2 Modified Convective Differencing Scheme
### Table of Contents

3.4.2.1 Model Description 94  
3.4.2.2 Results 95  
3.4.3 Pressure Correction Scheme 97  
3.4.3.1 Retarded Pressure Function 97  
3.4.3.2 Upwind Scheme 99  
3.4.3.3 Blended Differencing Scheme 99  
3.4.3.4 TVD Type Limiters 102  
3.4.3.5 Comparison of Schemes 103  
3.4.4 Grid Dependency Results 105  
3.4.5 Nozzle k-ε Specification 106  
3.4.6 Discussion of Numerical Issues 107  

3.5 Test Cases - Comparison to Experimental Data 110  
3.5.1 Chuech [16], NPR = 2.27 and 2.59 110  
3.5.2 Stickland et al. [7], NPR = 2.5, 3.5 and 5.0 113  
3.5.3 Donaldson and Snedeker [6], NPR = 2.69 and 6.76 115  
3.5.4 Hu and McLaughlin [9], NPR = 3.18 and 9.15 116  

3.6 Downstream Mixing Predictions 117  

3.7 Pseudo Source Calculations 118  
3.7.1 Moderately Underexpanded Jets 120  
3.7.2 Highly Underexpanded Jets 122  

3.8 Comparison to Previous Computational Studies 125  

3.9 Closure 128  

3.10 Figures 130  

**Chapter 4. Combustion Methodology** 204  

4.1 Introduction 204  

4.2 Review of Methods for Non-Premixed Combustion 204  
4.2.1 Chemical Closure - The Need for Combustion Models 204  
4.2.1.1 Reaction Mechanisms 204  
4.2.1.2 Chemical Reaction Rates 205  
4.2.1.3 Turbulence - Chemistry Interactions 207  
4.2.2 Conserved Scalar Approaches 208  
4.2.2.1 Fast chemistry 209  
4.2.2.2 Presumed Pdf Model 209  
4.2.2.3 Laminar Flamelet Models 210  
4.2.3 Coherent Flame Sheet Models 211  
4.2.4 Eddy Dissipation Concept 211  
4.2.5 Choice of Combustion Model 213  

v
4.3 Extinction Phenomena 215

4.4 Numerical Implementation 221
  4.4.1 Conserved Scalar 221
  4.4.2 Energy Equation 222
  4.4.3 Conserved Scalar for Enthalpy 224
  4.4.4 Thermo-Chemistry 225
  4.4.5 Calculation of Thermodynamic Properties 226
  4.4.6 Numerical Treatment of Energy and Scalar Transport Equations 226

4.5 Combustion Models 228
  4.5.1 Fast Chemical Reacting System 228
  4.5.2 Presumed PDF Model 230
    4.5.2.1 Numerical Implementation 236
  4.5.3 EDC Model 236
  4.5.4 Extinction Mechanisms 238

4.6 Closure 239

Chapter 5. Reacting Results 241

5.1 Introduction 241

5.2 Mixing Calculations 241
  5.2.1 Effect of TVD scheme 241
  5.2.2 Comparison to Experimental Data 242
  5.2.3 Pseudo Source Calculations 245

5.3 Energy Calculations 245
  5.3.1 Comparison to Constant Enthalpy Assumption Solution 245
  5.3.2 Effect of TVD scheme 245

5.4 Reacting Subsonic Jets 246
  5.4.1 Computational Setup 246
  5.4.2 Results 247

5.5 Reacting Underexpanded Jets 249
  5.5.1 Computational Setup 249
  5.5.2 Energy Equation 250
  5.5.3 EDC Models 251
  5.5.4 FCRS Model 253
  5.5.5 PDF Model 254
  5.5.6 Extinction Models 255
  5.5.7 Comparison to Experimental Data 259
    5.5.7.1 Lift-Off Height Predictions 259
    5.5.7.2 Downstream Data 264
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.6 Pseudo Calculations</td>
<td>266</td>
</tr>
<tr>
<td>5.7 Closure</td>
<td>268</td>
</tr>
<tr>
<td>5.8 Figures</td>
<td>271</td>
</tr>
<tr>
<td>Chapter 6. Conclusions</td>
<td>317</td>
</tr>
<tr>
<td>Appendix A. Staggered Grid</td>
<td>320</td>
</tr>
<tr>
<td>Appendix B. Numerical Diffusion</td>
<td>322</td>
</tr>
<tr>
<td>B.1 Convective Differencing</td>
<td>322</td>
</tr>
<tr>
<td>B.2 Pressure Correction Schemes</td>
<td>323</td>
</tr>
<tr>
<td>B.2.1 Blended Difference Scheme</td>
<td>323</td>
</tr>
<tr>
<td>B.2.2 Retarded Pressure Scheme</td>
<td>323</td>
</tr>
<tr>
<td>References</td>
<td>326</td>
</tr>
</tbody>
</table>
Chapter 1. Introduction

1.1 Preamble

An underexpanded jet is formed when a gas at a sufficiently high pressure is vented through an orifice. The resulting jet contains a complex, repeating structure of shock cells, the properties of which are principally dependent on the pressure of the gas, relative to the ambient conditions. This study aims to provide a detailed modelling strategy for this type of jet, and the resulting flame should a jet of combustible gas be ignited.

Underexpanded jets are of considerable interest to many areas of engineering. In the chemical industry they are important in regard to accidental releases from high pressure gas pipelines. Here, a pressurised gas escapes through a sonic orifice forming an underexpanded jet. Such a release can be particularly hazardous if the released gas is toxic or flammable. In the case of toxic jets it is the dispersion of the gas and its ground concentrations that are of particular interest. For a combustible release, should ignition occur, then a large diffusion flame with high intensity, strong radiative heat transfer and a large lift-off height can be formed. An accurate predictive capability is desirable for risk assessment and hazard management.

In the aerospace industry the exhaust gases from military aircraft generally form underexpanded jets. These jets will subsequently interact with the afterbody and tail surfaces and can lead to large increases in drag and raise issues regarding fatigue. The fluid dynamics of afterbody configurations in jet propulsion aircraft, such as those that are found in High Speed Civil Transport and Advanced Short Takeoff and Vertical Landing (ASTOVL) aircraft, is an area of considerable current interest. Here a knowledge of the often supersonic flow through intakes, diffusers, jet nozzles and afterbodies is desirable which is complicated further by complex geometries, co-flow configurations and ground impingement. In addition, the underexpanded jets formed by the exhaust gases represent a significant component of the nozzle from military aircraft and it is principally due to noise considerations that the exhausts from civil aircraft run just choked and not underexpanded.

Underexpanded jets are also important for the propulsion of space launch systems, which were the motivation for much of the early studies into underexpanded jets. In particular, an accurate understanding of the exit flows of jet propulsion units was required in order to calculate accurately the thrust performance of the rocket engines. Underexpanded jets are
particularly common in rocket propulsion since as altitude increases the atmospheric pressure and hence sonic velocity decrease, leading to an increase in the pressure upstream of the nozzle exit relative to ambient and therefore more likely conditions for underexpanded jet formation.

Jets from convergent nozzle can be characterised into one of three categories: subsonic, perfectly expanded and underexpanded. Subsonic jets are well understood, containing a potential core surrounded by a mixing layer in which the jet fluid mixes with the ambient fluid. Where this mixing reaches the centreline the potential core ceases to exist. Further downstream the jet continues to expand and entrain the ambient fluid. In this region of the jet the velocity profile becomes self-similar. Perfectly expanded jets occur when the total pressure reaches critical \((NPR = 1.89, \text{ for } \gamma = 1.4)\) and the nozzle becomes choked. Although in theory no shock cell structure is found, in practice it is virtually impossible to design a perfect sonic nozzle, due to boundary layer effects, and a very weak normal shock is always apparent at the nozzle exit.

An underexpanded sonic jet occurs when the nozzle pressure ratio (NPR) of a convergent nozzle exceeds critical. Throughout this thesis NPR will be expressed as the ratio of total reservoir pressure to ambient static pressure; this is not always the case in the literature where other measures are also used, such as the ratio of jet exit static pressure to ambient. At critical NPR the flow at the nozzle exit becomes choked and any further increase in NPR can not lead to an increase in the nozzle exit velocity and the static pressure remains above the ambient pressure. Thus, expansion to the ambient pressure must occur outside the nozzle and the flow is underexpanded at the nozzle exit. The imbalance of static pressure between the flow immediately downstream of the nozzle and the ambient leads to the formation of a complex shock cell structure whose form is dependent on the pressure ratio. Underexpanded sonic jets are the result of NPR above 1.89 (for \(\gamma = 1.4\)) and can be categorised into two types. Moderately underexpanded jets occur up to around NPR = 3.8, whilst for higher NPR the jet is highly underexpanded.

Figure 1-1 shows a schematic diagram of the expansion waves in a moderately underexpanded sonic jet. The initial nozzle flow has a static pressure above that of the ambient pressure (region 1) and a Prandtl-Meyer expansion fan, centred on the nozzle rim, reduces the pressure of the flow to atmospheric pressure at the jet boundary (region 2). Close to the centreline of the jet (region 3) the pressure will drop below atmospheric due to the coalescence of expansion waves from opposite sides of the jet. In order that atmospheric

2
pressure be maintained at the boundary the incident expansion waves are reflected back into the flow as compression waves forming region 4, which is at atmospheric pressure. These compression waves tend to coalesce forming oblique shock waves, which cross the jet, and a high pressure region behind them (region 5). These shock waves will also be incident on the jet boundary where they will be reflected as expansion waves, and thus the process is repeated.

Figure 1-1. Shock Cell Formation and Pressure Regions of a Moderately Underexpanded Jet

In an ideal jet the pressure in region 5 would be equal to that in the nozzle (region 1), and this process would continue indefinitely; in reality the viscous effect of shear stresses will cause the energy of the flow to be dissipated and the potential core to erode away. Therefore the pressure in region 5 will be lower than that in the nozzle. After a transition region the downstream structure of the jet resembles that of a subsonic jet. Figure 1-2 shows the oblique shock cell structure and the gradual erosion of the potential core in an underexpanded sonic jet.

Highly underexpanded jets occur at higher NPR. As in moderately underexpanded jets an expansion fan forms. However, in this case irregular shock reflection occurs when the initial expansion fan is incident on the jet boundary. Along the centreline the pressure drops to levels that are so low that an oblique shock cannot perform the required re-compression. The reflected compression waves coalesce to form an oblique intercepting shock, which steepen to form a normal and reflected shock. Figure 1-3 shows a schematic of a normal shock, often
referred to as a Mach disk. Where the normal shock and the intercepting shock meet, forming an oblique reflected shock, is known as the triple point. Downstream of the normal shock there is a subsonic flow region which is separated from the supersonic flow which passed through the reflected shock by a slipline. Rapid mixing occurs in this region, quickly reaccelerating the subsonic flow region to supersonic velocities. Where the reflected shock meets the jet boundary another expansion fan is formed. Here conditions are often similar to those encountered at the nozzle exit and hence subsequent Mach disks or oblique shock cells may be formed. The effects of mixing on the core region damps out the shock structure and far downstream typical subsonic mixing occurs.

![Figure 1-2. Shock Cell Structure and its Erosion in a Moderately Underexpanded Sonic Jet](image-url)
In the case of convergent-divergent nozzles an additional class of jet may form, known as an overexpanded jet. Here, the exit velocity is supersonic and the static pressure is lower than the ambient pressure, such that the jet must be compressed to atmospheric pressure outside the nozzle and, similarly to underexpanded jets, this is achieved in the form of a regular shock cell structure. Underexpanded jets can also be formed in convergent-divergent nozzle, but the exit velocity will now be supersonic.

The unsteady features of underexpanded jets are of interest to the aerospace industry, since they are responsible for noise and fatigue damage. Large scale structures are present which interact with the shock cell structure to produce shock associated noise of two types, known as broadband shock associated noise and screech. The large scale structures are also responsible for increased mixing rates.

The understanding of turbulence is a key issue for both reacting and non-reacting underexpanded jets. Turbulence has a significant effect on the initial momentum layer thickness and the mixing rate, with the mixing rate having significant influence on the potential core length and the downstream profiles. In the case of highly underexpanded jets, additional mixing regions occur behind the normal shock where subsonic flow that has passed through the Mach disk mixes with supersonic flow that has not. Many of the turbulence effects in underexpanded jets are poorly understood, in particular the effects of both large scale structures and compressibility.
Chapter 1. Introduction

This chapter reviews the literature relevant to underexpanded jets and their computation. Section 1.2 deals with non-reacting jet literature, first covering experimental studies and the physical features of such jets (section 1.2.1), followed by a review of analytical methods (section 1.2.2) and finally numerical methods (section 1.2.3). The literature regarding unsteady features of underexpanded jets, which has important consequences for jet noise, is reviewed in section 1.2.4. Section 1.3 reviews the literature regarding reacting underexpanded jets. First attached subsonic diffusion flames are discussed in section 1.3.1. Section 1.3.2 considers the literature regarding lifted subsonic diffusion flames, whilst underexpanded flames are discussed in section 1.3.3. Finally, the objectives for the present study will be presented (section 1.4).

1.2 Review of Non-Reacting Underexpanded Jet Literature

1.2.1 Experimental Studies

Much of the early experimental work on underexpanded jets involved the measurement of global properties of the first Mach disk, such as its location and diameter. Love et al. [1] presented comprehensive experimental results for underexpanded jets exhausting into both still air and supersonic streams. The experiments considered the effects of pressure ratio, nozzle exit Mach number, and nozzle divergence angle on jet structure, jet wavelength and curvature of the jet boundary using a double Schlieren technique. This technique produced two Schlieren images, one accentuating the horizontal gradients, produced by the vertical knife edge and one the vertical gradients, produced by the horizontal knife edge. Both the primary wavelength and the curvature were found to increase with increasing NPR. The authors concluded that increasing the divergence angle of the nozzle increased significantly the range of pressure ratios over which Mach disks were formed, whilst having only a small effect on the primary wavelength. Increasing the exit Mach number decreased the range over which Mach disks were observed. In the downstream region of the jets, for all Mach numbers and divergence angles tested, the structure deflected from the axis in an alternate fashion, closer examination of which revealed that the jet broke down into a vortex pattern resembling a vortex sheet, and thereafter into a region of wide turbulent diffusion.

Other workers have also determined the location and dimensions of the first Mach disk. Crist et al. [2] measured the distance to the first shock cell and its diameter up to very high pressure ratios of around 100,000, with stagnation pressures of 100 bars and ambient pressure down to around 0.001 bars. The effects of different gases and increased stagnation...
temperatures were also examined. Measurements were taken by means of a type of Schlieren photography, with the authors reporting some difficulty in taking measurements due to many of the shock waves appearing with finite thickness due to their curvature. The results showed that the Mach disk location was insensitive to the ratio of specific heats of the gas, condensation, nozzle lip geometry and the absolute pressure level. However, the diameter of the Mach disk, jet boundary and intercepting shock were found to increase with decreasing ratio of specific heats and with increasing condensation. At very high pressure ratios the diameter decreased due to the high stagnation density where intermolecular forces were thought to become important. Ewan and Moodie [3] have also used Schlieren photography to measure the barrel length and Mach disk diameter of air jets up to a pressure of 30 bars using nozzle of two diameters. They found that the normalised barrel length and Mach disk diameters were independent of the nozzle diameter.

Some of the earliest work measuring the flow properties in underexpanded jets was done by Ladenburg et al. [4], who used Mach interferometry to measure the density fields and shadowgrams to look at the structure up to pressure ratios of 200. For jets with NPR between 2 and 8, exhausting into atmospheric conditions, shadowgrams were used to visualise the shock structure and interferograms were used to obtain density fringes, which were interpreted into density contours for the first shock cell in which shock waves were clearly visible. Further measurements up to a pressure ratio of 200 were achieved by exhausting into a vacuum chamber. Schlieren photography was employed to demonstrate the changing shock structure as the pressure ratio increased from moderately underexpanded levels to highly underexpanded.

A similar technique, Moiré-Schlieren, has been used more recently [5] to calculate fringe patterns relating to the density fields in both rectangular and circular underexpanded jets up to a pressure ratio of 20. The distance to the Mach disk was found to be the same for both circular and rectangular jets. The density distributions along the flow axis showed smeared shock waves. This was accounted to the asymmetry of Moiré shifts and the blur of the Moiré image caused by light interference.

Pressure probe measurements are the most common technique applied to the flow properties of underexpanded jets. Donaldson and Snedeker [6] used this technique to measure Pitot and static pressures profiles on the centreline of a moderately underexpanded (NPR = 2.69) and a highly underexpanded (NPR = 6.76) jet, from which velocity profiles were determined. The velocity profiles, along with pressure and jet spread rate for the two pressure ratios were
presented, including data within the shock-containing near field region. A low frequency flapping mode was observed, as is found in all free jets, which was a function of the jet setup. The use of a long pipe instead of a hole in a flat plate for the nozzle lowered the jet spreading rate. Stickland at al. [7] employed a five hole probe to measure the Mach number for validation of the Phoenics CFD code. Centreline axial Mach number plots were presented for NPRs of 1.25, 2.5, 3.5 and 5.0, along with a number of radial profiles for NPR = 3.5. However, there is some question over the validity of these results since the Mach number shown at the nozzle exit in each case was significantly above 1. Eggers [8] provided benchmark velocity profile and eddy viscosity measurements for underexpanded jets. Unfortunately this data was limited to a convergent-divergent nozzle with an exit Mach number of 2.2. Total pressure measurements, taken using a pressure probe, were reduced to velocity profiles and then, using the momentum equations, to eddy viscosity profiles. Pressure probes and hot wire methods were used by Hu and McLaughlin [9] to measure axial and radial properties of two jets. The shock cell patterns appeared not to be well resolved. Seiner and Norum [10] also used pressure probes along with hot wire techniques to measure flow properties of underexpanded jets with the particular aim of noise analysis. The data was mainly limited to that from convergent-divergent nozzles where the exit velocity is supersonic. Finally, Norum and Seiner [11] presented axial static pressure plots for convergent nozzles at several pressure ratios from 2.08 to 7.70.

The use of pressure probes in flows such as underexpanded jets has its limitations. Unless the probe has a very small diameter in relation to the nozzle diameter then its sensing volume will be too large to adequately resolve features such as shock waves. This problem is often compounded by the desire for small nozzle diameters to reduce the capacity of compressed gas required. Further inaccuracies can also be introduced by the formation of additional shock waves due to the presence of the probes in supersonic flow. Different authors can often show significantly different results for what appear similar experimental set-ups. For example, in the work of Hu and McLaughlin [9] the centreline Mach number at pressure ratios of both 3.2 and 9.15 showed very little evidence of a shock cell structure downstream of the first shock cell. This is in contrast to the work of Stickland et al. [7] which measured seven shock cells for both NPR = 3.5 and NPR = 5.0.

A number of comprehensive experimental studies have ignored the difficulties of taking measurements in the supersonic, shock containing potential core and concentrated on the downstream regions only. Birch et al. [12, 13] took velocity measurement of air jets using

More recently laser techniques have been used to measure flow properties. One such technique is laser Doppler anemometry (LDA) [3, 14-16]. Although this technique is widely used for collecting data in the near field region of underexpanded jets, the results are effected by the response of seeding particles to the rapid changes of velocity across shock cells in supersonic regions [16], and the most reliable results are restricted to constant pressure regions.

Chuech [16] used LDA to measure mean and fluctuating velocities. Although the LDA setup was capable of measuring both subsonic and supersonic velocities, it was unable to resolve the rapid velocity changes found in the shock containing region of underexpanded jets. Laser-induced fluorescence (LIF) was also used to measure mean and fluctuating concentrations and mean static pressures with an iodine vapour seed. Limited by the range of pressure ratio studied (NPR = 2.3 and 2.6), it still amounts to some of the best data available, providing both axial and radial data. Reduced accuracy was reported across shock containing regions, where significant gradient broadening was observed due to the finite size of the measurement volume. The data was based on fully developed flow in the nozzle, whereas most experimental studies have used slug flow nozzles.

Other workers have used similar techniques to that of Chuech [16]. Marrone [17] used electron beam induced fluorescence to measure rotational temperatures in an underexpanded jet of nitrogen. Lemoine and Leporcq [18] reported pressure measurements in a moderately underexpanded sonic jet using LIF with iodine vapour as the tracer. The results showed promising ability to measure accurately the properties of shock cells, but only limited data was presented. LIF presents obvious benefits over traditional pressure probe measurements in that the method is non-intrusive. Compared to LDA methods, improvements to the shock cell resolution are obtained by using a vapour as the tracer where LDA typically uses either a solid or a liquid. The use of this technique is limited by the very corrosive nature of iodine vapour; its use is restricted to protected facilities.

Di Rosa et al. [19] demonstrated the use of a LIF type technique with NO as the seed for the simultaneous measurement of temperature, velocity and pressure in an underexpanded jet. Previous LIF studies were only able to measure one flow property at a time due to difficulties in handling multiple pulsed lasers and cameras. The technique reported in this paper
Chapter 1. Introduction

overcomes this problem. Near field measurements were presented for the centreline temperature, pressure, velocity and Mach number for NPR = 21.7. Some smearing of the normal shock was observed. Smith et al. [20] used planer Doppler velocimetry (PDV) with Mie scattering as the signal generator and an Iodine seed. Both instantaneous and averaged velocities were presented for overexpanded jets with little smearing of the shock cell structure. Since an iodine seed is used whose size reacts to the local thermodynamic conditions care has to be taken in extracting the velocity field. At high speeds the accuracy is limited by the need to find small enough seeding particles to follow the flow.

Oxygen flow tagging applied to underexpanded jets was reported by Miles et al. [21]. In this technique no flow seeding was required; flow tagging was stimulated by Raman excitation. After tagging the excited molecules moved with the flow for a time interval before being interrogated. The interrogation laser was focused into vertical sheets causing the excited molecules to produce fluorescence so that the downstream motion of each molecule could be observed and the streamlines visualised. These pictures can be imaged processed to obtain mean velocities and turbulence properties. However, only limited quantitative results with which to assess the technique were presented.

Krothapalli et al. [22] used particle image velocimetry (PIV) with 0.9μm Al2O3 particles as the seed for the jet and smoke particles in the range of 0.5 to 1.5μm for the ambient to study both supersonic (M = 2) moderately underexpanded and sonic highly underexpanded jets. From double exposure digital images the velocity field and also the vorticity field were derived. Shock cells appeared to be well captured in the two-dimensional representations. However, an example of the centreline velocity compared to similar results using pressure probes showed that the PIV results were in error after the normal shock. This was a consequence of particle lag, which could be corrected for using a particle dynamics model.

There is currently a lack of comprehensive data regarding underexpanded sonic jets, stemming mainly from the extreme difficulties encountered when measuring properties in the presence of highly fluctuating pressures and shock cells. Much of the data either totally ignores the near field region or the reliability of results in the region is questionable. Although new techniques are under development, mainly involving non-intrusive laser approaches, which hold the promise of moving nearer to finding a suitable method for the accurate determination of the properties of all flow variables in the near field shock containing region, at present work in these areas essentially focuses on method development rather than a database of quantitative data. This lack of experimental data has slowed down
the understanding of the physics of underexpanded jets and the development and validation of modelling techniques.

1.2.2 Analytical Methods

Complementing the experimental work are numerous analytical studies. Several works have presented empirical correlations for estimating the various properties of the shock cell structure in underexpanded jets [e.g. 1, 23, 24]. A detailed review of these was presented by Ramskill [25]. Correlations exist for the distance to the first normal shock, the diameter of the normal shock and the initial boundary layer thickness as well as the shock cell wavelength. However, many of these correlations are limited to a very narrow range of conditions and often give widely varying results from both other correlations and experimental data.

The method of characteristics has been applied to the near field region of underexpanded jets in several studies. Pack [26] applied the method of characteristics to predict the existence of shock waves, the point of their formation and their shape. The minimum pressure found behind the normal shock was also calculated, as was the shape and the initial inclination of the jet boundary. In the work of Adamson and Nicholls [27] the initial region, up to the first normal shock, was treated as an imaginary extension to the actual nozzle. In this region one-dimensional, isentropic flow was assumed and the centreline pressure distribution was calculated using the method of characteristics. The normal shock was assumed to form at the location where atmospheric pressure would be achieved behind it. Good agreement was found with the experimental data of Love et al. [1], but the model overpredicted the data of Ewan and Moodie [3] by 25%. However, according to both Ewan and Moodie [3] and Ramskill [25], the method of Adamson and Nicholls [27] was the most accurate available.

An approach that has been commonly applied to avoid the complexities of the shock containing near field region makes assumptions to create a fictitious set of approximate ‘pseudo’ nozzle conditions. Using these conditions a less complex analysis can subsequently be applied. Several methods have been used to approximate the conditions. Kalghatgi [28] and Gore et al. [29] extended the nozzle extension theory of Adamson and Nicholls [27] to calculate not only the location but also the properties behind the normal shock. These conditions were then used as a pseudo nozzle, hence assuming that no shock cell structure exists. In this way the underexpanded jet was approximated as a perfectly expanded jet located downstream of the true nozzle location.
Birch et al. [12, 13] developed a pseudo-diameter approach to correlate their far field concentration and velocity data using hyperbolic curves, which are often used for subsonic jets. For the concentration measurements [13], a pseudo-diameter approach was employed. Here, the pseudo nozzle was assumed to be choked, but ideally expanded and hence with atmospheric pressure at its exit. The diameter of the pseudo nozzle was calculated to ensure the pseudo nozzle had the same mass flow rate as the true underexpanded nozzle. For the velocity measurement [12] the method was extended so that both mass and momentum were conserved in the expansion and the velocity was no longer assumed to be sonic. This method also required an axial displacement of the pseudo nozzle, which was obtained empirically.

With the complexities of the shock containing region eliminated compressible turbulent jet theory [30] can be used to model the far field velocity profiles. Such approaches have been discussed by Ramskill [25] and Eggers [8]. Chuech [16] used the pseudo nozzle approach in conjunction with a CFD code to predict the downstream properties of underexpanded jets. Several different approaches were employed to obtain the pseudo conditions, although all the method produced very similar results, showing reasonable agreement with experimental data. However, no information on the shock containing region was available.

1.2.3 Numerical Studies

With the advent of more powerful computers numerical methods, such as CFD, are being applied more often to complicated flow problems. In many problems, such as underexpanded jet calculations, numerical studies can provide data which cannot currently be obtained experimentally due to measurement difficulties. However, numerical models must be comprehensively validated if the results are to be reliable. An underexpanded jet into quiescent condition represents a good test of any numerical scheme, since both high speed supersonic and low speed subsonic regions are encountered. In addition shear layers and both oblique and normal shock cells are present. Several levels of complexity have been applied in modelling underexpanded jets from Euler solution, which neglect all viscous terms, through to full Navier-Stokes solutions. In the following section some numerical studies of underexpanded jets will be discussed. A discussion on relevant numerical schemes is presented in section 2.1.2.

One of the earliest numerical studies of underexpanded jets [31] employed an inviscid, two-dimensional, time-dependent, finite difference method, known as the two-step Lax-Wendroff technique. This method was applied to an NPR = 7.85 underexpanded jet with promising
results. The region up to the Mach disk compared well to experimental Shadowgraph results, displaying typical features such as the curved boundary, normal shock and reflected shock. Some overshoots were observed at the leading edge of the normal shock, indicating numerical error, and the shocks were smeared over a number of cells, which were relatively coarse due to the available computational power. The coarse mesh also led to an inaccurate prediction of the location of the normal shock, although this may also be due to the application of a non-conservative numerical scheme leading to a loss of mass flux.

An Euler based scheme has been applied to highly underexpanded jets by Mehta et al. [32] using a Runge-Kutta time-stepping technique and a second order, central difference scheme in smooth regions with additional second order artificial dissipation reducing the scheme to first order accuracy in the vicinity of shock waves. For sonic jets, solutions for NPR = 10.0, 15.0 and 20.0, using a 271×51 grid, were presented and compared to the experimental data of Cobald [33]. The centreline pressure was in disagreement with the experimental data and the normal shock location was predicted upstream of that measured. In the downstream region the measured centreline total pressure increased due to mixing with the supersonic flow that had not flowed through the Mach disk, subsequently decreasing due to mixing with the outer shear layer and the ambient conditions. In the predicted results this behaviour was not observed; the centreline total pressure remained at atmospheric pressure after the normal shock, since the Euler solution can not model the mixing effects that were occurring. The authors reported an oscillatory phenomenon around the convergence criterion, to which they attributed the disagreement in their results.

Observations of unsteadiness in Euler calculations of underexpanded jets were also reported by Matsuda et al. [34]. They observed oscillations in moderately underexpanded sonic jets and suggested that a completely time-averaged solution independent of the grid resolution can not be expected. Only with large numerical damping, either by applying course grids or introducing excessive levels of artificial dissipation, could a stable solution be expected. The unstable behaviour of the jet was due to Kelvin-Helmholtz instabilities at high Reynolds number, excited by a feedback loop (see section 1.2.4). The oscillating or quasi-steady solution obtained was compared to Schlieren photographs with long (33ms) and short (1.1μs) exposures and showed reasonable qualitative agreement to the short exposure photographs. A time average of the quasi-steady solutions, on the other hand, showed reasonable agreement to the long time exposure images. To validate the code quantitatively, the shock cell wavelength, Mach disk diameter and its location were compared to experimental data [1]
with an excellent agreement. Although Euler methodologies are efficient and are able to model the essentially inviscid features of the initial shock containing region, downstream of this region the method is inappropriate. The mixing rate is dependent on viscous effects and these must, therefore, be adequately modelled if the shock cell decay, potential core length and downstream profiles are to be correctly predicted. The unsteady effects observed in these calculations will also be damped to some extent by the viscous terms present in Navier-Stokes solutions.

A parabolised Navier-Stokes (PNS) method, called SCIPVIS, has been developed by Dash et al. [35-37]. Parabolised methodologies assume that the shear stresses in the streamwise direction are small compared to those in the radial direction and are hence neglected. In the SCIPVIS code an inviscid analysis was employed for the shock containing near field region, with the PNS solver for the mixing layers and transitional regions. This model has been used in various studies incorporating several variants of two-equation turbulence models. Calculations employing the SCIPVIS code required a co-flow of around 9% of the maximum jet velocity to be applied in order to stabilise the calculations. An analysis of the effect of this co-flow [16] found that even low levels of co-flow tended to reduce the mixing rates and hence increase the length of the shock containing potential core region. Extrapolation of the results suggested a 20% increase in the potential core length, for a co-flow of 9%.

The SCIPVIS methodology was shown by Dash et al. [37] to predict accurately many of the features of supersonic ($M_e = 2$), moderately underexpanded jets, including the first shock cell location and its wavelength. However, the shock cell structure was found to be underpredicted when using the $k$-$\varepsilon$ turbulence model and thus the dissipation, either numerical or physical, was too large. This was improved by the inclusion of a compressibility correction within the turbulence model, which applied a factor to reduce the turbulent viscosity. Seiner et al. [38] applied the same model to sonic as well as supersonic moderately underexpanded jets and found that for sonic jets the shock cell structure was grossly overpredicted, compared to available experimental data. It appeared that the model was totally incapable of modelling the much reduced shock cell structure that occurs with sonic jets compared to supersonic jets. The use of a compressibility correction for sonic jets reduced the accuracy further, since the compressibility correction reduced the turbulent viscosity and hence also the already underpredicted mixing rate.

Abdol-Hamid and Wilmoth [39] employed the SCIPVIS code to assess multiscale turbulence effects in moderately underexpanded jets by using a two length scale turbulence model. The
results showed similar trends to those found by Dash et al. [37] and Seiner et al. [38]. For supersonic jets the shock cell decay was reasonably predicted, but for sonic jets the structure was overpredicted. Better results could be obtained by using more corrections to the turbulence models. However, it was not clear whether these modifications were addressing physical issues or correcting inaccuracies caused by the numerical scheme. The SCIPVIS code, being a parabolised solver, can not account for elliptic effects shown to be important in sonic jets. The effect of the imposed co-flow may also differ between sonic and supersonic cases.

Chuech [16] applied the SCIPVIS code to moderately underexpanded jets, both sonic and supersonic, in order to assess the effects of the nozzle flow profile on the downstream structure. Two nozzle conditions were considered, slug flow and fully developed pipe flow. However, since the SCIPVIS model is inviscid in the shock containing region, it is difficult to imagine what effect the nozzle conditions might have on this part of the flow. Predictions for the two conditions were compared to corresponding experimental data sets for the shock containing region. However, slug flow was only applied to supersonic jet calculations, whilst fully developed flow was applied to sonic jets. For supersonic, slug flow the shock cell structure was slightly underpredicted, whilst for sonic, fully developed flow it was grossly overpredicted. This was believed to be the results of the profile of the nozzle flow, since the SCIPVIS model would essentially see both slug flow and fully developed flow no differently, whilst experimentally the results could differ. However, it is clear from the results presented in previous work using exactly the same model [38], that this difference was primarily due to the failure of the model to deal satisfactorily with the increased mixing rate occurring in sonic jets. It is therefore difficult to draw conclusions from this work as to the effect of nozzle profiles on the calculations. It is clear, however, that PNS methodologies are unsuitable for sonic underexpanded jet calculations.

An axisymmetric laminar Navier-Stokes model has been applied by Obayashi [40] to the underexpanded supersonic afterbodies of rockets with specific application to the space shuttle. The model employed a high order TVD scheme. Good results were found using this model at near flight conditions, even though the model was laminar. For application to aerospace and especially to combustion from accidental releases a laminar model is inappropriate; turbulent mixing is significant to the growth of the shear layers and turbulence is a key parameter in combustion.
A highly underexpanded jet of NPR = 6.76, corresponding to the experimental data of Donaldson and Snedeker [6], has been modelled with both Euler and Navier-Stokes codes by Palacio et al. [41] using the Phoenics computer code [42]. Both methods employed a first order accurate finite volume scheme, which is generally reported to be too dissipative and smear shock cells unacceptably. This smearing was greatly reduced by using very fine grids. For NPR = 6.76, the grid had 100 axial by 30 radial cells, with 80 cells in the first 3 axial diameters and 20 radial cells in the nozzle. Although a fine grid was employed, the number of cells for the computation was kept to a modest level by using a very small domain, 4.5 by 1 diameter, obviously limiting the data to the near field shock cell structure. The centreline Mach number and contours were presented, showing a comparison to the experimentally measured Mach disk location of Donaldson and Snedeker [6]. However, no comparisons were shown to the centreline pressure or velocity data from the experimental data. For both the inviscid and viscous solutions, a Mach number of 3.4 before the normal shock was predicted; behind the shock the viscous solution had a Mach number of 0.56 whilst the inviscid solution was almost stationary. Both solutions predicted two Mach disks, but their locations were considerably downstream of the experimentally measured locations. Donaldson and Snedeker [6] measured two Mach disks at this pressure ratio; in contrast Ewan and Moodie [3] only observed a second Mach disk for NPR greater than 14. The Mach number contours showed the expected Mach disk features for the first Mach disk, although the normal shock had a very small diameter. The second Mach disk did not display any of the expected features, with no normal or reflected shock cells apparent. Without a more detailed comparison to the available literature it is difficult to determine the performance of this first order model and whether the application of a very fine mesh successfully overcomes the problems of artificial dissipation, common to all first order methods. In particular, there was no comparison of results applying different mesh resolutions. This approach may be successful for the near field region, however its more general application is restricted by excessive computational requirements.

Kim et al. [43] applied a Reynolds averaged Navier-Stokes code called PARC to both sonic and supersonic moderately underexpanded jets. The code attenuated the downstream shocks too rapidly, but with grid refinement especially in the axial direction this could be reduced. The initial coarse grids had 141x71 cells for a sonic jet of NPR = 3.323. The predicted results showed attenuation of the centreline Mach number after the third shock cell. The fine grid, with 421x71 cells, predicted seven shock cells, with very good agreement to the
experimental data. Unfortunately, the presented results only extended for 12 axial diameters so it is impossible to assess its ability to model the potential core length and downstream profiles. In addition, no information is given as to the overall domain dimensions or the use of any mesh expansion which are required in order to allow the mesh spacing to be calculated.

Lakshmanan and Abdol-Hamid [44] employed an implicit, upwind, Navier-Stokes methodology to study the effect of corrections for compressibility, pressure dilatation and asymmetry on the accuracy of the k-ε model. They also considered the effect of inlet boundary velocity profiles. Only supersonic moderately underexpanded jets were considered and not sonic nozzles. Reasonably good agreement was found with the experimental data of Seiner and Norum [10] for the shock containing region, although the shock cell structure was slightly underpredicted. The effect of radial grid resolution was found to be small, whilst the axial resolution was not considered. The correction to the k-ε model only affected the solution after the third shock cell, reducing the shock cell damping and increasing the wavelength. No downstream results were presented.

Both moderately underexpanded and highly underexpanded jets have been studied by Cumber et al. [45, 46] using the same Navier-Stokes solver and the k-ε model, with application to pipeline release problems. The model was a second order, Godunov type scheme, with a compressibility corrected k-ε turbulence model. An adaptive rectangular mesh was employed, with adaptation being achieved by overlaying successive layers of grids. No more detail were given as to the nature of the adaptive meshing or the numerical methods employed.

For moderately underexpanded sonic jets three cases were considered. The first corresponded to the NPR = 2.27 case which was studied experimental by Chuech [16], with a fully developed exit flow from a sonic nozzle. Radial mean velocity and turbulent kinetic energy (k) profiles, taken five diameters downstream of the nozzle, were presented to show the effects of grid refinement. The grid resolution study showed that, as expected, the resolution of the shear layer improved with increasing levels of grid refinement; it did not show the effect of grid resolution on the shock cell structure or the downstream mixing. Radial profiles of the mean velocity, taken 10 diameters downstream of the nozzle exit, comparing the turbulence model with and without the compressibility correction, showed an excellent agreement with the experimental data [16] with the compressibility correction. In the case of
the turbulent kinetic energy profiles, considerable disagreement was found, both with and without the compressibility correction. The level of agreement was found to decrease at an axial location $20$ nozzle diameters downstream of the nozzle. The centreline axial profile was also presented, but the scale used showed the downstream profile rather than the near field shock containing region. In the nearfield region the experimental results do not show the oscillating shock cell structure because the experimental technique employed (LDA) which can not sufficiently resolve these feature. However, the measured mean velocity was considerably lower than the predicted mean velocity in this region.

The second two sonic jets cases were for an air jet, $\text{NPR} = 3.88$, corresponding to the velocity data of Birch et al. [12] and a natural gas jet, $\text{NPR} = 3.56$, corresponding to the mixture fraction data of Birch et al. [13]. The results presented for both cases were for the far field only and showed a better agreement with the experimental data without the inclusion of compressibility correction.

The results for sonic jets did not consider the shock cell structure, only the downstream mixing. However, the shock cell structure was shown, and compared to the data of Seiner and Norum [10], for a supersonic jet with an exit Mach number of $2.0$ and $\text{NPR} = 2.74$, but in this case the downstream mixing was not shown. For the standard $k$-$\varepsilon$ model the shock cell structure was attenuated far too rapidly, whilst the compressibility corrected version improved the results considerably, but the agreement to the experimental data [10] was still inadequate. Results showing good agreement to the experiments were achieved by reducing one of the modelling constant in the $k$-$\varepsilon$ model and scaling the axial co-ordinate to match the shock cell wavelength. Similarly to the results from SCIPVIS, discussed earlier, the shock capturing performance is not clearly reported for sonic jets, where the shock cell structure is more difficult to predict accurately than for supersonic jets.

For highly underexpanded jets only sonic nozzles were studied by Cumber et al. [46]. The effect of grid resolution was again only shown on a single radial profile, in this case for $\text{NPR} = 6.76$, and thus the effect on the shock structure was not known. The predicted Mach disk diameter and location were compared with several experimental data sets [1, 3, 23, 24] and a reasonable agreement was shown, with the compressibility correction having no effect. For $\text{NPR} = 6.76$ several radial profiles were compared to the experimental data of Donaldson and Snedeker [6], with good agreement. All other results presented and compared to the literature considered only downstream velocity or mixture fraction profiles. It was found that the better downstream results were obtained using the compressibility correction; the opposite to that
found for moderately underexpanded jets. As might be expected, the accuracy of the results decreased with increasing pressure ratio. At these pressure ratios a more complex compressibility correction was employed including a pressure dilatation term; this was found not to improve the results. Mach number contours at NPR = 6.76 were also presented showing clearly the Mach disk and its features. A second Mach disk as suggested by Donaldson and Snedeker [6] at this pressure ratio and modelled by Palacio et al. [41] was also predicted here, whilst the centreline plots at higher pressure ratios show no shock structure after the initial Mach disk. This behaviour was observed experimentally by Ewan and Moodie [3].

Finally, it is worth mentioning the effect that an adaptive meshing technique may have on the results. It was stated in both papers by Cumber et al. [45, 46] that up to five levels of grid refinement were used in the calculations. This suggests that different grids could be employed in each case and as the results and particularly the shock cell resolution will depend on this, some effects may be those of the mesh refinement. For example the increased shock cell resolution found with supersonic jets and the compressibility correction could be due to a finer grid that may have been generated by the adaptation technique because higher gradients will be found in mixing layers with the compressibility correction, because of reduced spreading rates. It is also the case that with a rectangular grid, refinement at one location will affect all other point on the same grid line.

Although considerable progress has been made in the numerical modelling of underexpanded jets, few models have been presented in the literature that can model both the shock containing region and the downstream mixing, especially for sonic jets and without an imposed co-flow. Euler solutions cannot deal with the downstream mixing; results are limited to the predicting the first few shock cells. PNS methods, although reasonably successful for supersonic flows, fail to model the rapid dissipation of the shock cell structure in sonic jets, and also require a co-flow to be imposed. Navier-Stokes methodologies have been shown to be effective for either the near field or the far field results, although issues such as turbulence compressibility and numerical dissipation must be considered. However, few models have been shown capable of solving both the near and far field region especially for highly underexpanded sonic jets. This may partly be due to the lack of data covering both the near and far field of highly underexpanded jets.
1.2.4 Unsteady Features

From the earliest experimental studies of underexpanded jets, unsteady behaviour has been observed. Love et al. [1] observed the jet deflecting from the axis in an alternate fashion, with a vortex pattern resembling a vortex sheet. Powell [47] observed that strong density gradient existed in the turbulent region of underexpanded jets, displacing it laterally in an alternate formation.

Donaldson and Snedeker [6] observed a low frequency flapping instability whilst taking pressure probe measurements in moderately and highly underexpanded sonic jets. Long time exposure Schlieren photographs (20ms), which were effectively time averaged, were employed to demonstrate the considerable dependence of the jet spread on the pressure ratio. Two distinct regions were found as the pressure ratio was increased. Intense instabilities occurred as the pressure ratio increased from NPR = 2.18, decreasing again by NPR = 3.0. Even greater instabilities were then observed as the NPR increased further, seemingly centred on NPR = 3.41. By NPR = 3.78, when the first Mach disk was observed, the instabilities decreased, and did not increase again in the range of pressure ratios studied. The authors suggested that this behaviour was a unique function of the apparatus used. However, other work has shown that, although the behaviour can be influenced by, for example, the presence of reflecting surfaces and the nozzle lip thickness, the behaviour observed here is common to all underexpanded sonic jets.

Gutmark et al. [48] used Schlieren photography to study underexpanded jets in the NPR range 2 to 15. For NPR = 2.14, a weak shock cell structure was observed in the first three diameters, followed by a more turbulent flow downstream. This jet structure was axisymmetric. At NPR = 2.42 the now stronger oblique shock cell structure was followed by a braided structure; asymmetric vortex structures appeared to be excited from around three diameters downstream of the nozzle. This lead to a substantial increase in the apparent jet spread rate. By NPR = 4.25 a normal shock was observed in the first shock cell accompanied by a decrease in the jet spread rate. As the pressure ratio continued to increase then so did the size of the Mach disk, leading to an increased jet spread rate in the region of the first shock cell. By NPR = 14.62 a strong Mach disk dominated the flow and strong acoustic waves appeared to emanate from the jet.

The noise from underexpanded jets is known to consist of three components, turbulent mixing noise, broadband shock associated noise and screech. The noise from perfectly
Chapter 1. Introduction

expanded supersonic jets consists entirely of turbulent mixing noise, thus allowing the turbulent noise to be studied separately from any shock related noise components.

Turbulent mixing noise contains two components. Small scale turbulence is composed of small random fluctuations, whilst large scale structures are organised, wavelike structures which may exhibit length scales of an order of magnitude similar to the mean flow. As shown in perfectly expanded supersonic jets, the large-scale turbulent structures are the dominant turbulent noise producers [49, 50] and can be modelled as hydro-dynamic wavelike instabilities, using quasi-linear stability theory [51, 52]. The peak turbulent mixing noise appears in a region of 60° to the downstream jet axis and contains a broadband spectra with a peak Strouhal number of between 0.1 and 0.25, depending on the jet temperature and Mach number. Upstream of the nozzle the spectra is of a much lower intensity. This lower intensity noise is thought to be due to fine scale turbulence.

For shock containing jets, broadband shock associated noise is the dominant noise component in the upstream direction. At large angles to the downstream axis (q) there is a well defined peak frequency. As q decreases the peak frequency increases and the bandwidth becomes more spread. The mechanism suggested for this noise component is the weak interaction between the large scale structures of the jet flow and the oblique shock cell structure. Based on this mechanism a simple theory for the peak broadband frequency and a noise intensity scaling factor were developed [53]. Models for the near and far field acoustic spectra for slightly underexpanded [54] and moderately underexpanded jets have also been developed [55].

Screech tones are high amplitude discrete frequency tones observed only in shock containing jets. The frequency and number of tones observed is heavily dependent on the pressure ratio and the tones are principally radiated upstream of the nozzle. Screech is the least understood noise mechanism in underexpanded jets and at present its prediction is limited. The main reason for this is its sensitivity to external factors, such as the presence of reflecting surface and the nozzle lip thickness [56, 57].

Experimental observations have highlighted the strong relationship between the large scale structures in jet flows and screech tones. From his observation of large scale structures in jets, Powell [47] developed a feedback mechanism for screech. In the mechanism small disturbances are shed at the nozzle and propagate downstream, increasing in amplitude. Their subsequent interaction with the shock cell structure around the third or fourth shock
cell cause oscillations, producing sound waves which propagate back upstream towards the nozzle, where they induce the small disturbances, completing the feedback loop.

The frequency of the dominant instability mode decreases rapidly as the fully expanded jet Mach number increases [58]. However, for circular jets, the frequency-NPR curve is not smooth, it consists of a number of overlapping curves each of which corresponds to an oscillation mode of the jet. This is the cause of the variations of jet spread rate observed by Gutmark et al. [48] and Donaldson and Snedeker [6]. Powell et al. [59] identified 3 mode types, varicose (toroidal, axisymmetric), sinuous and helical, split into 4 stages on the frequency curve for underexpanded jets up to a pressure ratio of 6, whereas Tam [56] and Gutmark et al. [48] observe only toroidal and helical modes. Where the curves overlap more than one mode exists at that pressure ratio giving rise to more than one screech tone. Switching between helical and axisymmetrical modes, and its effect on jet spreading rate, has been studied using Schlieren photography and near field pressure measurements by Gutmark et al. [48], who found that although 2 modes appeared to be observed under certain conditions this was actually a rapid switching between the two modes.

The modelling of screech tones is at present limited, although the principal mechanism involved is well known. Tam et al. [60] presented an empirical formulation that showed a reasonable agreement with experimental results for the dominant frequency. However, an empirical method such as this cannot account for many of the effects of, for example, nozzle lip diameter [57] reported in the literature. Few other prediction methods for screech frequency and no predictive methods for screech amplitude have been published.

The use of CFD to model the acoustic properties of supersonic jets has been limited. Mankbadi et al. [61] demonstrated the application of large-eddy simulations (LES) to the computation of supersonic jet noise, obtaining the noise field directly from the Navier-Stokes solver. However, the model was axisymmetric and the authors note that their results were only meant to show qualitative agreement to the literature. For underexpanded jets Seiner et al. [38] used the SCIPVIS code to obtain the shock-cell wavelength for use in an empirical calculation of broadband shock noise. Kim et al. [43] modelled the mixing noise in imperfectly expanded sonic and supersonic jets, but not the broadband shock noise or screech components. They used the PARC code, employing the $k$-$\varepsilon$ model, as previously developed for shock free supersonic jets to calculate turbulent shear stresses. An analytical method was then employed to obtain sound pressure levels for the turbulent mixing noise.
1.3 Review of Lifted Diffusion Flame Literature

A reacting underexpanded jet will occur when a combustible gas at high pressure, issued through an orifice, is ignited by a suitable ignition source. At the boundary of the release, where mixing is occurring, the mixture fraction will be within combustible limits. However, in these regions, close to the nozzle, the strain rate will be such that a flame can not be sustained. Some distance downstream, usually beyond the potential core, the strain rate will be such that a flame can be stabilised and a large, high momentum diffusion flame will form. The distance to the base of the flame from the nozzle rim is known as the stand-off or lift-off height.

Experimental studies of non-premixed combustion in underexpanded jets are very few and the measurements taken are very limited. This is essentially due to the extreme difficulties and costs involved in taking measurements of large flames. However, lifted subsonic diffusion flames have been studied in more detail. In many ways subsonic diffusion flames are very similar to their underexpanded counterparts, once the initial shock containing region has been dissipated. Numerical modelling of underexpanded reacting jets has been performed even less, with no references to whole field computations found anywhere in the literature.

In this section a review will be made of work relating to underexpanded reacting jets. However, initially a brief review of subsonic attached and lifted diffusion flames is presented. A discussion of modelling details will not be presented here; this can be found in section 4.2.

1.3.1 Attached Diffusion Flames

The basic structure of a diffusion flame is well documented, and is described in most standard combustion texts [e.g. 62-65]. A diffusion or non-premixed flame occurs when initially separated fuel and oxidant come together in the reaction zone through the processes of molecular and, in the case of most practical systems of interest, turbulent mixing. In diffusion flames combustion occurs at the interface of the fuel and oxidant streams and the rate of combustion is principally dependent on their rate of mixing; the mixing time is usually more than an order of magnitude greater than the chemical time. In laminar flames the molecular mixing is the controlling factor, but in turbulent flames the turbulent mixing will dominate the molecular mixing.
Most work concerning non-premixed combustion considers annular diffusion flames where a central fuel supply is surrounded by a concentric air supply. Two types of flame may be formed in this arrangement. Underventilated flames occur when the supplied air results in an overall mixture fraction below that required for stoichiometric combustion and a fan shaped flame results. Overventilated flames are the result of an overall mixture fraction above stoichiometric giving rise to a closed elongated flame shape. In the work considered here, the diffusion flame occurring when an underexpanded jet of a hydrocarbon issuing through a circular aperture into quiescent air is ignited will form an overventilated annular diffusion flame. Although no concentric co-flow of oxidant will be imposed, an induced co-flow will develop due to the flow physics.

Typically a hydrocarbon diffusion flame appears as a luminous yellow or orange coloured flame. This colour is due to the oxidation of soot in the flame. Because the soot may react away from the main reaction zone the visible height of a diffusion flame is significantly higher than the true height of the flame. This has given problems in the measurement of flame heights, since the only accurate method to determine the true flame height is to measure the properties within the flame, such as species concentrations to determine the location of the reaction zone. As a result many experimental studies have measured the visible height of diffusion flames.

A large body of experimental data is available in the literature relating to diffusion flames. This data ranges from simple flame observations, such as visible flame heights, to more recent, non-intrusive measurements of quite detailed properties of flames. However, much of this more detailed measurement is restricted to idealised flames, often of low speed and therefore data for high momentum flames is often limited to the more basic properties. This is particularly the case for underexpanded diffusion flames.

The visible flame heights of subsonic diffusion flames have been studied by various workers [e.g. 28, 66, 67] and many empirical relationships are available. Flame heights for laminar diffusion flames have been shown analytically and experimentally to be proportional to the volumetric flow rate of the fuel and inversely proportional to the molecular diffusivity. However, in the case of turbulent flames the flame height is not dependent on the flow velocity, only the diameter of the nozzle.

Sonju and Hustad [67] performed experiments using both methane and propane for small and large scale experiments. Nozzle diameters between 2mm and 80mm were employed, with jet
exit Mach numbers between 0.03 and 1. Temperature profiles, mean concentrations, flame heights and lift-off heights were all measured. It was found that flame heights and diameters scaled with Froude Number. Gunther [68] presented a comprehensive review of turbulence measurements in both premixed and non-premixed flames, whilst Becker and Yamazaki [69] measured temperature, momentum flux and temperatures with exit velocities up to 100ms$^{-1}$.

More recently many Laser based technique have been used for flame measurements [e.g. 70-75]. These techniques include CH and OH LIF, PIV, Mie scattering, Raman scattering and LDA, measuring mean and fluctuating component of mixture fraction, velocities, temperature and species concentrations, in addition to properties such as the scalar dissipation rate. However, this data is limited to simple geometries on a small laboratory scale.

Much work has been performed on the numerical modelling of low velocity diffusion flames. Since mixing is often the rate limiting factor, it is reasonable in many systems to assume that the chemical rate is infinite. This leads to a situation where the stoichiometric contour is viewed as an interface between burnt and unburned gases, and can thus be seen as the location of a very narrow reaction zone or flame sheet [e.g. 76]. Therefore, with an assumption of infinite rate chemistry, it is the role of the combustion and turbulence modelling to predict the location and shape of the flame sheet, and to determine the properties of the fluids at the interface. This is an idealised situation since the actions of heat and mass transfer allow reaction to occur on each side of the flame sheet; the reaction zone is wider than that found in premixed combustion. Generally, the flame front is assumed to exist at the location of maximum temperature, which coincides with the location of maximum concentration of the major products. This type of idealised profile has been validated experimentally [e.g. 77]. Several excellent reviews of the numerical study of attached diffusion flames can be found in the literature [e.g. 76, 78, 79].

1.3.2 Lifted-Diffusion Flames

Lift-off and blow-out are important features of many flames, both premixed and non-premixed. A subsonic jet diffusion flame becomes detached from its burner and forms a stable lifted flame when the flow velocity is increased beyond the lift-off stability limit. If the velocity continues to increase beyond the blow-out limit then the flame will blow itself out.
Lift-off heights were studied extensively by Kalghatgi [28], for hydrogen, propane, methane and ethylene flames with a wide range of diameters and velocities. It was found that the lift-off height was independent of the nozzle diameter for a given gas and varied linearly with jet velocity. In addition the lift-off height was found to be inversely proportional to the maximum laminar flamespeed squared. With appropriate non-dimensional grouping the lift-off heights for the four gases could be collapsed onto a single curve. For blow-out [80] it was found that the blow-out velocity is linearly dependent on the nozzle diameter.

A number of studies have computed lifted turbulent diffusion flames, either to predict the flame properties or the lift-off height. Fairweather et al. [81] developed a model to predict high momentum reacting jets in a cross-flow, based on the $k$-$\varepsilon$ turbulence model and a laminar flamelet model using a prescribed probability density function (pdf) for the mixture fraction. In this model the chemistry is assumed to be fast compared with the mixing rate. Lift-off was modelled with a mixing rate switch, whereby when the turbulence time scale fell below a critical value no reaction occurred. This model was further developed [82] to predict soot concentrations and radiation from reacting non-premixed flames in a cross-flow.

Sanders and Lamers [83] employed a stretched laminar flamelet model with the $k$-$\varepsilon$ model for lifted turbulent diffusion flames. Temperature contours and centreline axial velocity were presented for a $71\text{ms}^{-1}$ methane flame. The velocity showed a reasonable agreement to experimental results except in the region close to lift-off, but no experimental comparisons were shown for the temperature. Beeri et al. [84] used the coherent flame sheet model together with a model for soot generation and oxidation, and the discrete transfer radiation model for lifted, high momentum vertical and horizontal flames. The predictions were in good agreement with published experimental data, apart from those for radiation.

Only a limited number of studies have been found that present predictions of lift-off height as a function of velocity. Lift-off height predictions based on cold flow simulations have been reported [83, 85, 86] where the lift-off height is extracted by applying a condition based on a strain parameter at the stoichiometric contour. Sanders and Lamers [83] employed both the cold flow and reacting calculations to predict the lift-off height for jet velocities of $40\text{ms}^{-1}$ to $71\text{ms}^{-1}$. Various models were compared and a good agreement was found between the measured and computed lift-off heights. Bradley et al. [87] employed a partially premixed flamelet model and again found good agreement to experimental lift-off heights over a range of $20\text{ms}^{-1}$ to $100\text{ms}^{-1}$. Byggstoyl and Magnussen [88] also found a good agreement between
the computed and measured lift-off heights, although the model had to be recalibrated for different nozzle diameters.

1.3.3 Underexpanded Jet Diffusion Flames

Few references containing experimental data relating to underexpanded jet diffusion flames have been found in the literature. McCaffrey and Evans [89] considered very large methane diffusion flames and measured lift-off heights and flame heights for flames up to 500MW both subsonic and sonic. For sonic jets an effective Mach number was proposed to characterise the jets. Lift-off height data was presented as a function of this effective exit Mach Number. The lift-off height was defined in this work as the distance from the lowest visible luminosity of the flame to the plane of the nozzle. The data presented was quite scattered, although it appeared to be independent of the nozzle diameter, with no change in trend observed at the transition to sonic flow. The recorded lift-off heights were very large, up to 5m in some cases. The data regarding lift-off height was not complete enough and contains too much scatter to provide quantitative data for analysis. The flame height data was less scattered and was presented as flame height normalised by the actual nozzle diameter, against effective exit Mach number; this seemed to be adequate to scale the data.

Lift-off heights for underexpanded jets have been studied more thoroughly by Birch and Hargrave [90]. Two measuring procedures were employed in this study, based on the findings of Birch et al. [91], where the relationship was established between blow-out, orifice diameter and stagnation pressure using a pseudo-diameter analysis [12]. For subsonic jets the blow-out velocity is an approximately linear function of diameter. However with a sonic exit velocity and a diameter where blow-out for subsonic jets would have occurred, it was found that restabilisation could be achieved if the pressure was increased sufficiently. It was also found that for diameters above around 30mm a stable flame was attained for all driving pressures. The data was correlated successfully by the pseudo-diameter approach. Below the critical diameter the flame was only stable once the pressure was increased sufficiently. This destabilisation pressure was found to increase as the nozzle diameter decreased.

For unconditionally stable nozzle diameters, (50.6mm and 111.2mm) steady state measurements were recorded, whereby the lift-off height was recorded 50 times a second for at least 25 seconds at several pressure ratios. The second procedure was used for those flames that were not unconditionally stable. Here the pressure ratio was reduced transiently
and the lift-off height recorded as the pressure ratio fell. Data in this way was obtained for six more orifice diameters.

It was found that as the pressure ratio increased then so did the lift-off height, asymptoting at higher pressure ratios. The lift-off height \((H)\) increased with increasing diameter, whilst the lift-off height normalised by the nozzle diameter \((H/D)\) decreased. For smaller diameters the asymptotic lift-off height reached a minimum value of around 1.8 meters as the diameter of the orifice was reduced. This was similar to the findings in subsonic jets where lift-off heights are independent of nozzle diameter [28]. The authors suggested that the increased lift-off height at large diameters was likely to be linked to the potential core and the shock cell structure. If \(H\) was to remain constant as the diameter increased then this would lead to \(H/D\) decreasing. In underexpanded jets the potential core length normalised by diameter is constant, and thus as the diameter increases the flame stabilisation zone would eventually move into the shock containing region. Due to high strain rate this is not possible and hence the flame stabilises further downstream.

Only one study, that of Gore et al. [29], has been found in the literature that measures properties in underexpanded jet flames. Here, measurements were taken of mean temperatures along the axis of seven large scale natural gas diffusion flames, with 96% methane. Measurements of total pressure near to the nozzle exit indicated that the flames were underexpanded with NPRs in the range 2.9 to 4.2. The tests were divided into two groups, those with 76mm diameter nozzles giving around 100MW flames and those with 102mm nozzle diameters resulting in around 200MW flames. The temperature measurements were taken using an array of twenty thermocouples supported by 24m high towers, but unfortunately no other variables were measured and the accuracy of the results was severely limited by the varying wind conditions. The flames observed were up to 30m high and were blue in the lower third of the visible portion and yellow in the remainder and were lifted from the burner by between 15 and 20 diameters, although no measurements of the lift-off heights were presented.

The work of Gore et al. [29] also represents the only numerical predictions of underexpanded jet flames found in the literature. Calculations were performed by employing a pseudo-source, such that the initial shock containing region was not computed, and thus the calculations were insensitive to the initial conditions of the experiments. The computations applied a laminar flamelet combustion model and the results showed only limited agreement to the experimental measurements. The disagreement of the computed and experimental
results was mainly attributed to the effect of wind disturbance on the flames; wind speeds of up to 2\( \text{ms}^{-1} \) were recorded during the tests. It was also noted that the effects of flame lifting was not adequately treated and that the methods for treating the effects of the underexpansion were not satisfactory.

Work has been reported in the literature regarding the prediction of supersonic hydrogen-air diffusion flames \[92\] employing a laminar flamelet model and extending it to account for compressibility effects. Although this case possesses some similarities to the underexpanded jet flames studies here, without the complication of the shock containing region and because hydrogen-air supersonic flames are attached to the nozzle rim the modelling requirements are significantly different.

Traditionally, high speed flows have been computed with density based methodologies which are accurate and efficient for high speed flow, but at best inefficient for low speed flows. For low speed flows, including studies of diffusion flames, incompressible, pressure based codes have been employed. In order to be able to predict the whole field of underexpanded diffusion flames accuracy is required for both the high speed, compressible, shock containing region and also for the downstream, lower speed flow regions where reaction occurs. It is for this reason that the numerical prediction of this problem is difficult and has not been attempted often. In addition, uncertainties regarding turbulence and combustion modelling for high speed flows and the need to predict lift-off heights accurately increases the complexities of the problem, whilst a lack of suitable experimental data makes validation difficult.

1.4 Objectives

The aims of this work can be split into two areas. The first is the development of an accurate and efficient flow solver for computing non-reacting, underexpanded jet flows at all pressure ratios. The second is the implementation of suitable combustion models to enable underexpanded diffusion flames to be computed.

Pressure based methodologies have previously been employed for the study of underexpanded, non-reacting jets with pressure ratios that lead to a maximum Mach number of less than 2.0. The use of a pressure based methodology extended to compressible flow is desirable since it is applicable to all flow regimes. The first objective of this work is to extend compressible, pressure based methods to allow the computation of flow at all Mach numbers, without reducing the shock capturing capability, and in particular to allow highly
underexpanded jets containing normal shocks to be computed. This will focus on developing better numerical schemes for the pressure correction equation. In addition to developments of the numerical schemes for the pressure correction equation modern, higher order numerical schemes will be applied to all equations in order to improve the accuracy of the flow solver. Further improvements in accuracy are also sought by considering compressibility effects on turbulence, grid resolution and boundary conditions. Extensive evaluation of the model in regard to the available experimental data will then be performed. Of particular importance for the subsequent reacting calculations is the ability to predict accurately the downstream mixing properties and particular attention will be paid to this.

Previous numerical studies of underexpanded jet diffusion flames are very limited, and no previous whole field studies have been reported in the literature. The objective here then is to implement well known combustion models into the previously developed non-reacting methodology in order to predict underexpanded jet diffusion flames. These flames are lifted from the nozzle rim and special attention will be paid to the prediction of this lift-off height. The model for lift-off will be validated by computing subsonic lifted diffusion flames that have previously been studied more frequently and underexpanded flames for which experimental data is available. Other experimental data for underexpanded jet flames is severely limited and therefore validation of the results will be based on the validation of the various components of the methodology.
Chapter 2. Non-Reacting Methodology

2.1 Introduction

2.1.1 Requirements of the Methodology

An underexpanded jet issuing into quiescent surroundings is a severe test of any numerical scheme. The scheme must be robust and accurate for both compressible, supersonic regions and for incompressible, subsonic regions where the flow may stagnate. In addition shock waves, both oblique and normal, must be adequately resolved, as must compressible, turbulent, shear layers.

Many methods are available that can treat certain aspects of the flow. Density based methods are typically applied to compressible flows, and a large literature exists in this area. However, these methods are at best inefficient in the incompressible limit. Pressure based methods on the other hand, developed for incompressible flow, have been successfully applied to many applications. They are used in almost all commercial codes. In recent years they have been extended to high speed compressible flows but, although robust at all speeds they are known to excessively smear shock waves.

In this chapter a review of numerical methods for high speed flows will first be presented, followed by a discussion of their application to flow at all speeds and the need for a pressure based scheme. Pressure based schemes will then be reviewed and in particular their application to compressible flows. Following this the methodology for the work in this thesis will be presented. Firstly the governing equations, including the treatment of turbulence and compressibility effects, followed by an explanation of the numerical techniques employed. Finally some solution details will be discussed.

2.1.2 Numerical Methods for Shock Containing Flows

There are two distinct methods for calculating flows containing shock waves in the field of computational fluid dynamics. Shock fitting schemes use the conservation equations to calculate the flow field and the likely location of shock waves, but employ analytical methods, such as the Rankine-Hugoniot relations, to calculate the actual properties of the shock wave. In contrast, shock capturing techniques apply the conservation equations to the whole flow field including any shock waves, without any special treatment. In this way the shock waves are captured automatically. Shock fitting can be useful for many simple flows,
Chapter 2. Non-Reacting Methodology

however multi-dimensional flows containing many interacting shock structures become too complicated. Therefore, in this thesis shock capturing techniques will be the primary interest and shock fitting techniques will not be discussed further.

Early work applying numerical methods to capture shock waves were hampered by the generation of unphysical oscillations at the leading and trailing edge of shock waves. This occurred because a shock wave in atmospheric air has a thickness of around 0.3μm. It is unrealistic, therefore, to consider resolving the physical thickness of a shock wave and thus when calculated on a computational grid the velocity gradients, and hence viscous dissipation, will be considerably smaller than in reality. This leads to an underprediction of the total pressure loss, but the conservative form of the Navier-Stokes equations guarantee that the Rankine-Hugoniot relations are satisfied. Thus, the numerical method is forced to create additional viscous losses in order to achieve the correct total pressure drop and hence satisfy the Rankine-Hugoniot relations. This is achieved by the generation of under and overshoots at the leading and trailing edges of the shock waves.

To create non-oscillatory schemes requires an understanding of the truncation errors of discretisation schemes. This is often accomplished by formulating the modified equation, which is the actual partial differential equation solved by the numerical scheme as opposed to the initial governing equation. It is derived by a Taylor expansion of each term in the numerical algorithm and, by comparison to the initial transport equations, allows the truncation errors to be identified. These truncation errors can be either dispersive or dissipative; dispersive terms are generated by odd order truncation errors, whilst dissipative terms are generated by even order terms. It is the dissipative terms that enable a numerical scheme to become non-oscillatory. The additional numerical dissipation created by these dissipative terms enable the correct total pressure loss to be attained and hence the Rankine-Hugoniot relations can be satisfied without the need for under and over shoots. However, if too much numerical dissipation, often referred to as artificial viscosity, is added the resulting shock structure will be highly smeared over many grid cells.

Central difference schemes do not generate any dissipative terms and as such will always generate oscillatory solutions, unless some explicit artificial dissipation is added. Upwind schemes, on the other hand, generate large dissipative terms and produce very stable schemes. However, these are often inaccurate due to the large dissipative terms smearing shock waves and shear layers, since the artificial viscosity will significantly exceed the physical viscosity. The design of accurate non-oscillatory schemes for shock containing
flows is one of the major areas of research in CFD and has lead to many developments in
numerical methods for all types of flows. In particular, schemes with intelligent dissipation
terms have been developed, such that a minimum amount of dissipation is added to prevent
spurious oscillations. These will be discussed in the next section.

2.1.3 Review of Density Based Methods for High Speed Flows

There exists a huge body of research into shock capturing techniques for high speed flows
using density based methods. Classical schemes such as those of Lax and Wendroff [93, 94]
and MacCormack [95, 96] have been in common use for many years and have had
reasonable success in many flows. These schemes are relatively simple compared to many of
the more modern schemes, and hence require much less computational resources. However
better schemes are sought to improve accuracy and robustness.

The Lax-Wendroff scheme is a classic example of an explicit second order scheme with
combined space and time discretisation. It is the simplest, explicit, second order scheme
available and its limitations are well
In the presence of steep gradients spurious
oscillations will develop and stability is governed by the CFL (Courant-Friedrichs-Lewy)
condition.

Central differencing is successfully used in many modern schemes by explicitly introducing
artificial dissipation terms to control under and over shoots and allow shock capturing, whilst
preventing the formation of unphysical expansion shocks. This idea was first introduced by
Von Neumann and Richtmyer [97], and often takes the form of second and fourth order
dissipation terms [98].

A large proportion of modern high-resolution techniques can be classed as upwind
differencing schemes. Upwind schemes utilise concepts from characteristic theory in order to
determine the direction of spatial differencing. First order upwind methods are stable and
produce oscillation free solutions for all flows. This robustness comes at the expense of poor
shock capturing; unacceptable shock smearing results from this highly dissipative scheme.
Other sharp gradients, such as shear layers, can be equally devastated. Numerical analysis of
upwind schemes shows that they are equivalent to a central difference scheme with the
addition of artificial dissipation terms. Thus, upwind schemes are strongly linked to central
difference schemes.
Chapter 2. Non-Reacting Methodology

First order upwind is an example of a monotone scheme. A monotone scheme does not allow the creation of new extrema, or any unphysical discontinuities; very desirable features in the computation of shock containing flows. However they cannot have an order of accuracy greater than one.

There are two common classes of upwind schemes. Flux Vector Splitting schemes (FVS) [99-101] introduce information based on the sign of the Eigenvectors, leading to the flux terms being split and discretised directionally according to the direction and speed of the flow propagation. More information is introduced with Godunov’s scheme [102] where each cell is assumed to be a uniform slab of fluid with discontinuities at the cell interfaces. This gives a first order monotone scheme. If this discontinuity is treated as a local Riemann problem then various Riemann solvers, either exact [103, 104] or approximate [105-107], can be used to obtain the time evolution. These schemes are often referred to as flux difference splitting (FDS).

The upwind schemes described above are only first order accurate and very dissipative. To obtain the desired accuracy either very fine computational meshes in the region of high gradients, or higher order schemes are required. The extension of first order schemes to higher orders is straightforward; first order upwind space differences are replaced by their higher order counterparts. However, because higher order schemes can not be monotone, oscillations can develop, particularly when high Peclet number (Pe) flows are combined with steep gradients. Examples of higher order upwind schemes include the second order upwind scheme [108] and QUICK (Quadratic Upstream Interpolation for Convective Kinematics) [109].

The choice thus far appears to be between robust, oscillation free solutions with poor shock capturing ability which require the use of very fine meshes to give adequate shock capturing performance and hence incur large computational expense, or higher order upwind scheme with better shock resolution, but at the expense of over and undershoots. The solution to this problem are the non-linear limiters of bounded schemes.

Accurate shock capturing schemes, with low diffusive properties and no oscillations, can be constructed that switch between accurate, but oscillatory methods for smooth regions and non-oscillatory monotone schemes in the region of sharp gradients. An early example of this type of scheme are the flux corrected transport (FCT) schemes [110]. Here, an initial solution is obtained using a first order monotone scheme. This initial solution is then corrected by
adding higher-order terms to the solution, but only where oscillations are not generated. A limiter is applied that detects where unphysical phenomena occur and in these regions the added correction term is limited. Where necessary the limiter will prevent the addition of any higher-order corrections, thus maintaining the low order monotone scheme. In this way oscillation free solutions are obtained that are mostly higher order. These limiters, based on the local flow properties, are non-linear and are the basis for much of the current high-resolution shock capturing schemes. For both FVS and FDS, extensions to higher order can be achieved by flux reconstruction [111], such as the MUSCL (Monotone Upstream-Centred Schemes for Conservation Laws) [103] formulation and the application of a suitable limiter.

The most commonly used non-linear limiters are those that enforce the TVD (Total Variation Diminishing) condition as proposed by Harten [112]. These limiters combine accuracy with monotonicity and entropy conservation. TVD schemes are extensively used in many classes of methodologies, both upwind and central difference; implicit and explicit [e.g. 103, 106, 111-115]. In upwind schemes they are applied to limit gradients during higher order flux reconstruction. They can be combined with schemes such as Lax-Wendroff to enforce monotonicity where required. Some of the resulting schemes may not always be formally TVD, especially in multi-dimensions, but high resolution, non-oscillatory scheme still results. Swanson and Turkel [116] developed a TVD central difference scheme by using the TVD limiter to control the addition of artificial dissipation to the scheme. All the TVD type methods discussed are essentially one-dimensional schemes, extended to multi-dimensions by using an operator splitting method. More recently multi-dimensional upwind methods have been developed [117].

Another class of schemes are known as ENO (Essentially Non Oscillatory) [118]. These high-order schemes are based on Godunov’s scheme. In contrast to TVD schemes, which are first order accurate across discontinuities, ENO scheme are uniformly high-order accurate.

Earlier in this section it was stated that the time step for explicit schemes was limited by the CFL condition. This condition states that a wave should not be able to propagate a distance greater than the smallest cell dimension in any time step and thus restricts the time step that can be applied. Implicit schemes eliminate the time step dependence on the CFL condition; implicit schemes are unconditionally stable. Much larger time steps are allowable with obvious reductions in computational expense. However, the time steps for time dependent problems are still limited by accuracy requirements, since they must still be smaller than the
Chapter 2. Non-Reacting Methodology

The smallest time scale of the unsteady phenomena. On the down side, implicit schemes require more CPU time per cycle than explicit schemes.

2.1.4 Flow at all Speeds

The development of high resolution shock capturing techniques discussed above was essentially motivated for application to high speed aerodynamics, hydrodynamics and in particularly hypersonics and were therefore designed only for the supersonic and transonic regimes. Most methods formulate the continuity equation to calculate density in a simultaneous time marching scheme; the pressure is obtained via an appropriate equation of state and a suitable form of an energy equation to calculate temperature. When applied to subsonic flows, below a Mach number of around 0.3, density based schemes suffer from a considerable decrease in convergence rate and many can become unstable and inaccurate. This occurs because in the incompressible limit the density becomes constant and the pressure is then driven by machine round-off errors. To overcome this problem, several approaches have been used such as artificial compressibility [119] and preconditioning [120] which suppresses the acoustic waves. The need for these artefacts shows that a time marching solution of the conservation equations in their original form is not suited to low speed, viscous flows [121]. Indeed although some of these fixes work for subsonic flows, they are not able to handle mixed flows of low and high speed.

The weakness of density based methods to handle low speed flow is the very strength of pressure based methods, which were developed for incompressible flows and are successful in many applications, including those with recirculation and chemical reaction. In pressure based methods the continuity equation is reformulated into a constraint equation for either pressure or pressure correction. The principle advantage of using pressure as the primary flow variable is that pressure changes are finite at all Mach numbers, thus allowing schemes that are genuinely applicable to all flow speeds to be developed.

It is clear that an underexpanded jet exhausting into a quiescent domain contains regions at all speeds from zero flow regions to supersonic. It is therefore essential that the numerical scheme is capable of handling all flow speeds and therefore a pressure based method is the obvious approach. A review of pressure based methods and their extension to compressible flows is described in the next section.
2.1.5 Review of Pressure Based Methods

Early pressure based methods were generally of the pressure substitution type, of which the Marker and Cell (MAC) method [122] is the best known. This method employs a Poisson equation for pressure and a staggered mesh arrangement. The incompressible pressure correction scheme was originally developed in the form of the SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm [123] and has many similarities to the MAC type methods. However, in this case an equation is derived for pressure correction, rather than for pressure directly, from which a velocity correction is derived. The method is deemed as semi-implicit because all the conservation equations are solved implicitly, only the pressure correction equation is partially explicit. Specifically, the pressure-velocity linkage is explicit due to the truncation of the momentum equation in its formulation. In pressure correction methods the continuity equation is recast into an elliptic equation for pressure and the following steps are taken:

1. The implicit momentum equations are solved using a guessed pressure (or the last estimate of pressure) which will give a velocity field that does not satisfy continuity
2. A pressure correction is calculated that forces the velocity field to satisfy continuity
3. The pressure is corrected using the pressure correction
4. The velocities are updated using correction formulae
5. Other scalar equations are solved, for example temperature, turbulence or concentrations
6. The new pressure is now treated as the guessed pressure for the start of the next iteration

The SIMPLE family of schemes effectively form a Poisson equation for pressure or its correction and the continuity equation is seen as an equation constraining the pressure field to be that which results in a velocity field satisfying continuity.

Although not strictly part of the SIMPLE methodology, several features have traditionally been employed in conjunction with it, for incompressible flows applications. The use of central differencing in the pressure correction equation for the incompressible Navier-Stokes equations results in the well known odd-even decoupling problem which can lead to a checkerboard effect. This occurs because the pressure at any location is not directly affected by the velocity at that point, but only that of adjacent points (see Appendix A). The common
way to overcome this problem is to use a staggered grid. Alternatively, Rhie and Chow [124] overcame this problem on a collocated grid by introducing a smoothing procedure that amounts to an extra fourth order dissipation term. Collocated grids have considerable advantage for non-orthogonal grids and if techniques such as multi-grids are to be used.

The convective terms have often been discretised using rather crude first order upwind schemes. It is well known that second order central difference schemes are much more accurate than first order schemes, but as the Pe number increases above around two, then oscillation are generated. Hence the very dissipative upwind schemes, such as hybrid or power law [123] are commonly employed. More recently higher order upwind schemes have been applied such as QUICK [109], but care has to be taken over the method of implementation if a three point stencil is to be retained [125]. Although more resistant to spurious oscillations than central differencing, these schemes can still cause under and over shoots in the region of steep gradients. Bounded version of higher order upwind schemes, that become monotone where oscillation are likely to occur, have been used to reduce the artificial dissipation. Example of this type of limited higher order schemes include SHARP [126], and SMART [127]. These schemes are based very closely on TVD principles. Leonard and Drummond [128] have recently discussed why first order upwind schemes should not be used, presenting examples of better schemes.

The solution of the equations for pressure based methods usually differ from those of density based methods. Typically, density based methods solve all the equations in a coupled manner. In pressure based methods a segregated approach is almost always used. Here, each equation is solved separately within an iterative procedure. The two major advantages of this type of solution are the reduced matrix size, requiring less steps to solve, and the ease at which extra equations, such as for turbulence or scalar concentrations, can be implemented, without the need to alter any other equations. The major drawback of an iterative scheme is the requirement of under relaxation in order to give stability. This can severely reduce the convergence rate of complex flows. Time dependent calculations can be performed with pressure correction algorithms by retaining the time derivatives in the discretisation, such that at each time step a converged solution is obtained, with iterations within each time step as required. If sufficiently small time steps are used the need for iteration is reduced and often eliminated. Issa [129] has shown that the time marching technique applied to pressure correction algorithms is essentially the same as under-marching, proposing a relationship between the time step and under-relaxation factor.
Many variations of the SIMPLE algorithm have been proposed such as SIMPLER [123], SIMPLEC [130], and PISO [129], but all the methods follow the same basic principle. The variants are mainly aimed at improving efficiency and convergence behaviour.

The extension of pressure based methods to compressible flow was initially undertaken by Issa and Lockwood [131]. The main difference between compressible and incompressible pressure correction algorithms is the linkage between pressure and velocity, which must take into account density changes in compressible flow. The idea of the continuity equation as a constraint equation still remains, but now the correct pressure is that which results in velocities from the momentum and density from the equation of state which together satisfy continuity. Issa and Lockwood [131] proposed a linearisation of the mass flux in terms of density and velocity separately, such that fluctuations of both velocity and density became important. This linearisation of the mass flux has been employed in several subsequent studies [132-134].

In order to achieve stable and oscillation free solutions the density terms in the pressure correction equation were all upwinded adding rather large quantities of artificial dissipation. A stabilising mechanism was required in the compressible pressure correction method because the Poisson equation for pressure is elliptic in nature; information can travel in all directions. This is suitable for subsonic flows, but not supersonic flows where the hyperbolic nature of the equation set must be addressed in order to retain stability and capture shocks. Stable solutions for all Mach numbers were obtained by Issa and Lockwood [131] using the linearisation and density upwinding, however, the shock structure was severely smeared.

Ways of controlling the levels of artificial dissipation have been a major part of the research regarding pressure based scheme applied to compressible flows. Multi-grid methods and adaptive artificial dissipation were developed by Rhie [135] and Rhie and Stowers [136]. The adaptive scheme had similar limiters to those of TVD schemes to control the added dissipation. This method gave better shock resolution whilst still being oscillation free. Demirdzic et al. [137] used the linearisation of Issa and Lockwood [131] for a collocated pressure correction scheme. In this method a mixed discretisation of upwind and central differencing in a pre-defined ratio was applied to the density term in the pressure correction equation and also to the convective terms in the other transport equations. This was found to have a beneficial effect on the shock capturing since it reduced the added artificial dissipation. However, the amount of upwinding required was problem dependent and not adaptive, it was applied in all regions.
A different approach was used by McGuirk and Page [138], where momentum per unit volume \((\rho u)\) rather than momentum per unit mass \((u)\) was solved for in the momentum equations. This modification removed the need for a linearisation of the mass flux term; the momentum equation now gives a direct link between pressure and mass flux. Better shock resolution was also achieved, probably because the mass flux \((\rho u)\) varies much more smoothly than velocity across a shock wave. However, upwinding of the density terms in the pressure correction equation was prevented; the only density terms appearing were in the time derivative. Without this upwinding, unstable solutions occurred in supersonic regions due to the elliptic nature of the pressure correction equation. In order to stabilise the scheme a retarded pressure function was employed. This method is essentially an extension of the retarded density function [139] and amounts to the addition of an artificial viscosity term to the momentum equations. The retarded pressure function is dependent on the local flow conditions, therefore artificial dissipation was only added where the local Mach number was above a specified reference value. The method gave very promising shock capturing for one-dimensional nozzles, and has been shown by Page [140] to resolve accurately moderately underexpanded impinging jets up to a Mach number of 2.0. Above this the scheme became unstable.

Recently pressure based schemes have been used with TVD and ENO type limiters with the aim of reducing dissipation. Zhou [141] adopted many of the feature of McGuirk and Page [138], such as solving for mass flux in the momentum equations and a retarded density function (similar to retarded pressure). Several convective discretisation scheme were assessed such as hybrid, second-order upwind and MUSCL. Lai et al. [142] also used a TVD limiter for convective fluxes within a pressure based algorithm. Kobayashi and Pereira [143] developed a scheme based around ENO schemes. In this method a highly accurate oscillation free density based scheme was used in regions where the Mach number was above 0.3. Below this a conventional pressure correction type scheme was applied.

### 2.1.6 Outline of Methodology

Following a review of the relevant literature regarding pressure based methods applied to compressible flows, the following outline methodology is proposed for the present study.

The momentum equations will be solved for momentum \((\rho u)\) as opposed to velocity following the work of McGuirk and Page [138]. This gives substantial benefits to the shock capturing ability of the solution.
A staggered grid will be used to prevent decoupling and the well known checkerboard effects. It is noted that collocated grids can be employed with the addition of Rhie and Chow [124] smoothing, but on orthogonal grids no benefits would be gained from this.

A second order TVD scheme will be employed for the convective differencing. In addition the hybrid scheme will also be applied to assess the effects of the low order differencing schemes extensively applied in pressure based methodologies.

A dissipation mechanism, either implicit or explicit, is required to attain stability in pressure based methods applied to supersonic flow due to the elliptic nature of the pressure correction equation. Upwind differencing has been applied in several schemes either alone [130-134] or combined in fixed proportions with central differencing [137] to give schemes stable at all Mach numbers. Upwind schemes do excessively smear shock waves and shear layers. The alternative approach used central differencing with an explicit dissipation scheme such as retarded pressure [140], which only applies the dissipation in high speed regions. These methods are however, limited to a maximum Mach number of around 2. In the current work features of both schemes will be applied to give shock resolution equal to the retarded pressure scheme, but also stable over all Mach numbers. This will involve a local Mach number dependent blending of central and upwind differencing. In addition, modifications to the retarded pressure formulation will be presented in order to extend the range of pressure ratios over which it is applicable and the results obtained compared to those with the blended differencing scheme.

2.2 Governing Equations

2.2.1 Navier-Stokes Equations

The well known Navier-Stokes equations of motion for a compressible, viscous, Newtonian, heat conducting perfect gas can be written in conservative form using Cartesian tensor notation as:

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

Momentum:
Chapter 2. Non-Reacting Methodology

\[
\frac{\partial \rho}{\partial t} \left( \rho u_i \right) + \frac{\partial \rho}{\partial x_j} \left( \rho u_i u_j \right) = -\left( \frac{\partial P}{\partial x_i} \right) + \frac{\partial \tau_{ij}}{\partial x_j} \quad 2-2
\]

Total Enthalpy:

\[
\frac{\partial \rho}{\partial t} \left( \rho H \right) + \frac{\partial \rho}{\partial x_j} \left( \rho u_j H \right) = \frac{\partial P}{\partial t} + \frac{\partial}{\partial x_j} \left( u_i \tau_{ij} - q_i \right) + \dot{Q} \quad 2-3
\]

Scalar Transport:

\[
\frac{\partial \rho}{\partial t} \left( \rho Y_k \right) + \frac{\partial \rho}{\partial x_j} \left( \rho u_j Y_k \right) - \frac{\partial}{\partial x_j} \left( \frac{C_p \mu_i}{S_c} \frac{\partial}{\partial x_j} Y_k \right) = \dot{\omega}_k \quad 2-4
\]

The stress tensor, heat-flux vector and total enthalpy are given by:

\[
\tau_{ij} = \left( \mu' + \frac{2}{3} \mu \right) \frac{\partial u_i}{\partial x_j} \delta_{ij} + \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad 2-5
\]

where \( \mu \) and \( \mu' \) are the first and second viscosities respectively. For air the second viscosity is very small and it is therefore assumed here that \( \mu' = 0 \). The heat flux \( (q) \) is given by:

\[
q_i = -\frac{C_p \mu}{Pr} \frac{\partial T}{\partial x_j} \quad 2-6
\]

and the total enthalpy \( (H) \) is given by:

\[
H = h + \frac{1}{2} u_i u_i \quad 2-7
\]

where the specific enthalpy is defined in terms of the specific internal energy \( (e) \) as:

\[
h = e + \frac{P}{\rho} \quad 2-8
\]

2.2.2 Treatment of Turbulence

Ideally the preceding equation set would be solved directly to cover all length and time scales involved in the turbulent flow. Although this type of direct numerical simulation (DNS) has been applied to some simple flows, its application to real flows is limited by the available computer power and storage capacity [e.g. 144, 145]. A DNS calculation requires that the grid resolution captures the smallest eddies in the flow, with a time step capable of resolving the shortest time scales. The number of cells required for resolution of the smallest scales can be estimated as:

\[
N = \text{Re}^\gamma \quad 2-9
\]
Thus for a low Reynolds number flow of 5000, more than 200 million cells would be required. This would require the most powerful super computers available to solve. For more realistic Reynolds numbers of around 50,000 the number of cells required is of the order $10^9$, and is well beyond the capacity of any available computer. These requirements prohibit the use of a DNS methodology for practical studies, although they are used to great effect to obtain detailed information of simple fundamental flows which can not be obtained experimentally. This information can be used to develop and calibrate the models that are applied to more complex flows.

A second approach, known as large eddy simulation (LES) [e.g. 146, 147], uses a filter to separate the flow into two scales. The larger scale is solved directly, whilst the smaller scales are treated by subgrid models. In this way the very large resources required for DNS are considerably reduced. However, the computational resources required are still considerable and the technique has not been adequately applied to compressible and in particularly shock containing flows. This method has therefore not been considered for the current work.

The most common manner of dealing with turbulent flows, and the one used here, applies an averaging procedure, whereby the fluctuating phenomena are not resolved directly, but their effect on the mean flow equations is represented by turbulence models. There are two commonly applied methods, conventional time averaging (sometimes called Reynolds averaging) and mass-weighted averaging (also called Favre averaging). In the current work mass weighted averaging will be employed for all variables apart from pressure and density, since the resulting equations are of a simpler form, very similar to their laminar equivalents. Reynolds averaged equations lead to extra terms consisting of the products of fluctuating components that can be difficult to model. It has been recommended in several previous works that Favre averaging should be employed for both reacting flows and compressible flows [e.g. 148-150].

In conventional time averaging a mean quantity can be defined as:

$$\bar{q} = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{t-\Delta t}^{t+\Delta t} q(t) \, dt$$  \hspace{1cm} 2-10$$

The instantaneous pressure and density can then be expressed in terms of a Reynolds averaged and a fluctuating component:

$$P(x_i,t) = \bar{P}(x_i) + P'(x_i,t)$$  \hspace{1cm} 2-11$$

$$\rho(x_i,t) = \bar{\rho}(x_i) + \rho'(x_i,t)$$  \hspace{1cm} 2-12$$
A mass weighted mean velocity can be defined as:

\[
\bar{u}_i = \frac{\rho u_i}{\bar{\rho}}
\]

and the instantaneous velocity is:

\[
u_i(x,t) = \bar{u}_i(x) + u'_i(x,t)
\]

where \(u''\) is the superimposed velocity fluctuation. Multiplying the above equation by density gives:

\[
\rho u_i = \rho (\bar{u}_i + u'_i) = \rho \bar{u}_i + \rho u'_i
\]

and time averaging gives:

\[
\overline{\rho u_i} = \overline{\rho \bar{u}_i + \rho u'_i}
\]

From the definition in eq. 2-13

\[
\overline{\rho u_i} = \overline{\rho \bar{u}_i}
\]

Thus:

\[
\overline{\rho u'_i} = 0
\]

Static temperature, total enthalpy, static enthalpy and species mass fraction can be defined in a similar fashion to the velocity:

\[
T(x,t) = \tilde{T}(x) + T''(x,t)
\]

\[
H(x,t) = \tilde{H}(x) + H''(x,t)
\]

\[
h(x,t) = \tilde{h}(x) + h''(x,t)
\]

\[
Y_k(x,t) = \tilde{Y}_k(x) + Y''_k(x,t)
\]

where:

\[
\tilde{T} = \frac{\rho T}{\bar{\rho}}, \tilde{h} = \bar{\rho h}, \tilde{H} = \tilde{h} + \frac{1}{2} \bar{\rho} \bar{u} \bar{u}_i + \frac{1}{2} \frac{\rho u'_i u''_i}{\bar{\rho}}, \tilde{Y}_k = \frac{\rho Y_k}{\bar{\rho}}
\]

With the above relations, the mass weighted conservation equations can be defined.

**2.2.2.1 Continuity**

Substituting eq. 2-12 and eq. 2-15 into eq. 2-1 gives:

\[
\frac{\partial}{\partial t} (\bar{\rho} + \rho') + \frac{\partial}{\partial x_j} (\rho \bar{u}_j + \rho u'_j) = 0
\]
Chapter 2. Non-Reacting Methodology

Time averaging the terms in this equation leads to:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_j} (\overline{\rho \overline{u}_j}) = 0$$  \hspace{1cm} 2-25

### 2.2.2.2 Momentum

Substituting eq. 2-11, eq. 2-14 and eq. 2-15 into eq. 2-2 gives:

$$\frac{\partial}{\partial t} (\overline{\rho \overline{u}_i} + \rho u'_i \overline{u}_j) + \frac{\partial}{\partial x_j} (\overline{\rho \overline{u}_i \overline{u}_j} + \rho u'_i \overline{u}_j + \rho u'_j \overline{u}_i) = -\frac{\partial}{\partial x_i} (\overline{P} + P') + \frac{\partial \tau_{ij}}{\partial x_j}$$  \hspace{1cm} 2-26

Time averaging and rearranging gives:

$$\frac{\partial}{\partial t} \overline{\rho \overline{u}_i} + \frac{\partial}{\partial x_j} (\overline{\rho \overline{u}_i \overline{u}_j}) = -\frac{\partial \overline{P}}{\partial x_i} + \frac{\partial}{\partial x_i} (\overline{\tau_{ij} - \rho u'_i u'_j})$$  \hspace{1cm} 2-27

The last term on the right hand side represents the turbulent diffusion of momentum, often referred to as the Reynolds stress. Other than this extra term, the Favre-averaged momentum equations are identical to the laminar versions (eq. 2-2), but with the instantaneous terms replaced by the appropriate averaged equivalent.

### 2.2.2.3 Total Enthalpy

Substituting eq. 2-11, eq. 2-15 and eq. 2-20 into eq. 2-3 gives:

$$\frac{\partial}{\partial t} \left( \overline{\rho H} + \rho H' \right) + \frac{\partial}{\partial x_j} \left( \overline{\rho H \overline{u}_j} + \rho H' \overline{u}_j + \rho u'_j \overline{H} + \rho u'_j H' \right)$$

$$= \frac{\partial}{\partial t} (\overline{P} + P') + \frac{\partial}{\partial x_j} (u'_j \tau_{ij} - q_j) + \dot{Q}$$

Time averaging gives:

$$\frac{\partial}{\partial t} \overline{\rho H} + \frac{\partial}{\partial x_j} \overline{\rho H \overline{u}_j} = \frac{\partial}{\partial t} \overline{P} + \frac{\partial}{\partial x_j} \left( \overline{u'_j \tau_{ij}} + u'_i \overline{\tau_{ij}} \right) - \frac{\partial}{\partial x_j} \overline{q_j} - \frac{\partial}{\partial x_j} \rho \overline{H u'_j} + \dot{Q}$$  \hspace{1cm} 2-29

### 2.2.2.4 Scalar Transport

Substituting eq. 2-11, eq. 2-15 and eq. 2-22 into eq. 2-4 gives:

$$\frac{\partial}{\partial t} \left( \overline{\rho Y_k} + \rho Y_k' \right) + \frac{\partial}{\partial x_j} \left( \overline{\rho Y_k \overline{u}_j} + \rho Y_k' \overline{u}_j + \rho u'_j Y_k' + \rho u'_j Y_k' \right)$$

$$- \frac{\partial}{\partial x_j} \frac{C_p \mu l}{Sc} \frac{\partial}{\partial x_j} (\overline{Y_k} + Y_k') = \dot{\omega}$$

Time averaging gives:
Chapter 2. Non-Reacting Methodology

For the non-reacting model, described in this chapter, the energy and scalar transport equations are not required. In the place of the energy equation constant total enthalpy is assumed, which is described in the following section. The implementation of equations for energy and scalar transport are described in section 4.4.

2.2.3 Constant Enthalpy Assumption

For non-reacting flows the purpose of the energy equation is to provide the temperature field so that density can be derived from an equation of state. Thus, in incompressible regions the energy equation is redundant. In the Euler limit, assuming no heat addition, the total enthalpy equation (eq. 2-29) reduces to:

\[
\frac{\partial}{\partial t} (\tilde{P} \tilde{H}) + \frac{\partial}{\partial x_j} (\tilde{P} \tilde{u}_j) = 0
\]

The energy equation becomes important in highly compressible region where the Mach number is high, but the flow in these region does not exhibit particularly viscous behaviour since the Reynolds number is usually high and convection dominates. It therefore seems reasonable to apply eq. 2-32 for isenthalpic jet calculations. This applies to most typical experimental configurations where the total temperature of the plenum is equivalent to that of the ambient. For steady, compressible flows, eq. 2-32 reduces to Bernoulli’s equation. This implies that the total enthalpy is constant along a streamline, and for homenergic flows the enthalpy is constant. Thus, the energy equation can be approximated by a statement of constant enthalpy:

\[
\tilde{H} = \frac{\gamma}{(\gamma-1)} \frac{\tilde{P}}{\rho} + \frac{1}{2} \tilde{u}_i \tilde{u}_i = \text{const}
\]

The constant enthalpy assumption is applied to most of the non-reacting calculations in this thesis, to reduce computational effort and to aid stability. Many compressible pressure based methods employ a similar assumption to avoid computing a transport equation for energy because of the unstable behaviour that often results. However, for heated or reacting jet calculations the solution of an energy equation is usually required. A description of the steps taken to implement a full energy can found in section 4.4.6. The applicability of a constant enthalpy assumption for non-reacting jets has been assessed numerically and the results of this can be found in section 5.3.1.
2.3 Closure: Turbulence Modelling

In order to close the Favre averaged Navier-Stokes equations listed in section 2.2.2 the Reynolds stress and turbulent scalar gradient terms must be evaluated. There are many different closure methods or turbulence models available, all with differing complexities and performance.

2.3.1 Review of Available Turbulence models

The many turbulence models available range from very simple models which require very little computational effort, but are often only applicable to a very narrow range of problems, to very complex models that may require massive resources, but are generally more accurate over a wider range of applications. All models do have in common the need for empirical input in some form to obtain closure. At present the three main groups of turbulence model are first order models, higher order models and algebraic stress models.

2.3.1.1 First Order Models

Central to first order turbulence models is the assumption that there exists an analogy between the action of viscous stresses and Reynolds stresses on the mean flow. Bousseinesq proposed that the Reynolds stresses could be linked to the mean rate of deformation; in this way a turbulent viscosity \( \mu_t \) was defined. Similar gradient assumptions can also be made for the turbulent scalar fluxes. With the definition of a turbulent viscosity the Favre-averaged Navier Stokes equations become identical to those of laminar flow, with the laminar viscosity replaced by the effective viscosity - the sum of the laminar and turbulent viscosities. Several assumptions are implicit within the Boussinesq approximation, the most important of which assumes that \( \mu_t \) is isotropic, such that the ratio between Reynolds stress and mean rate of deformation is the same in all directions. This assumption does fail in many flows and can give inaccurate predictions.

The task of first order turbulence models is to compute the turbulent viscosity and they are generally classified by the number of additional partial differential equations (pde's) employed in order to do this. The simplest methods are the zero-equation or mixing length models. Since they do not introduce any additional transport equations they require very little computational effort, solving only algebraic expressions for the turbulent viscosity, which is obtained from either a specified or calculated mixing length. The most commonly used mixing length model is the Baldwin-Lomax model [151]. Zero-equation models have proved
reasonably successful for certain flows, particularly attached, thin, shear layers, although their accuracy decreases as separation approaches and they become seriously erroneous once separation occurs. However, their appeal remains as a very simple and cheap model that can give accurate results if applied within their limitations.

The next increase in complexity introduces the one-equations models. Here, one transport equation is solved, in most cases for turbulent kinetic energy ($k$). The turbulent viscosity is then obtained from $k$ and a specified mixing length. However, these models are not particularly popular since two-equation models offer a much more general solution for only a modest increase in computational expense. For this reason, two-equation models are the most widely used, since they are relatively simple, requiring modest resources and are comprehensively validated over a wide range of flows.

Two-equation models solve transport equations for turbulent kinetic energy and, in various forms, a length scale. By far the most popular of the two-equation models is the $k$-$\varepsilon$ model of Jones and Launder [152], although others models, such as the $k$-$W$ [153] model, where $W$ is loosely regarded as the average value of the fluctuations of the vorticity of the fluid, have also been applied in some cases. In the $k$-$\varepsilon$ model, transport equations are solved for turbulent kinetic energy ($k$) and the rate of dissipation of turbulent kinetic energy ($\varepsilon$). Compared to zero- and one-equation models, many more effects, such as the transport of turbulence by the mean flow and its production and destruction can be accounted for. The $k$-$\varepsilon$ model has received widespread use principally because of its good performance in many industrially relevant flows; particularly bounded flows. For unbounded flows the performance is usually somewhat less accurate, whilst, because of its widespread use and validation, the limitations of the model are very well known. Weak shear layers, curved flows, swirling flows and rotating flows are all poorly predicted, whilst the spread rates of jets are overpredicted when the excess velocity is low. It should also be noted that this model was developed for incompressible flow and many of its assumptions are not directly relevant to compressible flow. In many applications the $k$-$\varepsilon$ model is used because it represents a good compromise between simplicity and generality.

2.3.1.2 Reynolds Stress Models

If the turbulence can not be assumed to have isotropic Reynolds stresses, then more complicated and expensive models are required. The Reynolds Stress Model (RSM) [e.g. 154] solves transport equations directly for the six Reynolds stresses and for the rate of...
Chapter 2. Non-Reacting Methodology

dissipation of turbulent kinetic energy. Terms such as diffusion, dissipation rate and pressure-strain correlations require modelling and the specification of constants; this can effect the performance in certain flows. The model is the most expensive classical model (i.e. one that uses Reynolds or Favre averaged Navier-Stokes equations), requiring seven additional transport equations. Although Reynolds stress models calculate all the Reynolds stresses directly and give very accurate results for some flows, inaccuracies similar to some of those with the $k-\varepsilon$ model are observed in, for example, free jets and confined recirculating flows and for the same reason - the turbulent dissipation. A very similar turbulence dissipation equation is used as in the $k-\varepsilon$ model, requiring modelling for closure. In addition, combusting flows with their large variations in density give very complex models in which error free solution can be difficult to obtain [150, 155].

2.3.1.3 Algebraic Stress Models

Algebraic Stress Models (ASM) [e.g. 156] can also account for anisotropies of the Reynolds stresses. Here only two transport equations, those for $k$ and $\varepsilon$, are required, along with a series of approximate algebraic equations. This method is only slightly more costly than the $k-\varepsilon$ model, whilst providing improvements in some flows. However, since ASM models effectively assume that convection and diffusion of Reynolds stresses are negligible, erroneous solution occur where this is not the case. Both the RSM and ASM models are not as well validated as the $k-\varepsilon$ model and thus much more care is needed when applying to new flows. In addition, the weakest component of the $k-\varepsilon$ model, the modelling of $\varepsilon$, is retained in a very similar form. The modelling of $\varepsilon$ is even more problematic and requires more empiricism for compressible flows.

2.3.2 The $k-\varepsilon$ Turbulence Model

The incompressible $k-\varepsilon$ model [152] defines the turbulent viscosity as:

$$\mu_t = C_{\mu}\frac{\bar{k}^2}{\bar{\varepsilon}}$$  \hspace{1cm} 2-34

where $k$ is the mass averaged turbulent kinetic energy:

$$\bar{k} = \frac{1}{2} \frac{\rho \bar{u}_i \bar{u}_i}{\bar{p}} = \frac{1}{2} \bar{u}_i \bar{u}_i$$  \hspace{1cm} 2-35

and $\varepsilon$ is the dissipation rate of turbulent kinetic energy:
Chapter 2. Non-Reacting Methodology

\[ \overline{\varepsilon} = \frac{\nu}{2} \left( \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right)^2 \] 2-36

Following the Boussinesq relations, the Reynolds stress can be evaluated using:

\[ -\overline{p} \overline{u}_i \overline{u}_j' = \mu \left[ \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right] - \frac{2}{3} \delta_{ij} \left( \mu_{\text{eff}} \frac{\partial \overline{k}}{\partial x_i} + \overline{p} \overline{\varepsilon} \right) \] 2-37

So the stress term in the momentum equation can be approximated by:

\[ \overline{\tau}_{ij} - \overline{p} \overline{u}_i \overline{u}_j' = \left( \mu_{\text{eff}} \right) \frac{\partial \overline{u}_i}{\partial x_j} + \frac{2}{3} \delta_{ij} \left( \mu_{\text{eff}} \frac{\partial \overline{k}}{\partial x_i} + \overline{p} \overline{\varepsilon} \right) \] 2-38

where the effective viscosity is:

\[ \mu_{\text{eff}} = \mu_t + \mu_r \] 2-39

The gradient diffusion hypothesis is also applied to the turbulent flux of scalar variables:

\[ \overline{p} \overline{u}_i \overline{\phi}' = -\frac{\mu_t}{\sigma_t} \frac{\partial \overline{\phi}}{\partial x_j} \] 2-40

The high Reynolds number \( k-\varepsilon \) model equations are [150]:

\[ \frac{\partial}{\partial t} \overline{p} \overline{k} + \frac{\partial}{\partial x_j} \left( \overline{p} \overline{k} \overline{u}_j - \frac{\mu_t}{\sigma_t} \frac{\partial \overline{k}}{\partial x_j} \right) = P_k - \overline{p} \overline{\varepsilon} \] 2-41

\[ \frac{\partial}{\partial t} \overline{p} \overline{\varepsilon} + \frac{\partial}{\partial x_j} \left( \overline{p} \overline{\varepsilon} \overline{u}_j - \frac{\mu_t}{\sigma_t} \frac{\partial \overline{\varepsilon}}{\partial x_j} \right) = \frac{\overline{\varepsilon}}{k} (C_{t1} P_k - C_{t2} \overline{p} \overline{\varepsilon}) \] 2-42

where the turbulent production is defined as:

\[ P_k = -\overline{p} \overline{u}_i \overline{u}_j' \frac{\partial \overline{u}_i}{\partial x_j} \] 2-43

In the case of high Reynolds number flows it is usual to ignore the laminar viscosity, since the turbulent viscosity is considerably larger.

The standard values for the model [157] are shown in Table 2-1 and are widely applied. They were originally calibrated to reproduce the correct results for three simple flows: the decay in time of homogenous turbulence, measurements of shear layers in local equilibrium and the log law of the wall in boundary layers.

The implementation of the \( k-\varepsilon \) has to be treated carefully in order to maintain robustness. The major issue here is the positivity of \( k \) and \( \varepsilon \). From the definition of the turbulent viscosity (eq.
2-34) a negative value of $\varepsilon$ is nonsense; there is no mechanism for any turbulence effects to reduce the effective viscosity below that of laminar viscosity. $k$ must also remain positive; physically a negative energy has no meaning. If either becomes negative, numerical failure often occurs.

<table>
<thead>
<tr>
<th>$C_{\mu}$</th>
<th>$C_{\epsilon 1}$</th>
<th>$C_{\epsilon 2}$</th>
<th>$\sigma_k$</th>
<th>$\sigma_\epsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.09</td>
<td>1.44</td>
<td>1.92</td>
<td>1.0</td>
<td>1.3</td>
</tr>
</tbody>
</table>

Table 2-1. Coefficients for the $k$-$\epsilon$ Model.

Being the most applied turbulence model, much is know about both the strengths and weaknesses of the $k$-$\epsilon$ model. Considering the many assumptions involved in its derivation its performance is often somewhat surprising. For example the model should not be accurate for recirculating flows, but has been found to be so in many applications. The same is also true for time-dependent mean flows. However, its limitations are many and must be understood when applying the model. In particular it is unable to account for rotational strain or shear and as mentioned is unable to account for anisotropy in the Reynolds stresses. Some of these problems can be particular severe for three-dimensional flows. For example, when the stress tensor and Reynolds stress tensor are not parallel then erroneous solutions will result.

A compressible version of both the $k$ and $\epsilon$ can be derived, to allow application of the $k$-$\epsilon$ model to compressible flow. The complexities introduced by extending the turbulence model to compressible flows can be demonstrated by examining the turbulent kinetic energy equation. Extension to compressible flow gives rise to the following equation [158]:

$$\frac{\partial}{\partial t} \overline{\rho k} + \frac{\partial}{\partial x_j} \overline{\rho \vec{u}_j \vec{k}} = -\frac{\partial}{\partial x_j} D_j + P_k + \phi + W - \overline{\rho \overline{\epsilon}}$$

where the diffusion ($D_j$), production ($P_k$), mean velocity-pressure interaction ($\phi$) and velocity-pressure fluctuation interaction ($W$) are defined as:

$$D_j = \frac{1}{2} \overline{\rho u_j u_j} \frac{\partial}{\partial x_j} \overline{\rho \vec{u}_j \vec{u}_j}$$

$$P_k = -\overline{\rho \vec{u}_j \vec{u}_j} \frac{\partial \overline{u_j}}{\partial x_j}$$

$$\phi = -\overline{u_j} \frac{\partial \overline{P}}{\partial x_j}$$
The increased number of terms in the compressible $k$ equation creates new closure problems; many of the required quantities are not available or easily modelled. The production, $P_k$, is obtained as for incompressible flow, whilst the dissipation is evaluated by its own transport equation. The diffusion term, $D$, can be modelled using the Boussinesq hypothesis:

$$\frac{\partial}{\partial x_j} D_j = \frac{\partial}{\partial x_j} \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j}$$

The terms representing mean velocity-pressure interaction and velocity-pressure fluctuation interaction can be combined to form what is commonly known as the pressure dilatation:

$$\phi + W = -u_j \frac{\partial P}{\partial x_j} + P' \frac{\partial u'_j}{\partial x_j}$$

This term has historically been neglected in many turbulence models. However, DNS analysis is beginning to show the importance of this term, even at moderate Mach numbers. At the present time several models have been proposed for this term. However, it is unclear how much advantage can be gained from the inclusion of such terms and which is the best to include. For these reasons the pressure dilatation has not been considered in the current work.

The above analysis simply considers the equation for $k$. A similar analysis for $\varepsilon$ [158] leads to more than twenty terms on the right hand side of the equation, all of which require modelling for closure. Since the $\varepsilon$ equation appears in both $k-\varepsilon$ and Reynolds stress models, much work is currently considering which are the important terms and how to achieve the most accurate modelling of them. Much of this work employs DNS, since it is virtually impossible to obtain the detailed information required via experimentation.

### 2.3.3 Turbulence in Compressible Flow

The treatment of turbulence in compressible flows is an area into which much work is required. Many of the complex effects that occur are either poorly understood or not known at all; a review of the effects of compressibility on turbulence has been presented by Lele [159].

Turbulence modelling in compressible flows is often handled by invoking Morkovin's hypothesis [160, 161]. This states that for Mach numbers below 5, the influence of density...
fluctuations on turbulence in turbulent boundary layers is negligible, although for compressible jets it may only be true for Mach numbers below 1.5 [161]. Thus, it would appear feasible to employ incompressible turbulence models to compressible flows up to moderate Mach numbers. For moderate Mach numbers, characteristics are observed similar to those for incompressible turbulence. For much larger Mach numbers strong interactions between vortices and shock waves cause acoustic phenomena to dominate. However, even for flows of Mach number less than 3, as the relevant Mach number in the turbulent flow increases, so the density and pressure fluctuations grow accordingly. Eventually, compressibility induced effects alter the structure and dynamics; resulting principally in a reduced spreading rate of mixing layers. This effect has been studied by several authors. Papamoschou and Roshko [162] performed the most extensive experimental study. The shear layer development was measured between two supersonic streams of various gases at free stream Mach numbers ranging from subsonic to high supersonic. In this way the effects of compressibility could be isolated from those of density and velocity ratios. Previous work [163, 164] had, in general, considered the effects of a single supersonic stream, where trends of decreasing growth rate with increasing Mach number were found, but their explanations often attributed this to the decreasing temperature and increasing density that accompanied the rise in Mach number. Papamoschou and Roshko [162] derived a frame of reference that allowed the spread rate to be solely dependent on the convective Mach number \( M_c \), which is the Mach number in a frame of reference convecting with the wave speed \( C_r \).

\[
M_c = \frac{U_i - C_r}{a_i}
\]

Data for the normalised shear layer growth rate against convective Mach number was presented, which showed that much of the reduction in spreading rate occurs whilst the convective Mach number is still subsonic, although the freestream velocity may be supersonic. This eliminated shock waves as the cause of reducing mixing, since they will not occur in the shear layer until the convective Mach number becomes supersonic.

Several reasons for the reduced growth rates are discussed. One theory is based around the increased removal of energy from the shear layer as the convective Mach number increases thus reducing the growth rate. This energy removal was thought to occur because a disturbance in a shear layer is more likely to perturb the flow away from the vortex sheet rather than in it as the convective Mach number increases.
Recently DNS work has begun to reveal the physical structure of compressible turbulence and shown that compressibility effects may be more important than previously thought. DNS on two-dimensional turbulence [165] has shown that when the initial density fluctuation levels \((p'/\rho)\) and the turbulent Mach number \((M_t)\) were sufficiently large, the initial large scale vortex structures of solenoidal turbulence decayed into shock like structures, embedded within the flow. Lee et al. [166] performed DNS on three-dimensional decaying isotropic turbulence to investigate the presence and influence of these ‘eddy shocklets’. They found that although dissipation due to compressible phenomena only accounted for 10% of the total dissipation, around the eddy shocklets the compressible dissipation was an order of magnitude higher than the solenoidal dissipation.

Based on these DNS findings, two works have developed a more physically based correction, with more general applicability. Zeman [167] and Sarkar et al. [168] independently identified dilatational dissipation as the cause of compressible effects on turbulence, and particularly the reduced spreading rate of compressible shear layers. The existence of pressure dilatation terms (see eq. 2-50) in both Reynolds Stress and turbulent kinetic energy equations have been well known for sometime, but are neglected in almost all turbulence models. A further term containing dilatation \((d')\) was found to be present in the \(e\) equation. This term appears to be an additional dissipation term and is therefore known as the dilatational dissipation \((e_d)\):

\[
\bar{p} e_d = \frac{4}{3} \mu \left( \frac{\partial u_i}{\partial x_j} \right)^2 = \frac{4}{3} \mu d'^2
\]

This term should only be significant if \(d'\) is large. In order to allow the pressure dilatation term to be neglected this is usually assumed to be small.

The effect of this dilatation is to generate a second dissipation term \((e_d)\) in the \(k\) equation. In the standard \(e\) equation (eq. 2-42), \(e\) is that due to solenoidal dissipation (now referred to as \(e_s\)), which is dissipation due to the transfer of the energy cascade into small scale turbulence. Thus the total dissipation then becomes:

\[
\bar{p} e = \bar{p} e_s + \bar{p} e_d
\]

Several models have been proposed for the dilatational dissipation. Zeman [167] modelled the dilatational dissipation as a function of the turbulent Mach number \((M_t)\), and the Kurtosis of the velocity field \((K)\), which is a function linked to the PDF such that:

\[
e_d = e_s c_d F(M_t, K)
\]
Sarkar et al. [168] used an asymptotic analysis to show that the compressible component of dissipation was a function of the turbulent Mach number squared:

\[ \varepsilon_d = \alpha_t M_t^2 \varepsilon, \]

where \( \alpha_t \) is a constant, whereby calibration using the data of Papamoschou and Roshko [162] led to a value of unity. Although both Zeman [167] and Sarkar et al. [168] found the dilatational dissipation to be dependent on the turbulent Mach number, the expressions derived give very different dependencies.

The model of Sarkar et al. [168] has been implemented in a RSM [169] and tested on a number of cases. The model reproduced the functional dependency of the mixing layer growth rate on the convective Mach number. The model has also been implemented into two-equation turbulence models [45, 170].

There are many works in the literature that apply the standard \( k-\varepsilon \) model to compressible flows with varying success [e.g. 134-143], many of them failing to consider the effects of compressibility on turbulence. More recently some of the effects of compressibility on turbulence have been considered, usually through empirical correction to the \( k-\varepsilon \) model so as to reproduce the experimentally measured growth rate dependence on convective Mach number.

Page [140] applied the Favre averaged \( k-\varepsilon \) model to impinging underexpanded jets using a pressure based method. Although no modifications were applied to the standard model, they were discussed. Pressure dilatational terms were neglected on the grounds that more knowledge of their performance for simple flows should be obtained before considering their application to complex flows. The dependence of the shear layer spread rate on the convective Mach number was acknowledged by the author as having a likely significant role and therefore desirable to model. However, the alternative models discussed were empirical in nature and could not be applied generally. It was therefore preferred not to introduce possible unknown difficulties, at the expense of not modelling the compressibility effects.

Dash et al. [37] applied a scaling to the turbulent viscosity:

\[ \mu_t = K C_{\mu} \rho \left( \frac{k^2}{\varepsilon} \right). \]

The scaling factor, \( K \), was a function of the characteristic Mach number, \( M_r = \sqrt{k_{\text{max}}/a} \), where \( k_{\text{max}} \) was the maximum turbulent kinetic energy for each slice of the solution and \( a \) the
local sonic velocity at the location of $k_{max}$. The function $K(M_c)$ was derived empirically so as to reproduce various sets of experimental data. A similar approach was taken by Chuech et al. [15]. Again an empirical scaling was applied to the turbulent viscosity as in eq. 2-56. However, in this case $K$ was a function of the overall convective Mach number and was constant over the whole solution domain. $K$ was calculated to reproduce several sets of experimental observations, in particularly those of Papamoschou and Roshko [162] giving:

\[
\begin{align*}
M_c < 0.55 & \quad K = 1.0 \\
0.55 \leq M_c \leq 0.95 & \quad K = 2.03 - 1.87M_c \\
0.95 < M_c & \quad K = 0.25
\end{align*}
\]

As can be seen above, for convective Mach numbers greater than 0.95 the turbulent viscosity is only 25% of the incompressible value, over the whole domain.

A $k$-$\varepsilon$ model for compressible free shear flows based on two length scales was proposed by Brescianini [171]. The first length scale was that from the standard $k$-$\varepsilon$ model:

\[
l_e = C_\mu \frac{k^2}{\varepsilon}
\]

whilst the second was based on a characteristic width $y_s$:

\[
l_s = \lambda_\varepsilon y_s
\]

The two length scale were combined by calculating a dissipation rate based on this second length scale and choosing the minimum of this and $\varepsilon$ from the standard $k$-$\varepsilon$ model:

\[
\varepsilon = \max \left[ \varepsilon, C_\mu \frac{k^2}{l_s} \right]
\]

Under conditions where the modified length scale is used to determine $\varepsilon$, the $\varepsilon$ equation becomes redundant and the two-equation model is reduced to a one-equation model with an algebraic equation for the length scale.

Abdol-Hamid and Wilmoth [39] also used a multi-scale version of the $k$-$\varepsilon$ model. However, in this case two extra transport equations were required. The turbulent kinetic energy was split into three components, large scale energy production ($k_p$), intermediate energy transfer ($k_i$) and small scale dissipation ($k_d$), but was reduced to two in high Reynolds number flow by assuming that $k_d$ was negligible. A transport equation was required for each of the two components of turbulent kinetic energy. In each case the left hand side is the same as eq. 2-41. However, the source terms become:
such that the energy dissipation of the large scale becomes the production for the transfer scale. This requires two dissipation rates to be calculated, $\varepsilon_p$, the rate of transfer from large scale to intermediate scale and $\varepsilon_i$, the rate of dissipation of the intermediate scale. Again the LHS is that of the standard $k$-$\varepsilon$ model (eq. 2-41 and eq. 2-42) with the following source terms:

$$Q[\varepsilon_p] = \frac{\varepsilon_p}{k_p}(C_{n_p} \rho_k - C_{r_p} \rho \varepsilon_p)$$ 2-62

$$Q[\varepsilon_i] = \frac{\varepsilon_i}{k_i}\rho(C_{n_i} \rho_k - C_{r_i} \rho \varepsilon_i)$$ 2-63

Two further empirical constants are required in order to close the equation set. This method has also been coupled with the compressibility correction of Dash et al. [37], described previously.

### 2.3.4 Compressibility Corrected k-$\varepsilon$ Model

From the discussions in the previous section, the inclusion a treatment for the effects of compressibility on turbulence, at least for comparison to the standard $k$-$\varepsilon$ model, appears very desirable. The model chosen for this work is that of Sarkar et al. [168], because it is based on physical phenomena and has been employed in a number of studies. In addition, the model is simple, has only one constant and incurs virtually no additional computation expense. The standard model will be referred to as $k$-$\varepsilon$, whilst that with the compressibility correction will be referred to as $k$-$\varepsilon$-CC.

In order to implement this model the $k$ equation is modified to include an extra sink term, that for the dilatational dissipation:

$$\frac{\partial}{\partial t} \rho \overline{\kappa} + \frac{\partial}{\partial x_j} \left( \rho \overline{\kappa} \overline{u}_j - \frac{\mu}{\sigma_k} \frac{\partial \overline{\kappa}}{\partial x_j} \right) = P_k - \overline{\rho \varepsilon} - \overline{\rho \varepsilon}_d$$ 2-64

where:

$$\varepsilon_d = \alpha_1 M_i^2 \varepsilon_i$$ 2-65

and $\alpha_1 = 1.0$. 

---

$$Q[k_p] = P_k - \rho \varepsilon_p$$ 2-60

and

$$Q[k_i] = \rho(\varepsilon_p - \varepsilon_i)$$ 2-61
Chapter 2. Non-Reacting Methodology

The \( \varepsilon \) equation is modified to become an equation for \( \varepsilon_r \):

\[
\frac{\partial}{\partial t} \rho \varepsilon_r + \frac{\partial}{\partial x_j} \left( \rho \varepsilon_r \frac{\partial u_j}{\partial x_j} - \frac{\mu_t}{\sigma_e} \frac{\partial \varepsilon_r}{\partial x_j} \right) = \frac{\varepsilon_r}{k} \left( C_{\mu} P_r - C_{\varepsilon_2} \rho \varepsilon_r \right) \tag{2-66}
\]

and the turbulent viscosity is modified to give:

\[
\mu_t = C_{\mu} \rho \frac{k^2}{\varepsilon_r + \varepsilon_d} \tag{2-67}
\]

This implementation is similar to those of Cumber et al. [45] and Dash et al. [170]. In the latter the \( \varepsilon \) equation differs in that the incompressible turbulent viscosity, i.e. that based on the solenoidal dissipation only, is used for the turbulent fluxes. In addition, the algebraic expression for the dilatational dissipation is given by:

\[
\varepsilon_d = \varepsilon_r \left( \alpha_t \tilde{M}_t^2 + \beta \tilde{M}_t^4 \right) \tag{2-68}
\]

where:

\[
\tilde{M}_t = M_t - \lambda \tag{2-69}
\]

\( \alpha_t \) is unity, \( \beta = 60.0 \) and \( \lambda = 0.1 \). This give rise to much larger dilatational dissipation for high turbulent Mach numbers.

### 2.4 Summary of Governing Equations

With the preceding relations defined, the final set of governing equations for the non-reacting calculations can be summarised:

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}_j}{\partial x_j} = \mathbf{Q} \tag{2-70}
\]

\[
\mathbf{U} = \begin{pmatrix} \rho \\ \rho \tilde{u}_j \\ \rho \tilde{k} \\ \rho \tilde{\varepsilon}_j \end{pmatrix}, \quad \mathbf{F}_j = \begin{pmatrix} \rho \tilde{u}_j \\ \rho \tilde{u}_j \nabla y + \tilde{P} \delta_{ij} - \left( \tau_{ij} - \rho \tilde{u}_j \tilde{u}_i \right) \\ \tilde{k} \tilde{u}_j - \frac{\mu_t}{\sigma_k} \frac{\partial \tilde{k}}{\partial x_j} \\ \tilde{\varepsilon}_j \tilde{u}_j - \frac{\mu_t}{\sigma_\varepsilon} \frac{\partial \tilde{\varepsilon}_j}{\partial x_j} \end{pmatrix} \tag{2-71}
\]
Chapter 2. Non-Reacting Methodology

\[ Q = \begin{pmatrix} 0 \\ 0 \\ P_k - \bar{\rho} \bar{\varepsilon}_z - \bar{\rho} \bar{\varepsilon}_d \\ \frac{\bar{\varepsilon}_r}{k} \left( C_{el} P_k - C_{el2} \bar{\rho} \bar{\varepsilon}_r \right) \end{pmatrix} \]

where:

\[ \tau_{ij} - \bar{\rho} \ddot{u}_i \ddot{u}_j = (\mu_r + \mu_r) \left[ \frac{\partial \ddot{u}_i}{\partial x_j} + \frac{\partial \ddot{u}_j}{\partial x_i} \right] - \frac{3}{2} \delta_{ij} \left[ (\mu_r + \mu_r) \frac{\partial \ddot{u}_i}{\partial x_k} + \bar{\rho} \ddot{k} \right] \]

\[ \varepsilon_d = \alpha_r M_r^2 \varepsilon_s \text{ for } k-\varepsilon-CC \]

\[ \varepsilon_d = 0 \text{ for } k-\varepsilon \]

\[ \mu_r = C_{el} \bar{\rho} \frac{k^2}{\varepsilon_s + \varepsilon_d} \]

\[ P_k = -\bar{\rho} \ddot{u}_i \ddot{u}_j \frac{\partial \ddot{u}_i}{\partial x_j} \]

2.4.1 Axisymmetric Co-ordinate System

In an axisymmetric co-ordinate system, eq. 2-70 expands to:

\[ \frac{\partial U}{\partial t} + \frac{\partial F_r}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} \left( r F_r \right) = Q \]

whilst the dilatation term in eq. 2-73 becomes on expansion:

\[ \frac{\partial u_k}{\partial x_k} = \frac{\partial u}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} \left( r v \right) \]

In addition the source term for the radial momentum contains an extra term representing the force due to the Reynolds stress normal to the \( x-r \) plane:

\[ Q[\bar{\rho}v] = \frac{1}{r} \left[ -\bar{F} + 2(\mu_r + \mu_r) \ddot{v} - \frac{3}{2} \left( (\mu_r + \mu_r) \frac{\partial \ddot{u}_k}{\partial x_k} + \bar{\rho} \ddot{k} \right) \right] \]

2.5 Discretisation

This section describes the discretisation of the governing equations and their computational implementation.
2.5.1 Finite Volume Technique

The governing equations, described in section 2.2, are discretised on a Cartesian mesh with a two-dimensional, axisymmetric co-ordinate system. A staggered mesh is employed to overcome the well known pressure-decoupling, described in Appendix A. All variables except for velocity \( u \) or \( \rho u \) are stored at the cell centres, with the velocities displaced in the relevant direction such that they are located on the main control volume faces, as shown in Figure 2-1.

Figure 2-1. Staggered Grid Control Volume

The methodology employs a finite volume technique to ensure conservation. For a control volume, \( S \), enclosing volume \( \Omega \) eq. 2-70 becomes:

$$\frac{3}{\partial t}\int_{\Omega} U d\Omega + \int_{\Omega} F_j \cdot ds = \int_{\Omega} Q d\Omega$$

2-81

In order to improve the shock capturing ability, the primary variables are defined as quantities per unit volume rather than per unit mass (see section 2.1.5). In this way momentum as opposed to velocity is the primary variable, with the velocity derived from momentum and density. Because the momentum terms are displaced on the staggered grid
Chapter 2. Non-Reacting Methodology

(Figure 2-1) whilst density is stored at the cell centres, either the momentum or the density must be interpolated in order to calculate velocity.

For the implicit discretisation, the governing equations are expressed in the form of a model convection/diffusion equation for any variable $\phi$:

$$
\frac{\partial \phi}{\partial t} + \frac{\partial}{\partial x} \left[ \phi u - \Gamma \frac{\partial}{\partial x} \left( \frac{\phi}{\rho} \right) \right] = Q_s
$$

where $\phi = [\rho u, \rho v, \rho e, \rho k]$, $\Gamma$ is the diffusion coefficient and $Q_s$ contains both terms that do not fit the model equation and the true sources. Defining $f_x$ and $f_y$ as the model face flux in the relevant directions eq. 2-81 can be expressed as:

$$
\int \delta U d\Omega + \int f_x ds - \int f_x ds + \int f_y ds - \int f_y ds = \int Q d\Omega
$$

where $\delta U$ represent the change of $U$ over volume $\Omega$ in time $\Delta t$ and the face fluxes are, for example:

$$
f_x = u\phi - \Gamma \frac{\partial \phi}{\partial x} \rho
$$

The model face fluxes are discretised implicitly, whilst the source term is discretised explicitly. The main discretisation tasks are, therefore, the implicit evaluation of the model fluxes at the control volume faces and the explicit treatment of the source term. In addition the temporal derivative must be evaluated.

In the following descriptions it will be assumed that the control volume is that shown in Figure 2-1, with an equally spaced grid and a variable stored at the main control volume such that the control volume faces occur at $(i \pm \frac{\Delta}{2}, j)$ and $(i, j \pm \frac{\Delta}{2})$. For the momentum equations the indices must be increased by $\frac{\Delta}{2}$ in the relevant direction, such that for the $u$-momentum equation the control volume is centred at $(i + \frac{\Delta}{2}, j)$, with faces at $(i + 1, j)$, $(i, j)$, $(i + \frac{\Delta}{2}, j + \frac{\Delta}{2})$ and $(i + \frac{\Delta}{2}, j - \frac{\Delta}{2})$.

The model control volume surface fluxes consist of two terms, convection and diffusion. The diffusive flux is always discretised using central differencing:

$$
\left[ \Gamma \frac{\partial \phi}{\partial x} \rho \right]_{i+\frac{\Delta}{2},j} = \frac{\Gamma_{i+\Delta/2,j}}{\Delta x} \left[ \left( \frac{\phi_{i+1,j}}{\rho_{i+1,j}} \right) - \left( \frac{\phi_{i,j}}{\rho_{i,j}} \right) \right]
$$

The convective differencing requires rather more careful consideration to ensure numerical stability, and is described in the following section.
2.5.2 Convective differencing

For convection dominated flow a central discretisation of the convective fluxes leads to oscillations in the solution which are at best unsightly, but usually contaminate the solution causing rapid divergence. Artificial diffusion, often in the form of upwinding, is required to smooth out these oscillations and give a robust solution. Appendix B describes the dissipation terms that result from applying upwind differencing. Here, two methods are used for the application of upwinding in the convective differencing.

2.5.2.1 Hybrid Differencing Scheme

The first differencing scheme employed is the hybrid scheme [123], which is traditionally very popular with pressure based methods. This scheme is very stable and offers very robust solutions, but is rather crude and applies upwinding to any region where convection is dominant, introducing significant artificial diffusion that can swamp the physical diffusion in many flows unless a very fine mesh is employed. This artificial diffusion is a particular problem for flows not aligned with the mesh. The hybrid scheme employs a switch between first order upwind and central differencing when the local Peclet number (Pe) reaches a specified value. The Peclet number is the ratio of momentum to diffusion fluxes:

\[
Pe = \frac{\rho u \Delta x}{\Gamma} \tag{2-86}
\]

and as such is equivalent to a cell Reynolds number. For Pe less than a specified constant the convective fluxes, as well as the diffusive fluxes are centrally differenced:

\[
[u\phi]_{i+1/2,j} = \frac{u_{i+1,j} + u_{i,j}}{2} (\phi_{i+1,j} + \phi_{i,j}) \tag{2-87}
\]

The face velocity is extracted from momentum on the control volume face and density, interpolated from neighbouring cell centres:

\[
u_{i+1/2,j} = \frac{2(\rho u)_{i+1/2,j}}{\rho_{i+1,j} + \rho_{i,j}} \tag{2-88}
\]

In the case of the momentum equations, to calculate the face velocity, momentum must be interpolated, but the density can be obtained directly:

\[
u_{i+1,j} = \frac{\rho u_{i+1/2,j} + \rho u_{i+3/2,j}}{2\rho_{i+1,j}} \tag{2-89}
\]
When Pe exceeds the limiting value, the convective term is upwinded and the diffusive term
is assumed negligible, compared to the artificial diffusion introduced by the upwinded
convective term, and as such is not computed. For upwind differencing the control volume
face velocity is also determined by the face momentum and the interpolated density, but the
sign of this velocity is now employed to determine which value of $\phi$ should be used in the
calculation of the flux, such that:

$$[u\phi]_{i+1/2,j} = u_{i+1/2,j}^+\phi_{i,j} + u_{i+1/2,j}^-\phi_{i+1,j}$$

where

$$u_{i+1/2,j}^\pm = \frac{(\rho u_{i+1/2,j}^\pm |\rho u_{i+1/2,j}|)}{\rho_{i+1,j} + \rho_{i,j}}$$

are the positive and negative face velocities, of which at least one is always zero.

In all the work in this thesis employing the hybrid scheme, the limiting value for Pe is taken
to be 2, as recommended by Patankar [123]. When the Pe number exceeds 2 the central
scheme can generate oscillations [171] since the viscous damping is no longer sufficient to
damp out oscillations.

The hybrid scheme has several desirable properties, explaining why the scheme is very
popular for many applications. In low speed regions it is second order accurate, whilst across
shock waves the scheme is monotone and does not produce over or under shoots. However,
the monotonicity is enforced in all region of flow above Pe = 2, not just around shock waves
and hence the scheme is very dissipative, which can be devastating to some flows,
particularly those with important shear layers, since, as shown in appendix B, upwinding
results in an additional viscous like term with a coefficient of $\frac{1}{2} \Delta x |u|$, which can be the
dominant diffusion term. However, if the grid resolution is sufficient, accurate solution can
be obtained. The drawbacks of this scheme have been well documented [e.g. 128].

2.5.2.2 TVD

The second convective differencing scheme employed is a second order TVD scheme. In this
scheme monotonicity is enforced where required to prevent oscillations, whilst, as in the
hybrid scheme, other regions reproduce second order central differencing. However, the
TVD is much more refined and applies much less artificial dissipation. The is done by using
a non-linear limiter, based on monitor functions rather than the local Peclet number, which
apply upwinding over a significantly smaller proportion of the domain, and allows upwind and central differencing to be blended to give second order upwind differencing.

The TVD scheme always employs a base first order upwind scheme for the implicit discretisation of the model equation. Higher order terms (HOT) then correct this base scheme to give second order accuracy where possible. In the current implementation the higher order terms are added as explicit deferred corrections by appending them to the source term, in order to maintain a tri-diagonal matrix and ensure a consistent discretisation. Hayase et al. [125] demonstrated, through the QUICK scheme, that using a base first order upwind scheme in the implicit part of the calculation and appending all other terms to the source term is the only way of formulating a consistent scheme that obeys the four rules for discretisation given by Patankar [123], whilst retaining a three point stencil.

Thus, the convective term is discretised as:

$$[u\phi]_{i+1/2,j}^{+} = u_{i+1/2,j}^{+}\phi_{i+1,j} + u_{i+1/2,j}^{-}\phi_{i,j} + \text{HOT}$$

where $u^{\pm}$ are obtained using eq. 2-91. The higher order terms are evaluated by introducing a limiter function, $\Delta(r)$:

$$\text{HOT} = \frac{1}{2} \left( u_{i+1/2,j}^{+} \Delta_{i+1/2,j}^{+} - u_{i+1/2,j}^{-} \Delta_{i+1/2,j}^{-} \right) \left( \phi_{i+1,j} - \phi_{i,j} \right)$$

It is $\Delta(r)$ that defines the scheme and ensures monotonicity, employing forward and backward monitor functions ($r^{\pm}$) to detect potential oscillations in the flow where:

$$r_{i+1/2,j}^{+} = \frac{\phi_{i+1,j} - \phi_{i+1-1,j}}{\phi_{i+1-1,j} - \phi_{i,j}}$$

$$r_{i+1/2,j}^{-} = \frac{\phi_{i+1-2,j} - \phi_{i+1-1,j}}{\phi_{i+1-1,j} - \phi_{i,j}}$$

The function $\Delta(r)$ defines the nature of the scheme. For $\Delta(r) = 0.0$ there are no higher order terms and the first order upwind scheme is retained. For $\Delta(r) = 1.0$:

$$\text{HOT} = \frac{1}{2} \left( u_{i+1/2,j}^{+} \phi_{i+1,j} - \phi_{i,j} \right)$$

and central differencing is reproduced. When $\Delta(r) = (r^{\pm})^{-}$, which gives second order upwind differencing.
Figure 2-2. Limiter Region for Second Order TVD Schemes

Figure 2-2 shows the limiter region for second order accurate TVD schemes. For a limited scheme to be second order accurate then \( \Delta(r) \) must lie in the region bounded by \( \Delta(r) = r \) and \( \Delta(r) = 1.0 \). For a scheme to obey the TVD criteria the following must be satisfied:

\[
0 \leq \Delta(r) \leq \min(2r,2)
\]

Various limiter have been designed to meet these criteria and have varying properties. One of the earliest limiters is that due to Van Leer [173]:

\[
\Delta(r) = \frac{r + |r|}{1 + r}
\]

This is similar to the scheme of Van Albada [174]:

\[
\Delta(r) = \frac{r^2 + r}{1 + r^2}
\]

The minmod scheme defines the minimum bounds for second order TVD schemes and as such is the most robust. It is defined as:

\[
\Delta(r) = \max[0, \min(r,1)]
\]

The superbee scheme [175] represents the upper bounds of the second order TVD region and has been found to be particularly good for resolving features such as shear layers. The superbee scheme can be defined as:

\[
\Delta(r) = \max[0, \min(2r,1), \min(r,2)]
\]
A general limiter can be defined that represents schemes such as minmod and superbee where [176]:

\[ \Delta(r) = \max\left[0, \min(b r, 1), \min(r, \beta)\right] \]

The parameter \( \beta \) must obey \( 1.0 < \beta < 2.0 \) for the resulting scheme to be second order TVD. For \( \beta = 1.0 \) the minmod scheme is reproduced, whilst for \( \beta = 2.0 \) the superbee scheme is obtained. For \( \beta > 1.0 \) the limiter can become compressive and help to steepen discontinuities. For \( \beta < 1.0 \) the scheme is still TVD, but not second order accurate, whilst \( \beta = 0.0 \) reproduces first order upwind differencing.

The UMIST limiter [177] is designed to reproduce the QUICK scheme and is defined as:

\[ \Delta(r) = \max\left[0, \min\left(2r, \left(\frac{1}{4} + \frac{3}{4} r\right), \left(\frac{3}{4} + \frac{1}{4} r\right)^2\right)\right] \]

Figure 2-3 shows the TVD diagram for each of the above limiters. The effect of varying limiters on underexpanded jet calculations is discussed in section 3.4.2.2
2.5.3 Form of Equations

This discretisation leads to a set of implicit scalar equations for \( \phi \) that maintain a three point stencil. For a two-dimensional equation solved on the main control volume an equation of the following form results:

\[
\alpha_{i,j-1}\phi_{i,j-1} + \alpha_{i,j}\phi_{i,j} + \alpha_{i,j+1}\phi_{i,j+1} = Q_{i,j} + \Omega
\]

where the coefficients \( \alpha \) contain the implicit discretisation of the model fluxes. The source term, \( Q \), contains true sources, and the terms that are not contained in the model flux, which are principally viscous terms in the momentum equations. These terms are discretised explicitly, using central differencing. In addition, the source also contains the higher order terms when applying the TVD scheme. The temporal derivative is contained in an old time value within \( Q_{i,j} \) and a new time value within \( a_{i,j} \). Solution is by way of a Gauss-Seidel line solver.

2.6 Pressure Correction Scheme

The equations are coupled together and advanced in time using a pressure based approach, whereby the continuity equation is recast into an equation for pressure correction. Mass continuity is imposed by the linkage between density and pressure, via an equation of state, and the linkage between velocity and pressure, via a truncated form of the momentum equations.

2.6.1 Correction Equation

Within each cycle, the momentum equations are first solved as described in section 2.5 to give the momentum field. With the exception of in the converged state, this will not be the correct momentum field since the pressure is only a guessed pressure \( P^* \), taken as the latest value of pressure available. Therefore, the result of the momentum equations is an intermediate momentum field, \( \rho^* u^* \), which will not satisfy the continuity equation until convergence is reached, but give rise to a mass error \( (M_e) \):

\[
\frac{\partial}{\partial t} \rho^* + \frac{\partial}{\partial x_j} \rho^* u_j^* = M_e
\]

The continuity equation can be used to enforce continuity at the new time level \((n+1)\):

\[
\frac{\partial}{\partial t} \rho + \frac{\partial}{\partial x_j} \rho u_j = 0
\]
where no superscript indicates the new time level.

Subtracting eq. 2-106 from eq. 2-107 gives:

$$\frac{\partial}{\partial t}(p - p^*) + \frac{\partial}{\partial x_j}(\rho u_j - \rho^* u_j^*) = -M_e$$  \hspace{1cm} 2-108

Correction terms are now introduced, signified by $\phi'$, such that when added to the intermediate values give the correct values at the new time level:

$$\phi = \phi^* + \phi'$$  \hspace{1cm} 2-109

Using this correction, momentum at $(n+1)$ can be expanded to give:

$$\rho u_j = (\rho^* + \rho') (u_j^* + u_j')$$
$$= \rho'^* u_j^* + \rho'^* u_j' + \rho^* u_j^* + \rho^* u_j'$$

and hence eq. 2-108 becomes:

$$\frac{\partial}{\partial t}(p - p^*) + \frac{\partial}{\partial x_j}(\rho'^* u_j^* + \rho'^* u_j' + \rho^* u_j^* + \rho^* u_j') = -M_e$$  \hspace{1cm} 2-111

The double correction term is now neglected since, as convergence approaches, its magnitude is much smaller than the other two terms, and its rate of decrease is much more rapid.

The time derivative from eq. 2-111 is discretisation using a first order backward Euler scheme to give:

$$\frac{\partial}{\partial t}(p - p^*) = \frac{1}{\Delta t} \left[ (p - p^*) - (p^* - p^*) \right]$$
$$= \frac{1}{\Delta t} (p - p^*) = \frac{1}{\Delta t} \rho'$$  \hspace{1cm} 2-112

Substituting eq. 2-112 into eq. 2-111 gives:

$$\frac{1}{\Delta t} \rho' + \frac{\partial}{\partial x_j} (\rho'^* u_j^* - \rho'^* u_j') = -M_e$$  \hspace{1cm} 2-113

### 2.6.2 Transformation to Pressure Based Equation

In order to close eq. 2-113 the correction terms must be evaluated; the intermediate values of velocity and density are already known. This is achieved by introducing the pressure correction ($P'$).

The linkage between density and pressure corrections is obtained via an equation of state:
\[ \rho' = \frac{p'}{RT} \]

The linkage between velocity and pressure corrections is obtained via a truncated form of the momentum equations. Recalling eq. 2-27 and 2-105, the \( u \)-momentum equation can be expressed in the form:

\[ u_{i+\frac{1}{2},j}^* = \frac{1}{\rho_{i+\frac{1}{2},j}^{*}} \left[ \left( \frac{Q - (\frac{\partial p'}{\partial x})_{i+\frac{1}{2},j}}{\Omega} \right) \right] - \left( a_{i+\frac{1}{2},j+1}^{*} (\rho u)_{i+\frac{1}{2},j+1}^{*} + a_{i-\frac{1}{2},j}^{*} (\rho u)_{i-\frac{1}{2},j}^{*} \right) \]

where \( Q \) contains viscous terms that do not conform to the model equation (eq. 2-82) and, in the case of TVD convective differencing, higher order terms; for the momentum equations there are no true sources. The pressure gradient term is, however, not included in \( Q \) and is expressed separately. Using this form of the momentum equations for a linkage would lead to a huge stencil; each of the 4 face velocities are dependent on all their respective neighbour values. The solution of the resulting full matrix is not a viable option. To arrive at a tractable solution it is assumed that the dominant influence on the face velocity is the pressure gradient at the face. This effectively assumes that the coefficient \( a_{i+\frac{1}{2},j}^{*} \) is larger than those at neighbouring points and thus all the other flux terms are neglected. In addition the viscous and HOT terms, and hence \( Q \) can also be neglected.

With these assumptions eq. 2-115 is truncated to give:

\[ u_{i+\frac{1}{2},j}^* = -\frac{\Omega}{a_{i+\frac{1}{2},j}^{*}} \left( \frac{\partial p'}{\partial x} \right)_{i+\frac{1}{2},j} \]

This can be expressed in the form of a velocity correction by subtracting it from the truncated momentum equation for the time \( n+1 \) to give:

\[ u_{i+\frac{1}{2},j}^{n+1} = -\frac{\Omega}{a_{i+\frac{1}{2},j}^{*}} \left( \frac{\partial p'}{\partial x} \right)_{i+\frac{1}{2},j} = -\alpha_{i+\frac{1}{2},j} \left( \frac{\partial p'}{\partial x} \right)_{i+\frac{1}{2},j} \]

Substituting eq. 2-114 and 2-117 into eq. 2-113 now gives an equation for the pressure correction:

\[ \frac{1}{\Delta t} \frac{P'}{RT} - \frac{\partial}{\partial x} \left( \rho \alpha_{i+\frac{1}{2},j} \frac{\partial p'}{\partial x} + \frac{p'}{RT} u_{i}^{*} \right) = -M_{e} \]

This is a convection-diffusion equation for pressure correction. Incompressible pressure correction methods and many compressible forms only give rise to a diffusion or Poisson equation for pressure correction by ignoring the density correction and hence the linkage
between density and pressure. However, this is the dominant term as the Mach number increases and is essential for stability.

Examining eq. 2-118 reveals that all the terms on the LHS are the product of a correction term. As such, upon convergence these terms tend to zero and therefore only have a role in ensuring convergence and stability; they do not affect the accuracy of the final solution. This removes any inaccuracies that may be introduced by the truncation of the momentum equation (eq. 2-116). On the other hand, the terms on the RHS of eq. 2-118 do not tend to zero on convergence, although their sum does, and the accuracy of the final solution will depend on the discretisation of the RHS. It is this discretisation of the RHS that defines exactly which mass flux is conserved.

Eq. 2-118 is discretised to give an equation of the form of eq. 2-105 that can be solved in the same manner as all the other transport equations to obtain a pressure correction field. The pressure field is then updated by:

$$p_i^{n+1} = p_i^{*} + p_i'$$

as is the velocity field:

$$u_{i+1/2,j} = u_{i+1/2,j}^{*} - \alpha_{i+1/2,j} \left( \frac{\partial P'}{\partial x} \right)_{i+1/2,j}$$

### 2.6.3 Flux Construction

Discretisation of eq. 2-118 follows the same form as eq. 2-83. Here the whole of the face fluxes $f_j$ are treated implicitly, with the source term containing only the mass error, so that, for example, the x-direction flux on the $(i + 1/2)$ face is:

$$f_x = - \left[ \rho \alpha_{i+1/2,j} \left( \frac{\partial P'}{\partial x} + \frac{P'}{RT'} \right) \right]_{i+1/2,j}$$

Discretisation of this face flux using central differencing gives:

$$f_x = - \left[ \frac{\rho_{i+1,j} + \rho_{i,j}}{2} \alpha_{i+1/2,j} \frac{P'_{i+1,j} - P'_{i,j}}{\Delta x} + \frac{1}{2R} \left( \frac{P'_{i+1,j}}{T_{i+1,j}} + \frac{P'_{i,j}}{T_{i,j}} \right) u_{i+1/2,j}^{*} \right]$$

where $u_{i+1/2,j}^{*}$ is given as in eq. 2-88.
Chapter 2. Non-Reacting Methodology

The mass error term \( M_e \), as discussed earlier in this section, requires careful consideration since it is this term that governs the accuracy of the solution. The mass error term is calculated by applying the continuity equation:

\[
M_e = \frac{\partial }{\partial t} \rho^* + \frac{\partial }{\partial x_j} \rho^* u_j^*
\]

so that:

\[
M_e \Omega = \frac{\Omega}{\Delta t} (\rho_{i,j}^* - \rho_{i,j}^*)
\]

\[
+ (\rho u)_{i,j}^* S_{i,j} - (\rho u)_{i,j-1}^* S_{i,j} + (\rho v)_{i,j}^* S_{i,j} - (\rho v)_{i,j-1}^* S_{i,j-1}
\]

Because the pressure correction equation is an elliptic equation a central discretisation produces oscillation when the local flow velocity approaches or exceeds sonic. This is often remedied by the introduction of artificial dissipation techniques, such as the retarded pressure function \( \text{[138]} \) (see section 2.1.5). An alternative approach is to introduce upwinding into the pressure correction discretisation, such that the numerical dissipation is added implicitly. Applying upwinding to the discretisation of eq. 2-133 gives (for clarity the * has been removed from the density and velocity terms in subsequent equations):

\[
f_x = \left[ \left( \tilde{\rho}_{i+1,j} - \tilde{\rho}_{i,j} \right) \frac{P_{i+1,j} - P_{i,j}}{\Delta x} + \frac{1}{R} \frac{P_{i+1,j}^* u_{i+1,j}^* + P_{i,j}^* u_{i,j}^*}{T_{i,j} + u_{i,j}^*} \right]
\]

where \( u_{i,j}^* \) is calculated using equation eq. 2-91 and the upwinded interpolated density \( \tilde{\rho} \) is:

\[
\tilde{\rho}_{i+1,j} = \frac{u_{i+1,j}^* \rho_{i+1,j} + u_{i,j}^* \rho_{i,j}}{u_{i+1,j}^*}
\]

Since the LHS of eq. 2-118 only effects convergence and stability, upwinding must also be included in the mass error term such that, for example:

\[
(\rho u)_{i,j} = \rho_{i,j} u_{i,j}^* + \rho_{i+1,j} u_{i+1,j}^*
\]

Upwinding \( M_e \) gives the solution the desired stability at all speeds. However, upwinding is too dissipative for many applications and causes excessive smearing that can be disastrous for accurate shock capturing. In order to give stability and acceptable shock capturing performance a blended scheme is applied, such that upwind (UP) and central differencing (CD) are combined, based on local, directional, blend factors, \( b_x \) and \( b_y \):

\[
f_x = b_x \text{[UP]} + (1 - b_x) \text{[CD]}
\]
Chapter 2. Non-Reacting Methodology

Thus for $b_x = 1.0$ the upwind differencing scheme and for $b_x = 0.0$ the central differencing scheme are reproduced.

Applying to the mass error gives:

$$(pu)_{i+1/2,j} = (pu)_{i+1/2,j} - b_x \left[ \frac{1}{2} \left( \frac{P_{i+1,j} - P_{i,j}}{2R} \right) - b_x \left( \frac{1}{2} \left( \frac{P'_{i+1,j} - P'_{i,j}}{T_{i+1,j} - T_{i,j}} \right) \right) \right]$$

The blend factor can be specified by several methods. The most simple method defines a constant value for $b_x$ and $b_y$ dependent on the type of flow. Although this is a relatively crude method it gives surprisingly good results. However, much better results can be attained by using an adaptive blend factor that takes consideration of the local flow conditions. The most commonly used in this thesis, calculates the blend factor as a function of the local directional Mach number:

$$b_x = \max \left[ \min \left[ f_1 (M_x - f_2), 1 \right], 0 \right]$$

where $M_x = \frac{u_{i+1/2,j}}{\sqrt{kRT}}$ and $f_1$ and $f_2$ are specified constants. In this way central differencing is applied where the local directional Mach number is less than $f_2$; above this upwinding is introduced as a linear function of $f_1$, with full upwinding for $M_x \geq \frac{1}{f_1} + f_2$.

### 2.6.4 Retarded Pressure Scheme

An alternative to the blended differencing scheme described above, the retarded pressure scheme of Page [140], has also been employed in this thesis. In this scheme the pressure correction equation is formulated differently, resulting in a Poisson equation for pressure as in the SIMPLE algorithm of Patankar [123].

In the retarded pressure formulation, correction terms to the mass flux rather than velocity and density are introduced such that:

$$\rho u = (\rho u)^* + (\rho u)'$$

and therefore in variable density flows:
Chapter 2. Non-Reacting Methodology

\[ u \neq u' + u' \]

This leads to a modification of eq. 2-108:

\[
\frac{\partial}{\partial t}(\rho - \rho') + \frac{\partial}{\partial x_j}(\rho u_j - (\rho u_j))' = -M_e. \tag{2-134}
\]

and therefore eq. 113 becomes:

\[
\frac{1}{\Delta t} \rho' + \frac{\partial}{\partial x_j}(\rho u_j)' = -M_e. \tag{2-135}
\]

The linkage between the momentum and pressure correction equation is now achieved via:

\[
(pu)_{i+\frac{1}{2},j} = -\frac{\Omega}{a_{i+\frac{1}{2},j}} \left( \frac{\partial P'}{\partial x} \right)_{i+\frac{1}{2},j} = -\alpha_{i+\frac{1}{2},j} \left( \frac{\partial P'}{\partial x} \right)_{i+\frac{1}{2},j} \tag{2-136}
\]

This results in the following Poisson equation for pressure which contains no density or convective terms:

\[
\frac{1}{\Delta t} \frac{P'}{RT} - \frac{\partial}{\partial x_j} \left( \alpha \frac{\partial P'}{\partial x_j} \right) = -M_e \tag{2-137}
\]

This equation is solved in the same manner as for the blended scheme, except that all terms are now centrally differenced. In fact, it is not possible to upwind any of the terms on the LHS of eq. 2-137.

The pressure field is updated as in eq. 2-119, but the momentum is now updated as:

\[
(pu)_{i+1,j} = (pu)_{i\frac{1}{2},j} - \alpha_{i+\frac{1}{2},j} \left( \frac{\partial P'}{\partial x} \right)_{i+\frac{1}{2},j} \tag{2-138}
\]

Stabilising dissipation is introduced by the retarded pressure formulation \[139\]

\[
F_i = P_i + \mu_x (P_{i-1,j} - P_{i-1,j}) + \mu_y (P_{i,j} - P_{i,j-1}) \tag{2-139}
\]

where \( \mu_y \) is a function usually dependent on the local, directional flow velocity.

2.6.5 TVD Differencing

To reduce the amount of added artificial dissipation, TVD type limiters can also be applied to the differencing of density in the pressure correction equation, using a similar approach to that employed for the convective differencing (section 2.5.2.2). However, it should be noted that although a TVD limiter is applied, the differencing scheme does not attempt to meet the TVD criteria, the limiter is merely employed as a framework for developing intelligent, non-
linear functions to prescribe the blending of upwind and central differencing in the pressure correction equation.

Application of the TVD limiter to the pressure correction equation takes a slightly different form to that of the convective terms in the other transport equations. Here, it is only necessary to apply the limiters in the source terms, since it is only the mass error term that has an effect on the accuracy of the converged solution. Applying a TVD scheme to the implicit part of the discretisation in the pressure correction equation has no effect on the steady state solution when the pressure correction tends zero.

The monitor function are based on density differences and not pressure correction. This is because in the steady state the pressure correction values are very small and insignificant to the flow properties, but they form a very oscillatory field which would result in an almost fully upwind discretisation of the source term and therefore highly dissipative solutions.

Recalling eq. 2-123, the mass error term is equal to:

\[ M_i = \frac{\partial}{\partial t} \rho^* + \frac{\partial}{\partial x_j} \rho^* u_j^* \] 2-140

The second term on the RHS is a simple convective term and as such the TVD discretisation described in section 2.5.2.2 can be applied. However, in this case the HOT terms do not appear as a deferred correction, since the discretisation is explicit and all terms appear in the source term.

\[ [\rho u]_{x,i,j} = \frac{1}{2} (u_{x,i,j}^+ \Delta_{x,i,j}^+ - u_{x,i,j}^- \Delta_{x,i,j}^-) (\rho_{i+1,j} - \rho_{i,j}) \] 2-141

where \( \Delta(r) \) is calculated using one of the limiters described in section 2.5.2.2 and the monitor functions \( r^2 \) are as in eq. 2-94 and 2-95 with \( \phi = \rho \).

2.7 Solution Details

The following section describes some specific numerical issues arising from the implementation of the numerical scheme.

2.7.1 Time Step Definition

A suitable time step must be chosen in order to meet both stability and accuracy requirements. It is well known that explicit schemes must not have time steps that violate the
Chapter 2. Non-Reacting Methodology

Courant-Friedrichs-Lewy (CFL) condition, which specifies that information must not be able to travel a distance greater than the smallest cell dimension within a single time step:

$$\frac{\Delta t}{\Delta x} |u + c| \leq 1$$  \hspace{1cm} 2-142

where $c$ is the wave speed and the quantity on the LHS of eq. 2-142 is usually referred to as the CFL number.

In theory for an implicit scheme there is no stability limit on the time step that can be used, although temporal accuracy may require a limit on the time step. The scheme used here is semi-implicit in that the model equations are solved implicitly, but source terms and those terms not conforming to the model equations are solved explicitly. In practice a CFL of around four gives reasonable speed of convergence without any loss in robustness. The time step for each cell is calculated based on a specified CFL number with the smallest value chosen for the whole domain:

$$\Delta t = \frac{\Delta x}{|u + c|} \text{CFL}$$  \hspace{1cm} 2-143

where $c$ in this case is the local sonic velocity.

This specification of time step can be very restrictive, since small time steps will result when either the velocity is high or the cell size is small. These can often occur in the same location leading to very small time steps, whilst there may be regions that are capable of using much larger time steps. However, for time accurate solutions this type of time step must be used.

When a steady-state solution is required it is not necessary to assign the same time step to every cell; a locally varying time step can be used without affecting the final solution, but reducing the number of cycles required for convergence, since for the majority of cells a much larger time step will be employed. However, the intermediate solution has no meaning, and does not necessarily represent the physical development of the flow. This non-time accurate technique is employed in many of the calculations in this thesis, and can be seen as specifying a constant CFL number, rather than a constant time. Iterations can be used within individual time steps to improve the convergence of the implicit equations. However, with the size of the time steps employed in the calculations, this was not found to improve convergence or temporal accuracy.
2.7.2 \( k-e \) Limits

The need to enforce positivity for the turbulence quantities was discussed in section 2.3.2. Numerically, negative turbulence values can be generated because the explicit source terms can be positive or negative, since both production and destruction of turbulence is physical. This situation must be prevented, since not only are negative turbulent quantities unphysical, they are also likely to lead to rapid failure of the numerical scheme. Negative values are prevented in practice by modifying the treatment of the explicit source term, so that part of the source is linearised so that it can be included in the implicit part of the discretisation.

For example, the source term of the turbulent kinetic energy equation (without the compressibility correction):

\[
Q[p_k] = P_k - \rho \varepsilon,
\]

is linearised as:

\[
Q[p_k] = P_k \frac{(\rho \varepsilon)^n}{(p_k)^n} - (p_k)^{n+1}
\]

The second term on the RHS is then in a suitable form for inclusion into the implicit coefficient \( a_{ij} \). In the case of the \( \varepsilon \) equation:

\[
Q[\rho \varepsilon] = \frac{\varepsilon}{k} (C_{\varepsilon} P_k - C_{\varepsilon2} \rho \varepsilon)
\]

the negative term can be directly appended to the coefficient \( a_{ij} \) for inclusion in the implicit part of the calculation. These steps greatly increase the robustness of the turbulence model, since the negative terms are handled implicitly. Of course \( P_k \) can still be negative, although this is not normally a problem.

Enforcing positivity is generally essential for iterative procedures. Time dependent problems are less susceptible to such problems since the marching procedure follows a physically valid path. However, these measures have always been included to improve the robustness of the code, primarily for calculations with large time steps, locally varying time steps or strong discontinuities in the flow.

In addition, two further measures have also been included primarily for problems with large locally varying time steps. The first guarantees that Schwarz’s inequality is satisfied [e.g. 178]. Schwarz inequality states for two randomly varying variables, \( x \) and \( y \), that:

\[
\overline{xy}^2 \leq \overline{x^2} \overline{y^2}
\]
Chapter 2. Non-Reacting Methodology

Applied to the fluctuating velocity components this states that:

\[ u''v' \leq \frac{3}{2} u'' v'' \]

Assuming:

\[ u'' = v'' = \frac{3}{4} k \]

and

\[ \frac{u''v'}{\rho} = \frac{1}{\rho} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \]

gives a constraint for the turbulent viscosity:

\[ \mu_t \leq \frac{3}{4} \rho k \]

The second condition imposes a maximum limit for the turbulent viscosity. Checks were always carried out to ensure that these limits were only enforced by the code during initial development and not in the steady state.

2.7.3 Equation of State

To close the equation set, density and temperature are derived from pressure, momentum and total enthalpy, noting that for non-reacting calculations the total enthalpy is constant. The scheme can be made more robust by a simple transformation of the equation of state into a more stable form. The equation of state can be expressed as:

\[ \rho = \frac{P}{RT} = \frac{P \left( \frac{\gamma}{\gamma - 1} \right)}{\left( H - \frac{1}{2} \left( \frac{\rho u_t}{\rho} \right)^2 \frac{\rho k}{\rho} \right)} \]

which can be rearranged to obtain:

\[ \frac{\gamma - 1}{\gamma} H \rho = P + \frac{1}{2} \left( \frac{\rho u_t}{\rho} + \frac{\rho k}{\rho} \right) \frac{\gamma - 1}{\gamma} \]

from which the density is calculated as:

\[ \rho = \frac{1}{H} \left[ \frac{P \left( \frac{\gamma}{\gamma - 1} \right)}{\gamma} + \frac{1}{2} \left( \frac{\rho u_t}{\rho} + \frac{\rho k}{\rho} \right) \right] \]
and the temperature from:

\[ T = \frac{P}{R \rho} \]  

Eq. 2-154 is more stable than eq. 2-152 for several reasons. The density in the modified form is included more implicitly than in eq. 2-152. Remembering that the density term is that from the previous cycle, whilst the implicit density in \( \rho u \) and \( \rho k \) would be for the new level. Further, in eq. 2-152 the velocity term and turbulent kinetic energy terms were subtracted, whilst in eq. 2-154 they are now added; this is more robust.

The density and temperature are updated at the end of each computational cycle, although in some cases it can be beneficial to update the density after the continuity equation using the new pressure and velocities.

### 2.7.4 Boundary Conditions

Three different boundary conditions are required for axisymmetric free jet calculations: jet, symmetry and constant pressure.

#### 2.7.4.1 Jet

The jet boundary is defined by specifying total pressure \( (P_o) \), total temperature \( (T_o) \) and the exit Mach number \( (M_e) \). For exit velocities below sonic, it is not sufficient to fix the boundary variables of pressure, density and momentum at calculated values. Some information must be interpolated from the interior so that disturbances from the interior can influence the boundary. However, once the nozzle is choked this is no longer a requirement and the inlet condition can be directly specified.

For a given total pressure, total temperature and nozzle exit Mach number, the exit pressure and temperature can be obtained from:

\[
P_e = P_o \left[ 1 + \frac{\gamma - 1}{2} M_e^2 \right]^{\frac{-1}{\gamma - 1}}
\]

\[
T_e = T_o \left[ 1 + \frac{\gamma - 1}{2} M_e^2 \right]^{1 - \gamma}
\]

The density at the inlet follows from the equation of state, whilst the momentum is calculated as:
The turbulence quantities are specified using defined length and velocity scales:

\[ k = \frac{3}{2} \left( u' \right)^2 \]  
\[ \varepsilon = C_k \frac{k^3}{l} \]

Typically \( u' \) is calculated as 5% of the nozzle exit velocity and \( l \) as 5% of the nozzle exit diameter (see section 3.2 and section 3.4.5).

### 2.7.4.2 Symmetry

For the symmetry boundary, a condition of zero mass flux through the boundary is imposed implicitly in the momentum equations. A zero pressure correction gradient is applied which sustains the zero mass flux boundary condition. In addition, a zero gradient is applied to all other variables, again in an implicit manner.

### 2.7.4.3 Constant pressure

A constant pressure boundary is very important for free jet calculations since it allows both inflow and outflow depending on the local pressure field. The pressure at the boundary is fixed to a specific value, such that a pressure gradient normal to the boundary can develop which controls the mass flux into and out of the domain through the momentum equation normal to the boundary. The momentum parallel to the boundary is calculated using a zero gradient assumption.

For all other quantities the boundary condition varies depending on the flow direction across the boundary. For outflow, turbulence quantities assume a zero gradient. For inflow these quantities are specified as their ambient values. For this boundary condition to be valid the flow at the outflow must be subsonic.

### 2.8 Closure

In this chapter the formulation of the non-reacting flow solver has been described. In the following chapter the performance of the formulation for application to underexpanded jets will be assessed.
Chapter 2. Non-Reacting Methodology

The basic methodology is an extension of the incompressible pressure based method of Patankar [123] to compressible flow, as has been attempted by several other workers [131-143]. However, in the current methodology attention has been focused on producing a numerical scheme that is robust at all flow Mach numbers, whilst not requiring the addition of excessively large quantities of numerical dissipation. This has been achieved by employing non-linear, TVD limiters to the convective differencing and Mach number dependent differencing in the mass error term of the pressure correction equation. Other differencing schemes have also been described and results obtained with the various schemes are compared in the following chapter.
Chapter 3. Non-Reacting Results

3.1 Introduction

In this chapter results obtained for non-reacting underexpanded jets are presented and discussed. Several numerical issues are addressed including the convective and pressure correction schemes, grid resolution, turbulence model and its compressibility correction, and the boundary conditions.

The performance of the optimised model is then compared to the available experimental data in sections 3.5 and 3.6, whilst computations employing a pseudo source approximation are presented in section 3.7. Finally, section 3.8 discusses the performance of the numerical scheme in relation to previous computational studies of underexpanded sonic jets.

3.2 Computational Setup and Grid Generation

The computational results presented in this chapter all employed an axisymmetric system, with cylindrical co-ordinates. The centreline boundary was specified as an axial symmetry line and the far field boundaries were all constant pressure boundaries. The inlet boundary comprised a jet boundary condition to represent the nozzle, with the remainder a constant pressure boundary. Figure 3-1 shows a schematic of the boundary conditions employed. The conditions applied to each boundary type were described in section 2.7.4.

For all the calculations the total temperature was specified as 288K and the ambient pressure was $1 \times 10^5$ Pa, with the jet total pressure obtained from this and the NPR. The thermodynamic properties were specified assuming air for both the jet and ambient. These conditions give rise to a range of jet Reynolds numbers, based on a nozzle diameter of 25mm and fully expanded conditions, from $1.0 \times 10^6$ for NPR = 2.0 to $2.7 \times 10^6$ for NPR = 20.0.

Specification of the boundary conditions was completed by the turbulence quantities. For the nozzle conditions the fluctuating velocity was taken as a percentage of the sonic velocity at the nozzle exit conditions and the length scale as a percentage of the nozzle diameter; for most of the calculations presented here both were set as 5%. In the absence of experimental data these turbulence conditions were arbitrarily specified with reference to previous computational studies of both subsonic and supersonic jets, and their effect is examined in section 3.4.5.
The majority of computations in this chapter employed a domain with dimensions of 40×15 diameters, and a nozzle diameter of 25mm. The location of the far field boundaries have been varied and found to have no effect on the solution away from the boundaries, provided that they are located sufficiently far downstream so as to ensure the flow is subsonic.

The computational grid was generated to give increased resolution in the region of the highest gradients, namely the shock containing region and shear layers. For the results in sections 3.3 to 3.5, unless otherwise stated, the same grid was employed with 300 axial cells and 105 radial cells. Moderate clustering was applied in both the axial direction, near the nozzle, and in the radial direction, around the lipline, giving a smallest spacing in both directions of 0.02 diameters and 80 axial cells in the first two diameters and 19 radial cells in the nozzle. Figure 3-2 shows the computational grid, whilst Figure 3-3 shows a close up of the near nozzle region. Many optimisations of the mesh have been carried out to allow accurate results to be generated without excessive computational expense; the effect of grid resolution and clustering will be discussed in section 3.4.4.

In all cases the timestep was specified as locally varying such that each cell had a CFL number of 3.0. The use of locally varying time steps allows efficient computations to be performed even when a high resolution of mesh is employed. With a constant time stepping method very small timestep constraints occur. For example, assuming a minimum grid spacing of 0.02 diameters with a 25mm nozzle giving a minimum cell size of around 0.5mm and sonic velocity results in a timestep of order $1 \times 10^{-6}$ s. Clearly, the computational requirements of such a small timestep can be very restricting. With a locally varying timestep the number of timesteps required for convergence is reduced by an order of magnitude, whilst not effecting the accuracy of the results for steady state computations.

For a 300×105 mesh and CFL = 3.0, convergent solutions for moderately underexpanded jets were obtained after 5000 cycles, taking around 100 minutes on a Silicon Graphics R10000 processor.

### 3.3 Predicted Flow Features

#### 3.3.1 Moderately Underexpanded Jets

The features of moderately underexpanded jets were described in section 1.1. Predicted Mach number contours for underexpanded jets of NPR 2.69 and 3.5 are shown in Figure 3-4 and Figure 3-5 respectively. The characteristic repeating shock cell structure can be clearly
observed, resulting in the distinctive curved shear layer. With increasing pressure ratio the shock cell structure becomes stronger and prevails further down the potential core. The higher pressure ratio and stronger shock cell structure increase the curvature of the jet boundary and give rise to a more rapid jet spreading rate. The shock cell wavelength and diameter are also increased by the increasing pressure ratio, as is their angle of inclination.

Corresponding centreline Mach number plots are shown in Figure 3-6 and Figure 3-7. The repeating shock cell structure appears as a decaying series of peaks and troughs. For NPR 2.69 a peak Mach number of 1.63 is predicted in the first shock cell, repeated over five shock cells. For NPR 3.5 the peak Mach number is somewhat higher, around 2.2, but again the shock cell structure decays over five shock cells. In both cases, since the shock cells are oblique the flow only becomes subsonic downstream of the shock cell structure, under the action of mixing in the shear layer, as the potential core decays. These figures show evidence of a degree of shock cell smearing.

The effect of NPR on the distance to the focal point of the first intersecting shocks for moderately underexpanded jets is shown in Figure 3-8 compared to the experimental measurements of Love et al. [1]. Excellent agreement is obtained between the computational and experimental data, indicating that the methodology is capable of predicting correctly the location of the shock cell structures in moderately underexpanded jets.

3.3.2 Highly Underexpanded Jets

The application of CFD codes to highly underexpanded sonic jets was reviewed in section 1.2.3. The complex phenomena occurring in these flows make their modelling very difficult and requires the use of very robust codes. Very few examples are recorded in the literature and these usually concentrate on either modelling the essentially inviscid near field shock cell structure or the far field subsonic regions, but not both together. In this section the successful application of the pressure correction methodology developed in chapter 2 to highly underexpanded jets is demonstrated.

The key feature of highly underexpanded jets that set them apart from moderately underexpanded jets is the appearance of a strong normal shock or Mach disk in the first and in some cases subsequent shock cells. Typical Mach number contours of the Mach disk structure at pressure ratios of 6.0 and 31.0 are shown in Figure 3-9 and Figure 3-10. The distinctive features of a Mach disk are clearly visible and can be compared to those in the schematic of a Mach disk structure (see Figure 1-3). The important features such as the
normal, reflecting and intercepting shocks, the triple point and regions of supersonic and subsonic flow are all well defined, indicating the ability of the pressure correction scheme to compute this complex flow phenomena. The effect of increasing the pressure ratio is to increase the diameter of the normal shock, whilst increasing the curvature of the boundary and increasing the maximum Mach numbers observed. In addition the Mach disk is located further downstream as the pressure ratio increases.

The centreline Mach number for a highly underexpanded jet of $NPR = 6.0$ is shown Figure 3-11. The normal shock is much stronger than the shock cells seen in moderately underexpanded jets resulting in a larger Mach number drop and subsonic flow behind it. The peak Mach number on the leading edge of the normal shock is 2.9, with a Mach number drop of 2.62 to give a Mach number of 0.28 on the downstream side. One-dimensional normal shock theory predicts a Mach number drop of 2.42 to give a downstream Mach number of 0.48 for an upstream Mach number of 2.9. This gives an error of around 8% in the Mach number drop across the normal shock, which can be accounted for by multi-dimensional and viscous effects. The subsonic region of the flow is then re-accelerated to supersonic velocities by mixing with the flow that has not passed through the Mach disk. Downstream, further expansion takes place via an oblique shock cell structure.

For $NPR = 31.0$ (Figure 3-10) the Mach number on the upstream side of the normal shock reaches in excess of 5.0, whilst the subsonic region immediately downstream of the normal shock has a Mach number of around 0.3. This represents a very large velocity gradient and requires a very robust scheme to be computed successfully.

As well as the problems associated with capturing strong normal shocks, highly underexpanded jets also present additional problems over moderately underexpanded jets. In particular, the mixing layers that develop downstream of the normal shock present a significant challenge. These shear layers separate region of subsonic and high supersonic velocities in the presence of both large gradients and absolute values of pressure. The rate of mixing between these two regions has a significant effect on the subsequent downstream shock cell structure and the recovered Mach number and must therefore be modelled accurately.

Figure 3-12 compares the effect of NPR on the measured distance to the normal shock in a highly underexpanded jet to the data of Love et al. [1]. This figure also contains the data for moderately underexpanded jets shown in Figure 3-8. As in the case of moderately
underexpanded jets the agreement between the computational and experimental results is excellent.

3.4 Numerical Issues

This section discusses the effects of various numerical issues on the accuracy of the computed solutions. In addition some improvements to the convective differencing scheme are described and tested.

3.4.1 Convective Differencing Scheme

As described in section 2.8.1, upwind differencing for the convective terms is first order accurate and leads to a truncation error, equivalent to a diffusion term with a coefficient proportional to the velocity and cell dimension. Central differencing is second order accurate, with a dispersive truncation error proportional to the cell dimension squared. Although central differencing would appear to be more accurate, it is well known to become unstable when convection dominates relative to diffusion. In particular, around discontinuities such as shock waves, monotonicity is required to prevent the production of under and over shoots.

The TVD scheme, described in section 2.5.2.2, gives both a second order accurate solution in smooth regions and oscillation free solutions by becoming monotone where required. Figure 3-13 compares the centreline Mach number for the upwind and TVD convective schemes for NPR = 3.5. The TVD scheme employed the minmod limiter, such that $\beta = 1.0$ in eq. 2-103, whilst the upwind scheme was achieved by setting $\beta = 0.0$. Surprisingly, the upwind solution appears to give the better shock cell resolution, with a significantly higher peak Mach number for each shock cell. Downstream, the potential core length decreases with the TVD scheme, thus appearing to show increased dissipation with this scheme.

The effect of the convective scheme on total pressure is shown in Figure 3-14. With the TVD scheme the total pressure initially increases with downstream distance, whilst with the upwind scheme it decreases. Across the first oblique shock cell the upwind scheme develops an overshoot, whilst with the TVD scheme the total pressure decreases by around 20%. Downstream of the first shock cell the upwind scheme maintains a fairly constant total pressure at the nozzle value, whilst the TVD scheme recovers a proportion of the total pressure loss due to entrainment from the shear layer, but continues to lose total pressure across each subsequent shock cell. Also evident is a high frequency oscillation of the total pressure with the TVD scheme close to the leading edge of shock cells. The total pressure
clearly demonstrates that the upwind scheme is behaving unphysically across stronger shock waves, whilst the TVD scheme is not preventing the formation of oscillations in the solution as it is designed to do.

Figure 3-15 compares the same two schemes, along with the hybrid scheme for $NPR = 2.69$. The hybrid scheme differs from the upwind scheme in that in regions where the Peclet number is less than 2 central differencing is employed, whilst in other region the scheme becomes upwind, but the physical diffusion terms are not included. Thus, it is expected that the hybrid scheme should give a slight improvement in shock cell resolution compared to the upwind scheme, since in high speed regions both convective schemes will be upwind, but the hybrid scheme does not include the additional dissipation in the form of the physical diffusion terms, although these will be small where the Reynolds number is high. This behaviour is shown in Figure 3-15. In the downstream region some switching to central differencing may occur with the hybrid scheme where Pe is low and this should increase the potential core length. However Figure 3-15 shows the opposite effect; the hybrid scheme predicts a shorter potential core. Similarly to the results for $NPR = 3.5$, the TVD scheme gives a significantly worse shock cell resolution and a reduction in the potential core length compared to the upwind scheme.

To eliminate any influence of the Mach number dependent pressure correction scheme the hybrid and TVD schemes have been compared in Figure 3-16 for $NPR = 3.5$ applying a full upwind solution to the density in the pressure correction equation. In addition to the hybrid, upwind and minmod schemes, a TVD scheme with $\beta = 0.5$ is applied, which represents a more diffusive limiter than the minmod scheme and satisfies the TVD criteria, but is not second order accurate (see section 2.5.2.2). As expected, the shock cell resolution has been reduced by the upwinding in the pressure correction equation, but the various convective schemes still give similar effects to those seen previously. The peak Mach number is reduced by the TVD scheme, and the $\beta = 0.5$ scheme gives a higher resolution than the less diffusive $\beta = 1.0$ (minmod) scheme. The hybrid solution still appears to give the best shock cell resolution, but only slightly better than the upwind scheme.

The effects of applying the minmod limiter to single transport equations, whilst upwinding all others equations, are shown in Figure 3-17 and Figure 3-18, again using a fully upwinded pressure correction formulation. Results are shown for applying TVD to none of the equations (i.e. the upwind scheme), the $u$-momentum, $v$-momentum, the turbulence equations ($k$ and $\epsilon$) and to all equations (i.e. the minmod scheme). It is clear that the
Chapter 3. Non-Reacting Results

differencing of the \( u \)-momentum equation has the major effect on the peak Mach number in the shock cells. Applying TVD to just the \( u \)-momentum gives a solution apparently more diffuse than when applying to all the equations. Applying TVD to the \( v \)-momentum equation increases the peak Mach number in the shock cells, whilst applying TVD to the turbulence model has little effect on the shock cell resolution. However, the reduction in potential core length observed with the TVD scheme is clearly the result of applying the TVD scheme to the turbulence model; the potential core length is insensitive to the convective scheme applied to the momentum equations.

To eliminate the influence of two aspects of the implementation two further convective differencing schemes have been considered. The effects of the switching within the limiter were examined by applying the well known higher order upwind scheme QUICK [109]. This scheme is third order accurate and unbounded. As such, the same scheme is applied at all locations and hence there is no switching. Implemented in a very similar manner to the TVD scheme, a base first order upwind solution is employed in the implicit part of the calculation with the higher order terms appended as a deferred correction to the source term. This implementation is the only consistent manner to implement the QUICK scheme, whilst retaining a three point stencil [125]. The QUICK scheme specifies:

\[
(u\phi)_{i,j} = u_{i,j}^* \phi_i + u_{i,j}^* \phi_{i+1} - \frac{1}{8} \left[ u_{i,j}^*(\phi_{i-1} + 2\phi_i - 3\phi_{i+1}) + u_{i+2,j}^*(\phi_{i+2} + 2\phi_{i+1} - 3\phi_i) \right] \tag{3-1}
\]

The second additional scheme considers the effect of the deferred correction technique on the solution. A 50% blending of upwind and central differencing was applied to the convective terms in similar manner to that of Demirdzic et al. [137]. This only requires a three point stencil, allowing evaluation of all terms in the implicit part of the calculation without the need for a deferred correction.

Results for these two schemes compared to the TVD and upwind schemes are shown in Figure 3-19 and Figure 3-20. Again the best shock cell capturing appears to be that of the upwind scheme. Compared to the full upwind scheme the 50% upwind, 50% central scheme results in a significant decrease in peak Mach number, whilst a further decrease is observed with the TVD scheme. The QUICK scheme, which is uniformly of higher order, gives apparently the worst shock cell capturing performance. In the downstream region, as might be expected the QUICK scheme gives the longest potential core, followed by the 50% central difference scheme and then the upwind scheme. However, the TVD scheme gives the
shortest potential core length of all, although this has already been shown to be due to the application of the minmod scheme to the turbulence model.

The effect of the convective scheme on highly underexpanded jets is similar to that observed for moderately underexpanded jets. Figure 3-21 compares the results employing the hybrid, upwind, minmod and $\beta = 0.5$ schemes for NPR = 6.0. The highest peak Mach numbers are predicted with the upwind and hybrid solutions, whilst the TVD scheme predicts considerably smaller Mach number drops across the normal shock. Both the hybrid and upwind schemes predict a Mach number at the leading edge of the normal shock of around 3.0, dropping to 0.15 in the subsonic region behind the normal shock. Normal shock theory for this Mach number at the leading edge suggests Mach number of 0.475 behind the normal shock. Thus, the hybrid and upwind schemes appear to undershoot behind the Mach disk. In contrast the minmod scheme predicts a lower Mach number of 2.8 prior to the normal shock suggesting a Mach number of 0.49 downstream of the normal shock according to normal shock theory. The predicted Mach number of 0.65 represents an underprediction of the normal shock strength.

The effect of mesh resolution and the TVD scheme is demonstrated in Figure 3-22 for NPR = 3.5, by comparing the solution employing the standard 300x105 mesh to that with a doubled resolution in both the axial and radial directions, giving a mesh size of 600x210. The higher resolution mesh gives an increase in the peak Mach number for each shock cell of around 7.5%. The potential core length and downstream profiles are not significantly effected. Clearly, these results show, as expected, that increasing the mesh resolution and hence decreasing the added artificial viscosity, increases the shock cell resolution. The effect of mesh resolution in each direction is shown in Figure 3-23. It is principally the axial mesh resolution that determines the shock cell capturing resolution of the scheme.

The results presented here for both moderately and highly underexpanded jets appear to show that higher order, less diffusive schemes predict a reduced resolution of the shock cell structure. However, increasing the mesh resolution shows, as expected, that decreasing the damping increases the shock cell resolution. This behaviour is not expected and suggests a problem with the applied methodology.

### 3.4.1.1 Subsonic Jet Calculation

Validation of the convective scheme by way of its application to a subsonic jet is considered in this section. The computational grid and boundary conditions were identical to those
described for underexpanded jets in section 3.2, apart from the jet conditions. In this case the static pressure at the inlet was determined by interpolating from the interior. The velocity, temperature and density at the jet exit were then obtained from a specified reservoir total pressure of 1.005 bar and total temperature of 288 K, by assuming an isentropic expansion, resulting in an inlet velocity of 28.7 m s\(^{-1}\). Turbulence kinetic energy was specified as 5\% of the inlet velocity and the length scale as 5\% the nozzle diameter.

In the case of an incompressible subsonic jet, the pressure correction equation reproduces the SIMPLE scheme of Patankar [123]; numerical dissipation is provided only by the convective scheme. Calculations were performed with the upwind and TVD schemes and also with TVD applied to either the momentum equations or to the turbulence model equations only. Figure 3-24 shows the predicted centreline axial velocity calculated using these convective schemes. Clearly, applying the minmod scheme to the turbulence model equations gives the most dissipative scheme, resulting in a significantly shorter potential core length. Similar behaviour was also observed in underexpanded jets (Figure 3-17), where applying the TVD scheme only to the turbulence model equations reduced the potential core length, but without effecting the shock cell resolution. The effect of applying the TVD scheme to the momentum equations can be seen more clearly in Figure 3-25, showing a slight increase in the potential core length indicating that the TVD scheme does have the desired effect in reducing the numerical dissipation.

Radial profiles of axial velocity at \(x/d = 1.0, 5.0\) and \(10.0\) are shown in Figure 3-26. Applying the TVD scheme to the turbulence model equations leads to a significant increase in the spreading rate of the shear layer even one diameter downstream of the nozzle exit plane. The reason for this increased spreading rate is seen in Figure 3-27 and Figure 3-28 which show the turbulent kinetic energy and turbulent viscosity at \(r/d = 0.5\). In the shear layer an increase of around 50\% in the turbulent kinetic energy is observed close to the nozzle exit plane. This results in an increase of more than 100\% in the turbulent viscosity in the same region. Close to the centreline no increase in turbulent kinetic energy or turbulent viscosity is observed (Figure 3-29 and Figure 3-30). Radial profiles of turbulent kinetic energy (Figure 3-31) also show the increase in turbulent kinetic energy close to the nozzle and the increased spreading of the shear layers. This is particularly evident at \(x/d = 1.0\) (Figure 3-31(a)).
3.4.1.2 Numerical Dissipation - the Effect of Momentum Upwinding

To understand the effects that have been observed with regard to the application of TVD convective differencing, in particular to the \( u \)-momentum equation, a further consideration of the modified equations and numerical dissipation is required.

The modified \( u \)-momentum equation, applying full upwinding and with \( \rho u \) as the dependent variable is (see Appendix B):

\[
\frac{\partial}{\partial x_j} (\rho u_j) = \frac{\partial P}{\partial x_i} + \mu \frac{\partial^2 u_j}{\partial x_j^2} + \frac{\partial}{\partial x_j} \left[ u_j \frac{\Delta x_i}{\Delta x_j} \frac{\partial (\rho u_i)}{\partial x_j} \right] + O\Delta x^2
\]

Here, the density weighted variable \( (\rho u) \) is the upwinded quantity.

In one-dimension the additional dissipation term becomes zero due to continuity, resulting in a second order scheme. Note that this would also be the case for multi-dimensional flows with streamlines predominantly parallel to a co-ordinate axis. However, for most multi-dimensions flows this is not the case and the dissipation term can be expanded as:

\[
\frac{\partial}{\partial x_j} \left[ u_j \frac{\Delta x_i}{\Delta x_j} \frac{\partial (\rho u_i)}{\partial x_j} \right] = \frac{\partial}{\partial x_j} \left[ \frac{\rho u_j \Delta x_i}{\Delta x_j} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left( u_j \frac{\Delta x_i}{\Delta x_j} \frac{\partial (\rho u_i)}{\partial x_j} \right) \right]
\]

In the case of \( u \) being the dependent variable in the momentum equation the modified equation is:

\[
\frac{\partial}{\partial x_j} (\rho u_j) = \frac{\partial P}{\partial x_i} + \mu \frac{\partial^2 u_j}{\partial x_j^2} + \frac{\partial}{\partial x_j} \left( \rho u_j \frac{\Delta x_i}{\Delta x_j} \frac{\partial u_i}{\partial x_j} \right) + O\Delta x^2
\]

Here, the primitive variable \( (u) \) is the upwinded quantity.

Unlike when \( \rho u \) is the dependent variable, the dissipation will not be zero across a shock wave in one-dimension, but will be large since the velocity gradient is large; this is also the case in multi-dimensions.

In incompressible regions, where density gradients are negligible, identical artificial diffusion terms are recovered in both cases, with a similar form to the physical diffusion. However, in compressible regions both terms in eq. 3-3 become significant. In cases where these terms are of opposite sign then the second term will act to reduce the artificial dissipation. This will occur whenever density and velocity are out of phase; this is the case across any shock wave including the oblique shock cells in a moderately underexpanded jet (Figure 3-32), and the normal shock in a highly underexpanded jet (Figure 3-33), where the density is a minimum where the axial velocity is a maximum.
Chapter 3. Non-Reacting Results

Across a shock wave the two terms in eq. 3-3 have opposite signs and the combined dissipation term will become of opposite sign to the physical diffusion when:

\[
\left| \frac{\partial}{\partial x_j} \frac{u_i u_j \Delta x_j}{2} \frac{\partial}{\partial x_j} \rho \right| > \left| \frac{\partial}{\partial x_j} \frac{\rho u_i \Delta x_j}{2} \frac{\partial}{\partial x_j} u_i \right| \tag{3-5}
\]

i.e. when the momentum is in phase with density but not velocity:

\[
\text{sgn}\left[ \frac{\partial}{\partial x_j} \frac{u_i \Delta x_j}{2} \frac{\partial}{\partial x_j} \rho \right] = \text{sgn}\left[ \frac{\partial}{\partial x_j} \frac{u_i u_j \Delta x_j}{2} \frac{\partial}{\partial x_j} u_i \right] = -\text{sgn}\left[ \frac{\partial}{\partial x_j} \frac{\rho u_i \Delta x_j}{2} \frac{\partial}{\partial x_j} u_i \right] \tag{3-6}
\]

Figure 3-34 shows the axial momentum and velocity at \( r/d = 0.02 \) for a moderately underexpanded jet. Clearly, momentum is out of phase with velocity in the shock containing region, such that momentum is in phase with density (Figure 3-35). This remains the case until the flow become subsonic. In the highly underexpanded case, shown in Figure 3-36, the relationship between the phases of velocity and mass flux is less clear. During the rapid acceleration phase, up to the peak Mach number and the first part of the normal shock the velocity and mass flux are out of phase, as in the moderately underexpanded jet. However, at the sonic point the mass flux inflects and becomes in phase with the velocity. The mass flux and velocity then remain in phase until the flow is re-accelerated to sonic velocity where the mass flux again inflects, becoming out of phase with the velocity once more. Thus in both underexpanded cases, the momentum is in phase with density wherever the flow is supersonic.

Therefore, wherever the flow is supersonic the effect of the upwinding of momentum will be a first order term which acts in the opposite sense to the physical diffusion and this will increase the shock cell capturing resolution. In the case of a TVD scheme with a base momentum upwind scheme, in smooth regions the limiter appends terms as a deferred correction to reproduce a central difference scheme therefore eliminates the anti-diffusive first order term, reducing the shock cell capturing resolution. Obviously this is not the desired effect, particularly as it is in unsmooth flow regions that the TVD scheme will not append terms and thus the anti-diffusive term will be applied in the very regions where the flow is most unstable. On the other hand, the upwind scheme will add the anti-diffusive terms everywhere.

It is well known that a dissipative term, either implicitly through upwinding or explicitly, must be added to centrally differenced convective schemes when convection dominates over diffusion (i.e. the Peclet No is high), and hence hybrid schemes have been popular for many
applications. In addition, artificial diffusion must be applied across shock waves in order to allow the Rankine-Hugoniot relationship to be satisfied on meshes that do not resolve the thickness of a shock wave, in order to avoid unphysical oscillations. The preceding discussions have described how in this case the upwind scheme does not result in a dissipative term in shock containing regions, but a term of opposite sense. However, the scheme remains stable and captures shock waves without oscillations. This is because the necessary dissipative terms are provided by the pressure correction equation in supersonic regions. In subsonic regions, where some dissipation may be required, density and velocity gradients are in phase and the effect of the upwinding is to add a diffusive term. Accordingly, the dissipation from the pressure correction equation has been found only to be necessary in transonic and supersonic regions.

The correct effect on the shock cell structure of a moderately underexpanded jet of reducing the dissipation can be seen in Figure 3-37 and Figure 3-38, which show the effect of decreasing the nozzle turbulent kinetic energy on the centreline turbulent viscosity and Mach number respectively. As shown by the turbulent viscosity, the level of the physical diffusion is decreased. The resulting Mach number profiles are as expected; the shock cell resolution and the potential core length both increase. Decreasing the added numerical diffusion from the upwinding of density in the pressure correction equation also has the same effect on the shock containing region. The effect of the nozzle turbulence specifications are discussed in more detail in section 3.4.5.

The effect of the convective differencing on the total pressure was discussed in section 3.4.1. This can also be explained by the preceding discussion of the effect of upwinding on the modified equation. It was shown that the upwind scheme leads to a sharp unphysical increase in the total pressure across the first oblique shock cell (Figure 3-14). This is caused by the anti-diffusive term being larger than the total dissipation term across the shock cell where the density gradient is very high. With the TVD scheme the peak does not occur because of the inclusion of some central differencing in the scheme, which does not contain the anti-diffusive terms. However, smaller oscillations are generated in order to satisfy the Rankine-Hugoniot relations. As the upwinding in the pressure correction equation is increased the sharp increase in the total pressure no longer occurs, although the total pressure loss across oblique shock cells is still lower with the upwind and hybrid schemes.

McGuirk and Page [138] demonstrated that solving for momentum rather than velocity gives better shock cell capturing applied to an inviscid one-dimensional convergent-divergent
nozzle problem using the retarded pressure scheme and upwind convective differencing. This was accounted to the change in momentum being reinterpreted as a change in mass flux and hence the mass conservation equation then only contained density explicitly in the time-dependent term. Page [140] extends this explanation stating that solving for momentum with the hybrid convection scheme gave much reduced numerical dissipation when the density field is varying because momentum is upwinded rather than velocity and momentum is constant through a normal shock, whilst velocity varies strongly. In the one-dimensional nozzle example, this is the case; due to continuity momentum will be constant at all points in the flow and there will be no numerical dissipation due to upwinding the convective terms. The results demonstrate the advantage of not including the rather diffusive terms of the velocity upwind scheme in supersonic regions. The scheme was subsequently applied to two-dimensional impinging, underexpanded sonic jets [140]. However, although good results were found for moderately underexpanded jets, the scheme was not able to compute very high Mach numbers or highly underexpanded jets. An explanation for this could be the inability of the retarded pressure scheme to provide enough dissipation to overcome the anti-diffusive terms of the momentum upwinding that increase with increasing Mach number and density variations and hence the Rankine-Hugoniot relations cannot be satisfied.

Other workers have also solved for mass flux components in the momentum equations in compressible pressure correction schemes. Zhou et al. [141] stated that the mass flux components vary more smoothly than velocity components across shocks, and thus solving for mass flux reduced discretisation errors. The mass flux and velocity across the oblique shock cells in an underexpanded jet are shown in Figure 3-34 and Figure 3-36. Clearly, in this case the mass flux varies more rapidly than the velocity, and it is the anti-diffusive effect of upwinding momentum rather than velocity that apparently improves the shock cell capturing resolution. In addition, schemes using momentum rather than velocity in the momentum equations have generally applied better methods than density upwinding for adding dissipation to the pressure correction equation and it is the combined effect of these two features that has improved the shock cell capturing resolution.

3.4.2 Modified Convective Differencing Scheme

In the previous section it was shown that upwinding momentum and not velocity had some undesirable effects in regions where the density gradients were large. In particular, this practice hinders the development of higher order schemes and requires the addition of often
Chapter 3. Non-Reacting Results

large amount of dissipation from the pressure correction equation in order to stabilise the scheme. In this section modifications to the convective differencing scheme, as presented in section 2.5.2, are described and results obtained using this are presented.

3.4.2.1 Model Description

Several options are available to correct the scheme such that the a dissipative diffusion term is reproduced by the upwind scheme. The most obvious method is it subtract a term equivalent to:

\[
\frac{\partial}{\partial x_j} \left( \frac{u_i \Delta x_j \phi}{2} \right) \frac{\partial \rho}{\partial x_j} \quad 3-7
\]

from the source term where upwinding is employed, and do nothing where the solution is centrally differenced. This does not require any modification to the calculation of the base scheme or the higher order deferred correction terms. However, implementation of this was found to give some instabilities in the solution, particularly for highly underexpanded jets. This is due to the monitor functions still detecting fluctuations in mass flux and not velocity. Additionally, this term must not be subtracted when \( \Delta(r) = 1.0 \), and only a proportion of this term when \( 0.0 < \Delta(r) < 1.0 \); this leads to some complexities to ensure the correct terms are subtracted. Hence, the approach chosen modifies the base scheme to remove the density gradient term. This modification is performed at all flow locations and ensures that the correct diffusive flux is obtained. The deferred correction is then modified to account for this change and to append the correct higher order terms.

The convective face flux is calculated as the sum of the base first order upwind scheme and higher order corrections:

\[
[u\phi]_{i+\Delta x_j} = \left( \frac{\rho u}{\rho_{i+1,j}} \right)^+ \phi_{i+1,j} + \left( \frac{\rho u}{\rho_{i,j}} \right)^- \phi_{i,j} + \text{HOT} \quad 3-8
\]

where \( \phi = [\rho u, \rho v, \rho k, \rho e] \)

The higher order terms are now evaluated as:

\[
\text{HOT} = \frac{1}{2} \rho_{i+\Delta x_j} \left( u_{i+\Delta x_j}^+ \Delta_{i+\Delta x_j}^+ - u_{i-\Delta x_j}^- \Delta_{i+\Delta x_j}^- \right) \left( \frac{\phi_{i+1,j}}{\rho_{i+1,j}} - \frac{\phi_{i,j}}{\rho_{i,j}} \right) \quad 3-9
\]

where the limiter functions \((\Delta(r))\) are calculated as described in section 2.5.2.2 and eq. 2-94 and eq. 2-95 are modified to become:
Chapter 3. Non-Reacting Results

\[ r_{i+1,j} = \begin{pmatrix} \phi_{i+1,j} \\ \rho_{i+1,j} \end{pmatrix} - \begin{pmatrix} \phi_{i,j} \\ \rho_{i,j} \end{pmatrix} \]

3-10

\[ r_{i+1,j} = \begin{pmatrix} \phi_{i+2,j} \\ \rho_{i+2,j} \end{pmatrix} - \begin{pmatrix} \phi_{i,j} \\ \rho_{i,j} \end{pmatrix} \]

3-11

With these modifications the scheme reproduces the based first order upwind scheme in unsmooth regions, where \( \Delta(r) = 0.0 \). When \( \Delta(r) = 1.0 \), the central difference scheme is reproduced, which is identical to the central difference scheme obtained with TVD and the momentum upwind base scheme.

3.4.2.2 Results

The centreline Mach number profiles for NPR = 3.5 using the modified convection scheme are shown in Figure 3-39, comparing the upwind and minmod TVD schemes. The results show the opposite trend to that in Figure 3-13. The TVD scheme now gives a better shock cell resolution than the more dissipative upwind scheme and without any unphysical oscillations. However, the potential core length is greater with the TVD scheme. This was shown in section 3.4.1 to be due to applying the TVD scheme to the turbulence model.

Similar results were also obtained for highly underexpanded jets. Figure 3-40 compares the upwind and minmod TVD schemes for NPR = 6.0. Again the better shock cell resolution is obtained with the TVD scheme as would be expected. Another benefit of the modified scheme for highly underexpanded jets appears to be the elimination of the undershoot in the subsonic region behind the normal shock. For an upstream Mach number of 2.8 normal shock theory predicts a downstream Mach number of 0.488, which is in almost exact agreement to that calculated.

The effect of applying the minmod scheme to individual transport equations is shown in Figure 3-41 and Figure 3-42 for NPR = 3.5. The highest shock cell capturing resolution is found when applying the minmod scheme to all equations. Applying to either momentum equations has a similar effect, with the u-momentum giving a slightly increased Mach number on the leading edge of the shock cell and the v-momentum giving better resolution behind the shock cell. Applying the minmod scheme only to the turbulence model has little
effect on the shock cell resolution, however the potential core length is reduced significantly. TVD applied to the \( v \)-momentum has no effect on the potential core length; applied to the \( u \)-momentum gives a very slight increase. Figure 3-43 shows the turbulent kinetic energy for the same calculations. Clearly applying the TVD scheme to the turbulence model equations leads to higher values of turbulent kinetic energy and also turbulent viscosity and hence the potential core lengths are reduced. This effect was also observed for subsonic jets (see section 3.4.1.1).

In addition to the minmod scheme several other TVD limiters have been compared. Figure 3-44 and Figure 3-45 compare the results for the various limiters described in section 2.5.2.2 for NPR = 3.5. The shock cell capturing ability is not effected significantly by the limiter employed, although the superbee scheme causes an increase in the minimum Mach number on the downstream side of the shock cell. The potential core length is effected more significantly by the limiter employed. This has been shown already to be the effect of the turbulence model equations. The shortest potential core length was given by the least dissipative superbee scheme, whilst the minmod scheme was found to be the most dissipative. The Van Albada scheme gives similar result to the minmod scheme, whilst the UMIST and Van Leer schemes give similar, moderate levels of dissipation.

For NPR = 6.0 (Figure 3-46 and Figure 3-47) the limiter has a more significant effect in the shock containing region. In particular, the length of the subsonic region downstream of the normal shock is larger with the more dissipative schemes. This region, behind the normal shock, is particularly sensitive to the scheme employed and turbulence model, with the predicted mixing rate determining the minimum Mach number here and also the recovered Mach number further downstream. The superbee, UMIST and Van Leer scheme are the least dissipative of the schemes, but give rise to the highest turbulence levels giving the shortest potential core lengths and also the smallest subsonic region and therefore the highest downstream Mach number recovery. The minmod scheme predicts the lowest mixing rate behind the normal shock because \( k \) is lower and hence the recovered Mach number is lower than for the other schemes. In addition, its increased dissipative properties lead to the prediction of a slightly lower maximum Mach number at the leading edge of the normal shock.
3.4.3 Pressure Correction Scheme

In this section the effects of applying various differencing schemes in the pressure correction equation, namely upwind, central, blended, TVD and retarded pressure, will be discussed, along with the reasons for adopting the blended differencing scheme for the reacting calculations.

3.4.3.1 Retarded Pressure Function

The retarded pressure scheme was shown by Page [140] to be capable of calculating impinging underexpanded jets up to NPR = 3.3 using the following formulation for the retarded pressure transformation (see section 2.6.4):

\[ \bar{P}_i = P_i + \mu_x (\bar{P}_{i,j} - \bar{P}_{i-1,j}) + \mu_y (\bar{P}_{i,j} - \bar{P}_{i,j-1}) \]

where the retarded pressure function in, for example, the axial direction (\( \mu_x \)) was calculated as:

\[ \mu_x = \max \left\{ 0, k \left[ 1 - \left( \frac{M_{ref}}{(M_x)_{ref}} \right)^2 \right] \right\} \]

with \( k = 0.5 \) and \( M_{ref} = 0.775 \). \( M_x \) is the local directional Mach number, calculated using the relevant component velocity.

In the current work underexpanded free jets up to NPR = 3.05 have been calculated successfully with a retarded pressure function of this form, employing the same convective differencing to that of Page [140] (the hybrid convective scheme based on upwinding density weighted variables). The calculations of Page [140] achieved higher NPRs with this function because a coarser mesh was employed leading to a reduced maximum Mach number.

In an attempt to increase the range of Mach numbers where stable solutions can be obtained the retarded pressure function has been modified to the form:

\[ \mu_x = \min \left\{ \max \left\{ 0, k (M_x - M_{ref}) \right\}, 0.5 \right\} \]

Compared to the function employed by Page [140] (eq. 3-2), this function is linear and limits the retarded pressure function to a maximum value of 0.5. It is shown in Appendix B that when the function \( \mu_x \) exceeds 0.5, the retarded pressure transformation will be increasingly influenced by nodes upstream of its nearest neighbour, a rather undesirable feature. Constraining the retarded pressure function to be less than 0.5 removes this unphysical and
numerically disastrous behaviour. The maximum Mach numbers were achieved with the constants $k$ and $M_{re}$ set to 0.85 and 0.9 respectively. In addition to the modification of the retarded pressure function, applying the equation of state as described in section 2.7.3 to calculate the temperature was found to improve the robustness when computing higher Mach numbers. With these modifications underexpanded free jets up to NPR = 3.5 were successfully calculated, employing convective schemes based on upwinding density weighted variables. However, unstable solutions were always found for pressure ratios above this. In fact, even at this pressure ratio under certain conditions and convective differencing schemes unstable results, or stable results containing obvious unphysical oscillations, were obtained. Unless employing a coarse mesh and thus increasing the damping of oscillations and reducing the shock cell resolution, the hybrid solution failed with the retarded pressure function at NPR = 3.5. However, the TVD convective scheme was able to compute a reasonable solution, representing a maximum Mach number of 2.05. Typical centreline Mach number profiles obtained using this form of the retarded pressure function are shown in Figure 3-6 for NPR = 2.69 and Figure 3-7 for NPR = 3.5.

With the modified convective differencing scheme, discussed in section 3.4.2, a larger range of NPR has been calculated successfully using the retarded pressure function. Figure 3-48 and Figure 3-49 show comparative results to those shown in Figure 3-6 for NPR = 2.69 and Figure 3-7 for NPR = 3.5. Similar results are obtained using the two convective schemes, although the upwinding of primitive and not density weighted variables leads to a reduction in the shock cell resolution especially for the upwind scheme since the anti-diffusive term has been replaced by a diffusive one. However, where schemes based on upwinding density weighted variables failed to give solutions above NPR = 3.5, the primitive variable based scheme is capable of calculating solutions at NPR = 4.0 and NPR = 5.0 (Figure 3-50), corresponding to a maximum Mach number of 3.0. Significantly, the solution at NPR = 5.0 contains a normal shock and is therefore a highly underexpanded jet, which had not previously been calculated with the retarded pressure scheme. Above this pressure ratio, solutions show increasing oscillatory behaviour with no solutions possible for pressure ratios of 6.0 and above.

Thus the range of applicability of the retarded pressure scheme to underexpanded free jets has been extended from NPR = 3.05, achieved using the formulation of Page [140] to 3.5 by modifications to the retarded pressure function and the implementation of the equation of state.
Chapter 3. Non-Reacting Results

state. Further increases up to NPR = 5.0 have been achieved by incorporating the TVD convective scheme based on upwinding primitive variables as described in section 3.4.2.

3.4.3.2 Upwind Scheme

Applying full upwinding to the pressure correction equation overcomes the Mach number limits imposed by the retarded pressure function, allowing solutions over a very large range of pressure ratios with any of the convective schemes; results presented in section 3.3.2 demonstrate the ability to attain stable calculations up to NPR = 30.

The centreline Mach numbers using the upwind scheme for the pressure correction is shown in Figure 3-51. The effect of the increased dissipation can be observed with a more smeared shock cell structure. This type of scheme was that used in almost all early compressible pressure correction schemes, producing unacceptable smearing.

3.4.3.3 Blended Differencing Scheme

The ideas behind a blended difference scheme were described in section 2.6 and are initially applied with convective schemes based on upwinding density weighted variables. The simplest method of applying blended differencing to the density in the pressure correction equation assigns fixed proportions of upwind and central differencing. The effect of applying 20% central differencing over the whole domain in each direction is shown in Figure 3-52 and Figure 3-53. The addition of 20% central difference in the radial direction produced only a very small increase in the peak Mach number in the first shock cell. However, applied in the axial direction it had a much more significant effect; the Mach number drop across the first shock cell increased by around 8%, whilst the increase was close to 25% across the second. The downstream region, beyond the shock containing potential core, was unaffected by the differencing employed in the pressure correction equation.

Better results can be obtained by using local Mach number dependent functions, in the form of eq. 2-131, to prescribe the proportions in which central and upwind differencing are blended. With this function, where the local direction Mach number is below $f_2$ the differencing will be purely central; above this Mach number a proportion of upwinding is introduced in a linear manner dependent on $f_1$. The effect of varying $f_1$, with $f_2$ fixed at 0.5, can be seen in Figure 3-54. As $f_1$ was reduced then so also was the proportion of upwind differencing, resulting in improved shock cell capturing. With $f_1 = 0.4$ the peak Mach
number in the first shock cell is 2.25, compared to 2.0 with $f_1 = 1.0$. Subsequent shock cells are also resolved more accurately.

There are obvious advantages of applying a locally varying blending scheme. In the case of $f_1 = 0.4, f_2 = 0.5$, full upwind does not occur until the local flow exceeds a Mach number of 3.0. For NPR = 3.5, the peak Mach number in the solution was 2.25 where the solution would be 70% upwind, 30% central differencing, whilst at the ideally expanded Mach number of 1.47 the blending would be 40% upwind and 60% central differencing. In addition, throughout almost the whole domain central differencing is retained in the radial direction due to the radial Mach number being below $f_2$, although as shown in Figure 3-52 the radial differencing does not have a significant effect on the shock cell resolution. One further advantage of this scheme is its ability to stabilise the jet development phase when employing locally varying time steps. During the transient phase it is possible to generate unphysical spikes in the solution. The damping of these spikes will be improved since the scheme will apply increasing amounts of upwinding during the development of these spikes.

With a TVD scheme based on upwinding primitive variables applied to the convection terms, much lower levels of dissipation in the pressure correction equation are required to obtain stable solutions. In fact, for NPR below 3.5 solutions can be obtained applying no upwinding in the pressure correction equation; this could not be achieved for any underexpanded jet applying momentum based upwinding for reasons already discussed in section 3.4.2.2. Figure 3-55 shows the solution at NPR = 2.69. This result show a significant improvement in the shock cell resolution over any other scheme. In this case the minimum amount of numerical dissipation is added to prevent the formation of oscillations and for much of the solution domain all differencing will be second order accurate. For NPR = 3.5 (Figure 3-56) an unphysical overshoot develops at the leading edge of the shock cell, and thus some dissipation is now required in the pressure correction equation. This is because even with upwinding in the convective terms at this point, the dissipation is not sufficient to overcome the effects of applying an elliptic equation for pressure to a non-elliptic situation.

Figure 3-57 shows the effect of increasing amounts of local Mach number dependent upwinding in the pressure correction equation, achieved by modifying $f_1$ and $f_2$. As the upwinding is increased the peak Mach number at the leading edge of the shock decreases and the Mach number drop becomes smeared across an increasing number of nodes, which decreases the Mach number gradient across the shock to give a smeared appearance. With full upwinding the solution is smeared across around half a nozzle diameter, or about twenty
nodes. In contrast with no upwinding the shock is captured across three nodes. However, the solutions downstream of the shock containing region are insensitive to the differencing employed in the shock containing region; only the upwind scheme, which is the only scheme which does not apply central differencing in low Mach number regions, is significantly different here.

Compared to similar results for upwinding based on density weighted variables for the convective scheme (Figure 3-54) the results in Figure 3-57 show similar peak Mach numbers in the first shock cell. However, the shock cells are captured with less smearing and are retained further downstream. This is due to the lower levels of upwinding that can be applied in the pressure correction with primitive variable based upwinding for convective terms.

Similar effects to those seen for moderately underexpanded jets are also found for highly underexpanded jets. The effect of varying $f_1$ for $f_2 = 0.7$ at NPR = 6.0 is shown in Figure 3-58 and Figure 3-59. Again as the upwinding is reduced the peak Mach number increases as does the Mach number drop across the shock cell giving a lower Mach number in the subsonic region.

Although the blended differencing scheme has been shown to be capable of computing solutions at all Mach numbers, it is necessary to modify the blend factors in order to obtain the best shock cell capturing resolution. As the maximum Mach number increases it is necessary to increase the amount of dissipation applied for a particular Mach number. The optimum values for various Mach number ranges are shown in Table 3-1. For low NPR no dissipation is required and the value of $f_2$ is arbitrary, since $f_1 = 0.0$.

<table>
<thead>
<tr>
<th>NPR range</th>
<th>$f_1$</th>
<th>$f_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1-3.4</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>3.5-5.0</td>
<td>0.1</td>
<td>0.9</td>
</tr>
<tr>
<td>5.0-10.0</td>
<td>0.2</td>
<td>0.7</td>
</tr>
<tr>
<td>10.0-30.0</td>
<td>0.5</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Table 3-1. Optimum Blend Factors as a Function of NPR

For a pressure ratio of 5.0 the maximum Mach number is around 2.8 giving a blend of 19% upwind and 81% central differencing, whilst at the ideally expanded Mach number of 1.7 only 6% upwind differencing is applied. For NPR = 10.0 the maximum Mach number is
around 3.3 giving 52% upwind and 29% upwind at the ideally expanded Mach number of 2.16.

The blended differencing scheme has been shown to be capable of predicting both moderately and highly underexpanded jets with good shock cell capturing resolution, but requiring the correct specification of the blend factors. Applying the primitive variable based TVD scheme to the convective differencing allows significantly higher proportions of central differencing to be employed in the blending, and for NPR below 3.5 full central differencing can be applied.

3.4.3.4 TVD Type Limiters

The TVD based pressure correction discretisation, described in section 2.6.5, only applied the TVD differencing to the source, or mass error term since this is the only significant term effecting the accuracy of the solution. The implicit pressure correction containing terms can be discretised using any suitable method in order to give stability. For moderately underexpanded jets the solutions obtained were independent of the discretisation applied to the implicit pressure correction terms, only the discretisation scheme applied to the source term was significant.

Figure 3-60 and Figure 3-61 compares the centreline Mach number solution obtained with the TVD scheme to those with full upwind and central differencing for NPR = 3.5. The TVD scheme has comparable shock cell resolution to that of the central differencing scheme, and all three solution are similar in downstream regions. The TVD scheme does not exhibit the overshoot on the leading edge of the first oblique shock cell, however an undershoot is observed which takes the Mach number below one, suggesting the presence of a normal shock, which should not be predicted at this pressure ratio. However, the Mach number contours (Figure 3-62) show some evidence of a small normal shock and no evidence of numerical oscillations usually observed with over- and undershoots. This undershoot is not observed with either of the other two schemes considered here. A further consequence of this behaviour is that the subsequent oblique shock cell structure is displaced downstream by around 0.2 diameter compared with the central differencing scheme.

Highly underexpanded jets have also been computed with the TVD scheme. In this case the type of discretisation applied to the implicit part of the pressure correction equation does become important. For NPR = 6.76, with the TVD scheme applied to the mass error term, applying central differencing to the discretisation of the implicit terms leads to a rapid
generation of instabilities and no solution can be obtained. Solutions have, however, been obtained with both upwinded and blended differencing applied to the implicit terms and these give identical solutions. Figure 3-63 compares the blended differencing and TVD solutions for NPR = 6.76, employing TVD convective difference based on primitive variable upwinding. The TVD scheme predicts a significantly higher Mach number at the leading edge of the normal shock, and a very similar resolution of the normal shock and minimum Mach number downstream of the normal shock, whilst the resolution of the oblique shock cell structure is also improved. However, this apparent higher resolution comes at the expense of some oscillations in the flow away from the centreline that can be observed in the Mach number contours (Figure 3-64). These become more significant with higher pressure ratios and eventually lead to numerical failure at higher pressure ratios.

3.4.3.5 Comparison of Schemes

The centreline Mach numbers for three pressure correction schemes are compared in Figure 3-65 for a moderately underexpanded jet with NPR = 3.5. Upwind differencing gives by far the most smeared shock cells due to its excessive numerical dissipation. The best shock cell capturing performance is that of the local Mach number dependent blended differencing scheme, although its performance is only marginally better than that of the retarded pressure function. In the potential core region the retarded pressure scheme gives a higher mean Mach number closer to the ideally expanded Mach numbers of 1.47. This is probably due to the retarded pressure function retaining its central differencing up to a higher value of the directional Mach number.

Figure 3-66 compares the same pressure correction schemes, but for a highly underexpanded jet of NPR = 5.0. In this case the maximum peak Mach number is given by the retarded pressure scheme, with a maximum Mach number of 2.96 compared to 2.84 in the case of the blended differencing scheme. Minimum Mach numbers of 0.77 and 0.50 are obtained respectively, compared to normal shock theory which calculates values of 0.478 and 0.485 respectively for the predicted maximum Mach numbers. Clearly, the blended differencing predictions agree very accurately with the normal shock, whereas the retarded pressure computations underpredict the normal shock strength. The resolution of the captured shock and its location are comparable for the retarded pressure and the blended differencing schemes.
Chapter 3. Non-Reacting Results

Figure 3-67 compares the total pressure obtained for each scheme. With the retarded pressure scheme an unphysical spike is observed in the total pressure at the leading edge of the normal shock. This indicates that the computations are beginning to show unstable behaviour, and that the high Mach number predicted by the scheme is an error due to this unstable behaviour. This is further demonstrated since any increase to the NPR causes the scheme to become unstable.

The dissipation terms associated with each type of differencing scheme were described in Appendix B. The retarded pressure scheme adds a dissipation term to the momentum equations, whilst the blended and upwind schemes add dissipation terms to the mass error term in the pressure correction equation. In addition to these terms, which are present in the steady state, during jet development transient terms are important to ensure stability. In the retarded pressure formulation the equation solved is of the form:

$$\frac{1}{\Delta t} \frac{P'}{RT} + \frac{\partial}{\partial x_j} \alpha_{ij} \frac{\partial P'}{\partial x_j} = -M_s$$

Where $\alpha_{ij}$ represents the linkage between the momentum equation and momentum correction. This equation is an elliptic Poisson equation for pressure correction.

In the case of the blended and upwind schemes the pressure correction equation is of the form:

$$\frac{1}{\Delta t} \frac{P'}{RT} - \frac{\partial}{\partial x_j} \left( \alpha_{ij} \frac{\partial P'}{\partial x_j} + \frac{P'}{RT} u'_j \right) = -M_s$$

This equation is a convection-diffusion equation for pressure correction.

In compressible flows it is necessary to account for both velocity and density changes simultaneously in the pressure correction equation in order to construct a stable scheme. Recalling eq. 2-110, the momentum was split to form three terms, $\rho^* u'$, $\rho' u^*$ and $\rho' u'$. These terms represent contributions from velocity corrections, linear density corrections and non-linear density corrections respectively. In the incompressible and retarded pressure formulations only the first term is included; the second term gives rise to the convective term in eq. 3.5 and will be large in high speed regions. The third term was neglected in all the formulations. In the steady state, all terms containing pressure correction disappear such that the accuracy of the pressure correction formulation is solely dependent on the mass error term. However, the correction terms are essential to ensure a robust convergence to the steady state and their omission from the retarded pressure formulation is a possible cause of
its failure for higher Mach number flows, whilst being of similar accuracy to the blended differencing scheme at moderate Mach numbers.

### 3.4.4 Grid Dependency Results

The preceding results employed a computational mesh of 300x105 cells, as described in section 3.2. The effect of increasing the mesh resolution has been considered by employing a mesh doubled in both the x and y directions, giving 38 cells radially within the nozzle and a minimum mesh spacing of 0.01 nozzle diameters (0.25mm) in both the axial and radial direction. With the doubled mesh, the computational time required to obtain a converged solution increases from 100 to 800 minutes on a Silicon Graphics R10000 processor, since the number of cells increases be a factor of four, and the reduced time step requires that around 10000 cycles are required. The centreline Mach number for a NPR = 3.5 moderately underexpanded jet employing the 600x210 grid is compared to that for the original grid in Figure 3-68. The doubled resolution leads to an increase in the peak Mach number in the first shock cell of around 5%, from 2.17 to 2.28. A similar improvement is also observed in subsequent shocks cells. Significantly, it is only the rate of attenuation of the shock cells that is effected by the increased grid resolution and not the location of these shock cells. Downstream, the potential core length is not effected by the increased resolution. The turbulent kinetic energy for both grids are compared in Figure 3-69 and radial Mach number profiles at four axial locations are shown in Figure 3-70, confirming that the shear layer predictions are not dependent on the mesh resolution. The predicted centreline turbulent kinetic energy is slightly higher with the 600x210 mesh as a result of the higher predicted velocity gradients leading to increased turbulent production terms. The 300x210 mesh gives essentially grid independent results for the shock cell locations, shear layers and downstream mixing in moderately underexpanded jets; only the shock cell strength is affected by increasing the mesh resolution further.

Figure 3-71 shows the effect of the radial and axial mesh resolution on the shock cell structure. The peak Mach number at the leading edge of the first shock cell is principally dependent on the axial mesh resolution; the radial resolution has a much less significant effect. Downstream of the first shock cell increasing axial resolution has the effect of increasing the Mach number, whilst increased radial resolution decreases this Mach number and hence increases the overall Mach number drop across the oblique shock cell.
The 600×210 and 300×105 meshes have also been compared for a highly underexpanded jet with NPR = 6.0 in Figure 3-72. As with moderately underexpanded jets the increased mesh resolution increases both the peak Mach number and the Mach number drop across the first shock cell, whilst having no effect on the downstream mixing. However, in the highly underexpanded case the recovered Mach number in the oblique shock region is dependent on the mesh resolution. In the subsonic region behind the normal shock the lower resolution mesh allow more rapid mixing between the subsonic and supersonic regions and thus this subsonic flow is accelerated more rapidly, giving both a shorter subsonic region and a higher Mach number downstream. This is reflected throughout the subsonic region.

The effect of mesh resolution on moderately underexpanded jets was studied by Kim et al. [179] using a commercial code. The authors assumed that it was only the axial resolution that affected the solution accuracy. For a sonic nozzle with NPR = 3.323 meshes of 141×71 and 421×71 were compared. No details are given as to the nature of the mesh, or the domain size so as to assess the grid spacing. Similar solutions of the centreline velocity were observed in the first shock cells. However, downstream of this, the shock cell structure with the coarse mesh was dissipated rapidly, with only 3 shock cells resolved. The fine mesh case predicted around eight shock cells and compared well to the experimental data.

3.4.5 Nozzle $k$-$\varepsilon$ Specification

As stated in section 3.2 many of the flow properties at the nozzle exit during experimental measurements are generally unknown, this is particularly the case for turbulence quantities. It is therefore necessary to specify sensible values for these quantities. For most of the work in this thesis $k$ was calculated by specifying a fluctuating velocity component of 5% of the mean velocity at the nozzle, whilst $\varepsilon$ was calculated assuming a length scale of 5% of the nozzle diameter.

Figure 3-73 considers the effect of the turbulent velocity scale by comparing centreline Mach numbers for solutions employing 10%, 5% and 1% as the turbulent velocity scale, whilst retaining the same length scale. Reducing $k$ leads to an increase in the potential core length and an increase in the shock cell strength, since the physical damping is reduced. Figure 3-74 shows the turbulent kinetic energy, whilst Figure 3-75 shows the turbulent viscosity plots for the same calculations. Clearly, the initial turbulence conditions have a significant effect on the solution obtained, particularly on the potential core length. This has important implications with regard to comparing computational results with experimental data.
Chapter 3. Non-Reacting Results

Encouragingly, the sensitivity to the initial turbulence conditions demonstrates that the numerical viscosity within the methodology does not dominate the physical diffusion. In particular, the potential core length is not sensitive to the scheme employed for either the convective or pressure correction differencing.

The ambient values for $k$ and $e$ did not have a significant effect on the computations.

3.4.6 Discussion of Numerical Issues

It has been shown that convective differencing based on upwinding density weighted variables gives additional first order terms in the modified equation that act to increase gradients in supersonic flow regions, i.e. compressive terms acting in the opposite sense to dissipation terms. This has been shown to result in theoretically higher order schemes, such as QUICK, TVD and blends of upwind and central differencing, giving apparently lower resolution shock cell capturing than pure upwinding. These anti-diffusive terms then require large quantities of dissipation to be added through some other method in order to maintain stability, and has led to the use of density upwinding in the pressure correction mass error term, or the use of methods such as retarded pressure or density. Results presented in this thesis have shown that the retarded pressure scheme can be extended to achieve solutions up to $NPR = 3.5$ with upwinding based on density weighted variables for the convective differencing. With density upwinding in the mass error term of the pressure correction term solutions above $NPR = 30.0$ have been obtained, however these results show excessive dissipation of the shock cell structures and shear layers. The blended differencing scheme was also shown to be capable of calculating solution up to $NPR = 30.0$ with improved accuracy. However, in very high Mach number regions the differencing would be almost totally upwind.

With a modified convective differencing scheme based on the upwinding of the primitive variables the shock cell capturing resolution is considerably reduced compared to that with density weighted variable based upwinding, when employing the same differencing in the pressure correction mass error term. However, the TVD scheme gives much improved shock cell capturing performance compared to the upwind scheme. With upwinding of the primitive variables the added first order terms are of the correct nature and supply stabilising dissipation. However, with the TVD limiters, the minimum dissipation is supplied on a local basis to maintain stability. This allows the dissipation supplied by the differencing of density in the mass error term or the retarded pressure scheme to be reduced, and for pressure ratios
below 3.5 removed completely; sufficient dissipation is supplied by the convective differencing. Thus, much improved shock cell resolution was obtained in these cases. Above NPR = 3.5, although some additional dissipation was required from the pressure correction equation, the quantities were significantly lower than previously required, allowing the retarded pressure scheme to be extended up to NPR = 5.0, including reasonably accurate prediction of a normal shock. The amount of upwinding in the blended differencing scheme could be also reduced, improving the shock cell resolution. Demirdzic et al. [137] employed a blending scheme in a pressure based method to all the transport equations. This blending scheme applied a constant level of upwind differencing over the whole domain for application to transonic and supersonic bump flows. Typically, 10\% upwind was added for a peak Mach number of around 2.0. In the current work, for a Mach number of 2.0 (assuming NPR < 5) 11\% upwind was added. However, this was only applied to the pressure correction terms, with TVD applied to the convective differencing in the other transport equations. Additionally, the level of upwinding was applied based on the local Mach number allowing lower or no dissipation in lower Mach number regions.

The requirements of the numerical scheme for the computations in this thesis is a scheme that is both stable and accurate over the whole range of pressure ratios. The upwind scheme, although robust at all the pressure ratios tested is inaccurate due to its excessive numerical dissipation. Central differencing is both stable and accurate for NPR below 3.5, but above this the solution is unstable. The TVD limiter has been shown to give very good shock cell capturing at pressure ratios up to around 7. However, instabilities are a problem for all highly underexpanded jets and there is some questions about its accuracy and tendency to predict normal shocks at too lower pressure ratios. This leaves the retarded pressure scheme and blended difference scheme which show comparable shock cell resolution. However, although the retarded pressure scheme has been shown capable of predicting Mach disks up to NPR = 5.0, extending the pressure ratio range from previous studies, above this NPR the solution fails. Thus the blended difference scheme is the seen to be the best option.

The major benefit of the blended differencing scheme is its ability to compute flows over the complete range of Mach numbers, although to obtain optimum shock cell resolution the blend factors must be modified for different ranges of Mach number. In the incompressible limit the scheme reduces to an incompressible pressure scheme, whilst at very large Mach numbers the scheme becomes predominantly upwind and hence very stable. It is for these
reasons that the local Mach number dependent blended differencing scheme will be predominantly employed in this work.

The choice for the convective differencing scheme is straightforward. Both the hybrid and TVD schemes are capable of calculating solutions at all the pressure ratios tested, however much improved shock cell resolution was obtained with the TVD scheme based on the minmod limiter, without any reduction in stability or significant increase in the computational requirements. Other TVD limiters have been employed, but the minmod scheme provides the best stability without a significant loss of accuracy.

It has been shown for both underexpanded and subsonic jets that the TVD scheme applied to the turbulence model equations decreased the length of the potential core, but when applied to only the momentum equations it increased this length. This behaviour was not found to be affected by including density in the upwinded term.

The modified $k$ equation with upwinding based on $k$ is:

$$\frac{\partial}{\partial t} \tilde{\rho} \tilde{k} + \frac{\partial}{\partial x_j} \tilde{\rho} \tilde{u}_j \tilde{k} - \frac{\partial}{\partial x_j} \Gamma_{\text{eff}} \frac{\partial \tilde{k}}{\partial x_j} = P_k - \tilde{\rho} \tilde{\varepsilon} + \text{HOT} + O \Delta x^2$$

where:

$$\Gamma_{\text{eff}} = \frac{\mu_t}{C_{\mu}} + |\tilde{u}_j| \frac{\Delta x}{2} = \frac{\mu_t}{\sigma_k} \frac{k^2}{\varepsilon} + |\tilde{u}_j| \frac{\Delta x}{2}$$

The additional first order dissipation term can be an order of magnitude equal to or greater than the turbulent viscosity and will act to increase the effective diffusion when the solution is upwinded, which will lead to lower levels of $k$ and hence $\mu_t$ in the shear layers. Additionally, since turbulent production is a function of the turbulent viscosity this will then also decrease in the shear layers. The effect of this will be to increase potential core lengths. With the hybrid scheme upwinding will predominate throughout the majority of the regions where $k$ is high and in particular the shear layers, since this differencing is based on the Peclet number. With the TVD scheme, the type of differencing is dependent on the $k$ solution and can be different from that used by the transport equations of other variables and therefore higher order terms will be significant throughout the majority of the domain and their effect will be to reduce or eliminate the additional diffusion coefficient. Therefore, with the TVD scheme applied to the turbulence model, $k$ and hence $\mu_t$ will be larger in the shear layers and give rise to the predicted increase in mixing and decrease in potential core lengths.
3.5 Test Cases – Comparison to Experimental Data

In the following section computations are presented over a range of pressure ratios and are compared to the available experimental data. The compressibility correction, described previously (section 2.3.4), is also assessed in light of the experimental data.

3.5.1 Chuech [16], NPR = 2.27 and 2.59

The work of Chuech [16] presents experimental data for two underexpanded jets with NPR = 2.27 and 2.59. Axial static pressure profiles were presented for both pressure ratios, whilst for the lower pressure ratio, axial and radial profiles of both the mean and fluctuating velocities were also obtained. The pressure measurements employed LIF and were significantly gradient broadened across shock waves, due to the finite size of the LIF measuring volume. Estimated experimental error, away from gradient broadened regions was 13%. Velocity measurements were taken using LDA which was found by the author to be adequate for measurements in the subsonic and sonic portions of the flow. However, the particles could not respond to the rapid changes of velocity encountered in passing through shock waves in the supersonic region. Estimated experimental error was 10% away from shock waves. In addition to these quantitative measurements a number of Schlieren photographs were obtained to demonstrate the effect of increasing pressure ratio on the shock cell structure.

Computations have been performed for both these cases employing a 300×105 cell mesh along with the minmod TVD convective differencing scheme and no dissipation in the pressure correction scheme, since for NPR < 3.5 this is not required (see section 3.4.3.3). For NPR = 2.27, Schlieren photographs showed a typical diamond shaped shock cell structure, with the action of viscous effects dissipating the shock cell structure after around 6-8 diameters from the jet exit. These observations are supported by the computations where the potential core region extends around 6.5 diameters with k-ε and 8 diameters with k-ε-CC. Comparison to the computed centreline axial velocity data, shown in Figure 3-76, demonstrates clearly the problems associated with obtaining experimental data for this kind of flow. Chuech [16] states that the experimental data is only reliable downstream of the potential core region and that the oscillating velocities, clearly observed in their flow visualisation studies and the present computations, could not be measured. Downstream of the potential core a reasonable agreement was found between the experimental and computational results. Radial profiles are also considered at three axial locations (Figure 3-
At $x/d = 5.0$ very encouraging results are obtained, indicating the ability to predict correctly the shear layer spreading rate, particularly with the compressibility corrected model. This axial location is within the potential core region, but downstream of the predicted shock cell structure. Very good agreement is also obtained in subsonic flow regions away from the supersonic flow around the jet centreline. At $x/d = 10.0$, which is just downstream of the potential core region, similar results are observed; excellent agreement is obtained away for the jet axis. Finally, results from the downstream region at $x/d = 20.0$ confirm the accurate prediction of the downstream mixing properties with the $k$-$\varepsilon$-$CC$ model.

In addition to the mean axial velocities, data for the fluctuating axial velocity was also obtained by Chuech [16]. By assuming isotropic turbulence a turbulent kinetic energy can be derived, which is compared to that obtained in the computations. Figure 3-78 shows the centreline turbulent kinetic energy. Qualitatively, the centreline turbulent kinetic energy compares well. Throughout the initial shock containing region the turbulent kinetic energy is low, increasing to a peak value as the potential core region is eroded away. The experimental results show a higher value of $k$ in the core region followed by an earlier increase in the turbulent kinetic energy and a higher peak. The $k$-$\varepsilon$-$CC$ results, which gave closer agreement for velocity, give the largest discrepancies for $k$. This could suggest that the nozzle $k$ values are higher in the experimental case than the computations. However, it is the value of $k$ in the shear layers that is most important in determining the mixing characteristics of the jet; $k$ has little effect on the shock containing region. Three radial profiles are shown in Figure 3-79 at $x/d = 5.0$, 10.0 and 20.0 diameters from the nozzle exit plane. In each case good qualitative agreement is found between the experimental data and $k$-$\varepsilon$-$CC$ computations, whilst good quantitative agreement is only found away from the centreline.

Several factors could influence the results presented here for $k$. As with the mean velocities, the larger differences between experimental and computational results occurred in the supersonic flow regions. Again, this could be due to experimental errors in these region. However, significant uncertainties exist with the application of the present turbulence treatment to compressible flows. Also, the derivation of $k$ from the experimental fluctuating axial velocity data requires the assumption of isotropic turbulence, for which there is no supporting experimental data. The $k$-$\varepsilon$ model, as with any first order turbulence model, does assume that the ratio between the Reynolds stresses and mean rate of strain is isotropic and hence reduces the ability of the model to predict anisotropic turbulence. Any deviation of the
turbulence from isotropic behaviour will effect both the derivation of $k$ from the experimental data and the accuracy of the turbulence treatment in the computations.

Improvements to these results could have been achieved by assuming fully developed pipe flow at the nozzle exit, instead of slug flow. However, the cases of interest in this thesis will be almost entirely of the slug flow type and therefore simulations have been restricted to these nozzle conditions.

The only extensive measurements of the shock containing regions are pressure profiles which are shown in Figure 3-80 and Figure 3-81 for NPR = 2.27 and NPR = 2.59 respectively. In both cases the results show the experimental and computational results to be out of phase.

One explanation for this problem is the use of a long pipe in the experimental configuration so as to obtain fully developed pipe flow at the nozzle exit, which can lead to inaccuracies in defining the correct nozzle exit plane. Clearly, the lower NPR pressure data has some error in this region since the experimental pressure measurements indicate an initial increase from below ambient with increasing axial distance from the nozzle; this is clearly not the case for an underexpanded jet. The location of the first pressure measurement was 0.1 diameters downstream of the nozzle with a pressure below ambient. For this pressure reading to be accurate the first oblique shock cell would have to have been located upstream of this point. However, data for the location of the first shock cell, such as that of Love et al. [11], indicates that the first shock cell is located around 0.3 diameters downstream of the sonic nozzle exit plane; very close to the computed value. A similar situation occurs for NPR = 2.59.

In order to obtain a more meaningful comparison the axial co-ordinate, the experimental data was translated downstream such that the first shock cell is positioned at the location measured by Love et al. [11]. The results with this translation are shown in Figure 3-82 and Figure 3-83. In both cases it appears that the wavelength of the shock cell structure is slightly overpredicted, as is the peak pressure in the first cell. For NPR = 2.27, subsequent shock cells show an underprediction of the shock cell structure, both in terms of the peak pressures in each cell and the number of cells predicted. For NPR = 2.59 the magnitude of the peak pressure in subsequent shock cells is predicted more accurately, as is the number of cells observed. It is expected that the computed shock cell structure will be better resolved with higher pressure ratios since the effect of damping will be less significant compared to the larger pressures involved. The experimental data shows that the shock cell structure is damped more quickly in the higher pressure ratio case; for NPR = 2.27 the tenth shock cell is
observed at $x/d = 6.0$, whilst for NPR = 2.59 the fifth and last measured shock cells occurs at $x/d = 4.5$.

3.5.2 Stickland et al. [7], NPR = 2.5, 3.5 and 5.0

Stickland et al. [7] obtained experimental axial Mach number profiles for NPR = 2.5, 3.5 and 5.0 and also radial profiles for NPR = 3.5. The data was attained by interrogating the flow with a five hole pressure probe, and deriving Mach number and static pressure data from this data. Some uncertainties are generated in the results due to the probe only being calibrated for $0.7 < M < 1.8$ and below $M = 0.1$; extrapolation was employed outside these ranges. For NPR = 5.0 Mach numbers of up to 2.5 were recorded. The limitation of pressure probe data was discussed in section 1.2.1, such as the effect of the probe on the surrounding flow and the need for very small probes so that the sensing volume is sufficiently small to allow shock cell structures to be adequately resolved. The results of Stickland et al. [7] show some smearing of the shock cell structure with, for example, the normal shock at NPR = 5.0 smeared over around 0.25 diameters (12.5mm). However, the relatively large nozzle ($d = 50mm$) will reduce the amount of shock smearing.

As with the data of Chuech [16] there are some uncertainties in the location of the nozzle exit plane. In this case a subsonic test with NPR = 1.25, giving an exit Mach number of 0.58, showed an initial flow acceleration to a Mach number of around 0.62. This was believed to be due to imperfections in the nozzle design. Any imperfections in the nozzle design will also have significant effects on the underexpanded jet data since features of an underexpanded jet, such as the wavelength of the shock cell structures, their strength and the number of shock cells occurring before the flow is damped, depend on the nozzle exit Mach number. The underexpanded jet results show Mach numbers above 1.0 at $x/d = 0.0$. For NPR = 2.5 this Mach number is recorded as 1.1, increasing to 1.15 for NPR = 3.5 and 1.25 for NPR = 5.0. This increased Mach number could be due to several effects, such as imperfections in the nozzle design, the location recorded as $x/d = 0.0$ being downstream of the actual nozzle exit, or inaccurate measurements or decomposition of the pressure data. A number of computations have been performed in an attempt to simulate the increased nozzle exit Mach numbers observed. However, assuming that the reservoir conditions are unchanged, an increase in the nozzle exit Mach number from 1.0 to 1.1 for NPR = 2.5 would give a decrease in the pressure at the nozzle exit from $1.32P_{amb}$ to $1.17P_{amb}$ and an increase to 1.25 for NPR = 5.0 would give a decrease from $2.64P_{amb}$ to $1.93P_{amb}$. Clearly, such
decreases effect significantly the shock structure, and in the NPR = 5.0 case lead to the Mach disk disappearing. Thus, as was the case for the pressure data of Chuech [16], a translation of the axial co-ordinate has been employed in the following results, such as to ensure that the first experimental data point coincides with the point in the computed results with an equivalent Mach number.

Figure 3-84 shows the centreline Mach number for NPR = 2.5. The experimental results predict a significantly stronger shock cell structure prevailing further downstream. The mean Mach number is also higher in the experimental case. For a sonic, NPR = 2.5 jet the ideally expanded Mach number, assuming isentropic flow, is 1.22. This is in almost exact agreement with the computed value. Thus, the higher value observed in the experimental data again raises suspicions about the accuracy of this data. The location of the shock cells and the wavelength show good agreement between the predicted and measured values. In addition, the length of the potential core and the downstream mixing \((x/d > 15.0)\) are in good agreement to the k-e-CC computational results.

Both axial and radial Mach number profiles were presented for NPR = 3.5. Very good agreement is obtained for the centreline axial Mach number (Figure 3-85) in the first shock cell, after which the predicted shock cell structure decays too rapidly. In addition, there is also an underprediction of the shock cell wavelength after the third shock cell. This may be due to excessive damping, either physical or numerical, since the k-e-CC model predicts an increased wavelength for the fourth and fifth shock cells. As with NPR = 2.5, the potential core length is well predicted by the k-e-CC model. For NPR = 3.5 the ideally expanded Mach number is 1.47, which is close to the computed value.

Radial profiles are presented in Figure 3-86 for \(x/d = 0.5, 2.3, 15.0\) and 30.0 diameters downstream from the nozzle exit plane. Away from the centreline very good agreement is achieved between the experimental and k-e-CC computational results. Close to the nozzle the increase in Mach number around the lipline is not predicted, although this effect is probably due to the nozzle exit profile.

Figure 3-87 compares the results for NPR = 5.0, representing a highly underexpanded jet. The agreement in this case is not as good as for the moderately underexpanded cases, apart from in the downstream region. The predicted normal shock has a significantly higher peak Mach number at the leading edge and a higher Mach number in the subsonic region than measured. Comparing to normal shock theory, for the computed upstream Mach number of
2.85, the downstream Mach number should be 0.485; for the experimentally measured upstream Mach number of 2.35, the downstream Mach number should be 0.530. The computed downstream Mach number is 0.47 compared to the experimental value of 0.15, indicating some error in the experimental measurements. Some deviation from normal shock theory can be expected due to the action of viscous forces and multi-dimensional effects, however these should tend to increase the Mach number in the subsonic flow region. The lower measured peak Mach number on the leading edge of the normal shock is likely to be the results of the location of the pressure measurements not coinciding with the exact location of the normal shock and also the inability of the pressure probes to measure the very high gradients present in a strong normal shock.

The mean recovered Mach number in the supersonic potential core is in good agreement as are the Mach numbers in the first and second oblique shock cells and the wavelength, but subsequent oblique shock cells are prematurely damped. The location of these shock cells are not well predicted even with the translation of the axial co-ordinate.

For NPR = 5.0 the ideally expanded Mach number is 1.71. Neither the experimental or computational results reach this Mach number in the supersonic potential core because flow through the Mach disk is not isentropic.

3.5.3 Donaldson and Snedeker [6], NPR = 2.69 and 6.76

Donaldson and Snedeker [6] present axial and radial velocity profiles for NPR = 2.69 and NPR = 6.76. The data was obtained using pressure probes. Figure 3-88 compares the axial velocity for NPR = 2.69. The experimental data has only limited data points in the shock containing potential core region, from which an accurate representation of the shock cell structure can not be obtained. In the downstream regions a reasonable agreement is obtained. Radial velocity profiles at $x/d = 1.96, 7.32$ and 11.7 are shown in Figure 3-89, which again show a reasonable agreement. The results shown here are not entirely conclusive as to whether the compressibility corrected model gives the best results. Generally, in the low velocity flow region the $k$-$\varepsilon$-$CC$ models is the most accurate, whilst the $k$-$\varepsilon$ model is more accurate in the higher velocity regions.

The centreline axial velocity for NPR = 6.76, representing a highly underexpanded jet, are shown in Figure 3-90 and Figure 3-91. Again the number of measurements in this region is limited, but it is possible to ascertain the shock cell structure. The peak velocity at the leading edge of the normal shock is in good agreement to the computational results, but the
computed subsonic velocity downstream of the normal shock is underpredicted. The recovered Mach number in the oblique shock cell containing region is in good agreement, but the rate of recovery has been shown in section 3.4.4 to be dependent on the mixing rate in the subsonic region, which requires accurate specification of the nozzle turbulence properties. In addition, the experimental results appear to show a second, but much weaker, normal shock, indicated by the flow becoming subsonic after the second shock structure. This is also the case with the $k$-$\epsilon$-CC computations, where the reduced mixing behind the normal shock leads to a longer subsonic region and a lower recovered Mach number for the second shock waves and subsequently a subsonic Mach number downstream of the second shock. However, although this suggests that a second normal shock is present, there is no evidence in the Mach number contours to suggest that this shock is a normal shock.

Radial profiles are also shown at three axial locations (Figure 3-92). The results for $x/d = 1.96$ are shown in Figure 3-92(a). This axial location is located behind the normal shock in the subsonic region, thus close to the centreline the velocity is subsonic, and as previously stated, underpredicted by the computations. The experimental results appear to show a sharper velocity gradient between the subsonic and supersonic regions, and suggests a failure of the $k$-$\epsilon$ model to model the correct mixing rates in this region. The $k$-$\epsilon$-CC results reduce the mixing here slightly, although this leads to a larger underprediction of the subsonic velocity in the core. However, the model does predict accurately the velocity in the supersonic region and also, in the case of the $k$-$\epsilon$-CC model, the outer shear layer. Radial profiles at $x/d = 7.32$ and 11.7 are both located in the supersonic core region and good agreement is found between the experimental and $k$-$\epsilon$-CC results.

### 3.5.4 Hu and McLaughlin [9], NPR = 3.18 and 9.15

The data of Hu and McLaughlin [9] was obtained using pressure probes for two very low Reynolds number jets ($Re = 8000$) of NPR = 3.18 and 9.15. These low Reynolds numbers were achieved by the use of a low pressure chamber and a small nozzle diameter. Attempts to model these conditions have caused severe numerical difficulties. However, Hu and McLaughlin [9] stated that the only significant effect of the low Reynolds number was a 10% decrease in the shock cell spacing and a shorter length over which there is a well defined shock cell structure. This was thought to be due to a thickening of the initial boundary layer at low Reynolds numbers. Computations have thus been performed using standard atmospheric conditions and therefore a much higher Reynolds number.
The experimental results presented display very different mixing properties to those of other experimental studies. The centreline Mach number for \( \text{NPR} = 3.18 \) is shown in Figure 3-93. Not only is the shock cell structure rapidly damped, but the potential core length is significantly shorter.

Figure 3-94 shows the centreline Mach number for \( \text{NPR} = 9.15 \). Here, much better agreement is obtained, although the potential core length is still overpredicted. However, the normal shock shows reasonable agreement and in both cases the supersonic region shows only very weak oblique shock cells. This type of behaviour has been supported by Ewan and Moodie [3] who observed that as the pressure ratio of highly underexpanded jets continues to rise the shock structure becomes more dominated by the normal shock and further shock cell structures become less apparent. Radial profiles at \( x/d = 4.06, 9.48 \) and 13.55 are shown in Figure 3-95, showing only qualitative agreement.

One particular consequence of the use of a very small diameter for the nozzle is the reduced resolution due to the sensing volume of the probe. Since the observed normalised shock structures are independent of diameter, for smaller diameters smaller probes are required to obtain the same resolution. The smearing of shock cells can be observed in the \( \text{NPR} = 9.15 \) case where the normal shock is smeared over around one diameter.

3.6 Downstream Mixing Predictions

Downstream velocity field data was obtained by Birch et al. [12] for pressure ratios between 2.5 and 75 and was presented in terms of a hyperbolic decay function:

\[
\frac{u}{c} = \frac{\lambda}{x/d - a}
\]

where \( c \) is sonic velocity at ambient pressure and jet total temperature, \( \lambda \) is the hyperbolic decay constant and \( a \) is the virtual origin displacement. The empirical values of the constants \( k \) and \( a \) were derived from data for locations at \( x/d > 175.0 \) and are shown in Table 3-2 for four pressure ratios.

Computations have been performed for the four cases in Table 3-2, employing a computational mesh with dimensions of 250×13 diameters and 400×105 nodes. With this mesh, computations took around 25 minutes per 1000 cycles on an SGI R10000 processor. Due to the extended domain size more computational cycles were required in order for the flow to converge close to the outlet, although employing suitable initial conditions could
reduce the number of cycles required. Generally around 10000 cycles were required taking 4.5 hours.

<table>
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<tr>
<th>NPR</th>
<th>( \lambda )</th>
<th>( \alpha )</th>
</tr>
</thead>
<tbody>
<tr>
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</tr>
<tr>
<td>9.05</td>
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<tr>
<td>30.99</td>
<td>24.21</td>
<td>44.38</td>
</tr>
</tbody>
</table>

Table 3-2. Hyperbolic Decay Function and Virtual Origin Displacement (Birch et al. [12])

The resulting velocity profiles are compared to those from the hyperbolic decay function (eq. 3-14) in Figures 3-96 to 3-99 for the four cases studied, with good agreement between the experimental and computational results.

Figure 3-96 shows the results for a moderately underexpanded jet of NPR = 2.96, with the near field shock cell containing region in Figure 3-100. For these cases the axial mesh resolution is reduced in the shock containing region in order to reduce the overall computational requirements when solving over large axial domains. This does not have a significant effect on the downstream mixing, as demonstrated in section 3.4.4, but only reduces the shock cell resolution. However, even with this reduced mesh, the shock cell structure is still well resolved.

The other three cases all represent highly underexpanded jets up to a NPR = 30. In each case the flow is dominated by the normal shock and only very weak oblique shock cell are observed. In the far field, the best results were obtained with the \( k-e-CC \) model, with the overall agreement reducing as the NPR increases. This may due to a lack of resolution of the normal shock, and thus an underprediction of the isentropic losses, because of the relatively low mesh resolution close to the normal shock.

### 3.7 Pseudo Source Calculations

The aim of the pseudo source approximation is to allow the computation of the far field properties of underexpanded jets without the need for resolving the shock cell structure. This could allow a numerical method with poor shock capturing ability to be employed or analytical techniques which are available for both subsonic and fully expanded supersonic jets. A number of the available nozzle approximation methods were discussed in section
1.2.2. The method developed here assumes an isentropic expansion of the jet to the ambient pressure and applies continuity to calculate the diameter of the pseudo nozzle. Unlike many of the other methods presented in the literature, this method ensures conservation of mass, momentum and energy. In addition, the pseudo nozzle is not displaced downstream, but is applied at the location of the real nozzle. This approximation results in supersonic, but fully expanded pseudo nozzle conditions.

For a given stagnation temperature and NPR, isentropic relations are used to calculate the true nozzle conditions, as is the case for underexpanded calculations:

\[ P_s = P_0 \left( \frac{2}{\gamma + 1} \right)^{\frac{\gamma}{\gamma - 1}} \]  
\[ T_s = T_0 \left( \frac{2}{\gamma + 1} \right) \]  
\[ (\rho u)_t = \frac{P_0 \gamma}{\sqrt{\gamma RT_s}} = P_0 \left( \frac{\gamma}{T_o R} \right)^{\frac{\gamma}{2}} \left( \frac{2}{\gamma + 1} \right)^{\frac{\gamma - 1}{\gamma - 2}} \]

The pseudo conditions are calculated by assuming a further isentropic expansion to ambient pressure. In this way mass, momentum and energy are all conserved and a supersonic fully expanded jet occurs.

\[ P_{ps} = P_{amb} \]  
\[ T_{ps} = T_o \left( \frac{P_{amb}}{P_o} \right)^{\frac{\gamma - 1}{\gamma}} \]  
\[ M_{ps} = \left[ \left( \frac{P_s}{P_{amb}} \right)^{\frac{\gamma - 1}{2}} - 1 \right] \left( \frac{2}{\gamma - 1} \right)^{\frac{\gamma}{2}} \]  
\[ (\rho u)_{ps} = \frac{P_{amb} \gamma M_{ps}}{\sqrt{\gamma RT_{ps}}} \]

Finally, the diameter of the pseudo nozzle \((d_{ps})\) is calculated by applying conservation of mass between the true nozzle and pseudo nozzle conditions:

\[ \frac{d_{ps}}{d_e} = \sqrt{\frac{A_{ps}}{A_e}} = \sqrt{(\frac{(\rho u)_t}{(\rho u)_{ps}})} \]
Nozzle turbulence was specified as for underexpanded calculations, using the exit velocity of the pseudo nozzle and the pseudo diameter. Computations were performed employing the pseudo nozzle diameter and the subsequent results were then normalised by the true nozzle diameter. Table 3-3 shows the calculated pseudo nozzle conditions for varying NPR with $T_o = 288K$.

### Table 3-3. Pseudo Nozzle Conditions

<table>
<thead>
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<th>$M_{ps}$</th>
<th>$d_{ps}/d_e$</th>
<th>$k$ (m$^2$s$^{-2}$)</th>
<th>$\varepsilon$ (m$^2$s$^{-3}$)</th>
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### 3.7.1 Moderately Underexpanded Jets

Results have been obtained using the pseudo nozzle approximation throughout the whole of the pressure ratio range over which underexpanded calculations were obtained. The results presented within this section employed the same meshes as used for the underexpanded calculations, although coarser meshes could have been employed since there is no shock cell structure to be resolved. The boundary conditions for all boundaries, apart from the jet, were the same as for the underexpanded calculations. For the jet boundary, the pressure was interpolated from the interior and eq. 3-19 and 3-20 were applied to specify the temperature, Mach number and hence velocity at the nozzle.

Figure 3-101 compares the centreline axial velocity solutions obtained with the pseudo model to those of the standard model and the experimental data of Chuech [16] for NPR = 2.27. The pseudo solution agrees very well with the mean underexpanded jet solution.
throughout the potential core region, but obviously does not predict the shock cell structure. The length of the potential cores are also in good agreement, although the pseudo model appears to predict a more gradual ending to the potential core regions. Good agreement is also found in the far field regions between the two $k$-$\varepsilon$ and also the $k$-$\varepsilon$-$CC$ solutions. Radial axial velocity profiles at $x/d = 5.0$, 10.0 and 20.0 are shown in Figure 3-102 with again very similar results for both the standard and pseudo models.

Turbulent kinetic energy results for the same case are shown in Figure 3-103 and Figure 3-104. For both the $k$-$\varepsilon$ and $k$-$\varepsilon$-$CC$ models the rapid increase of turbulent kinetic energy along the centreline occurs slightly earlier with the standard nozzle than with the pseudo nozzle, whilst both reach very similar peak values. The values in the potential core region are higher for the pseudo nozzles due to the higher velocity at the nozzle exit. In the downstream region the pseudo nozzles predict higher values than the equivalent standard models. The radial plots also show the increased turbulent kinetic energy near the centreline, but also show that on the outside of the jet the standard models predict a higher turbulent kinetic energy. Thus, the pseudo model predicts narrower shear layers than the standard model, although this does not have a very significant effect on the overall jet mixing rate, as shown by the velocity results. However, it may explain the more gradual ending of the potential core.

Mach number predictions are presented for NPR = 3.5, but only for the $k$-$\varepsilon$-$CC$ model. The centreline axial velocity is shown in Figure 3-105. The pseudo model predicts a higher velocity than the mean velocity from the standard model, but lower than the experimental data for Stickland et al. [7]. The potential core length and downstream solutions show very good agreement between both computational models and the experimental data.

The radial velocities, shown in Figure 3-106 for $x/d = 0.5$, 2.3, 15.0 and 30.0 respectively, also show a good agreement between the standard and pseudo nozzle solutions, at locations downstream of the shock containing region. The solutions at $x/d = 0.5$ and 2.3 are clearly effected by the fluctuating velocity due to the shock cell structure, which is not modelled with the pseudo model. However, the pseudo model also predicts a lower initial jet spreading rate. Even with a larger nozzle diameter, 1.075 true diameters for NPR = 3.5, by $x/d = 0.5$ the standard model predicts an increased jet width of around 0.5 diameters compared to the standard model. However, by $x/d = 30.0$ the pseudo and standard models are almost identical and also agree very well with the experimental data of Stickland et al. [7].
Chapter 3. Non-Reacting Results

The performance of the pseudo model in the far downstream region has been assessed by performing pseudo calculations on the moderately underexpanded case from the Birch et al. [12] data presented in section 3.6, with \( \text{NPR} = 2.96 \). Figures 3-107 to 3-109 show the axial velocity, turbulent kinetic energy and temperature respectively, compared to the standard model and, in the case of velocity, the experimental data. The results clearly show very good agreement away from the shock containing region.

3.7.2 Highly Underexpanded Jets

Highly underexpanded jets have also been successfully computed with the pseudo nozzle approximation. Figure 3-110 compares the compressibility corrected pseudo and standard models for \( \text{NPR} = 5.0 \). The velocity predicted in the potential core region is now significantly higher than the mean velocity of the shock cell structures predicted with the standard model. This is due to the total pressure loss across the normal shock and hence its non-isentropic behaviour. In the downstream region the agreement is very good between the two solutions and also the experimental data of Stickland et al [7]; the total pressure loss with the standard model results in only a very small decrease in the centreline axial velocity. The centreline turbulent kinetic energy is shown in Figure 3-111. The Mach disk, and its very large velocity gradients, leads to a significant turbulent kinetic energy production and a peak in \( k \); smaller peaks are also observed due to the oblique shock cells. Downstream of the normal shock, convection of \( k \) from its peak leads to an increase in \( k \) throughout the remainder of the potential core, but only to a level slightly higher than with the pseudo nozzle computations. Further downstream this behaviour in the potential core region appears to have little effect, with the pseudo model predicting slightly higher values of \( k \) downstream of 10 diameters.

The axial velocity for \( \text{NPR} = 6.76 \) is shown in Figure 3-112. The velocity predicted by the pseudo model in the potential core is again significantly higher than the mean centreline velocity for the underexpanded model. However, the radial plots in the shock containing region reveal that this is due to the structure of the Mach disk as well as the total pressure losses through the normal shock. Figure 3-113(a) shows the radial profile at \( x/d = 1.96 \), located in the subsonic region just behind the normal shock. Here, in the first 0.25 radial diameters the velocity is subsonic, representing the flow that has been compressed through the action of the normal shock. The slip line then separates the subsonic flow from the supersonic flow that has not passed through the Mach disk. Obviously, none of these
complex flow phenomena are represented by the pseudo model, which predicts a constant velocity across the jet width, and thus the centreline comparison is somewhat misleading. As shown in some of the moderately underexpanded jet cases, the standard model predicts a more rapid jet spread rate than the pseudo model; in fact the pseudo model has hardly expanded from its initial radius of $0.625d$. The more rapid expansion with the standard model is due to the curvature effects of the shock cell structure, which leads to the familiar barrel shaped appearance. Further downstream at $x/d = 7.32$ and 11.7 (Figure 3-113(b,c)) the flow in the first 0.5 radial diameters is affected by the oblique shock cell structure, but away from the centreline the agreement between the two solutions is good. Downstream of the potential core region, at $x/d = 39.2$ (Figure 3-113(d)), the solutions show reasonable agreement, however the pseudo model solution does show an increased velocity and larger diameter. This is because the standard model has lost total pressure due to the non-isentropic effects in the shock containing region, whilst the pseudo model assumes an isentropic expansion upstream of the nozzle.

The effect of the pseudo model on the downstream centreline axial velocity, turbulent kinetic energy and temperature for the NPR = 9.05, 19.07 and 30.99 are shown in Figures 3-114 to 3-122 respectively. As the pressure ratio increases the near nozzle velocities show more disagreement and over a larger region. However, reasonable agreement is still achieved for the velocities in the downstream region, although as the pressure ratio continues to increase this agreement is reduced, with the pseudo model predicting higher velocities than both the standard model and the experimental data of Birch et al. [12]. This occurs with both the $k-\varepsilon$ and $k-\varepsilon-CC$ models (Figure 3-120), although the effect is much more significant with the $k-\varepsilon-CC$ model. For NPR = 30.99 the pseudo model predicts far field velocities around 20% larger than the equivalent standard model. The turbulent kinetic energy shows less reaction to the normal shock in these results than for NPR = 5.0 (Figure 3-111). This is likely to be to the result of the lower mesh resolution used for these calculations with larger domain sizes, leading to lower velocity gradients through the normal shock. Downstream higher centreline values are predicted by the pseudo model, again this effect is more significant for the $k-\varepsilon-CC$ model. The temperature solutions show considerable differences in the shock containing region due to the fluctuating velocities. For the lower pressure ratios, by the end of the potential core region the two solutions have converged. However, for NPR = 30.99, the pseudo and standard calculation with the $k-\varepsilon-CC$ model do not converge until around 150 diameters. This again demonstrates the effect of non-isentropic behaviour which causes the
Chapter 3. Non-Reacting Results

standard model computations to dissipate more rapidly. These differences in temperature may have had a more significant effect on the solution had the full energy solution been employed for the underexpanded calculations.

The results presented above show that for moderately underexpanded jets the pseudo nozzle approximation can represent the behaviour of an underexpanded nozzle, downstream of the shock containing region, and even in the shock containing region the correct mean velocities are predicted. They also demonstrate that the shock cell structure has little effect on the overall properties of the jet. However, for highly underexpanded jets this is not the case. The non-isentropic effects in the shock containing region are not accounted for by the pseudo model and lead to an overprediction of the velocities in the downstream regions, particularly for very high pressure ratios. This downstream behaviour could be corrected by employing a coefficient of discharge in the pseudo nozzle specification. However the coefficient would have to be a function of the nozzle pressure ratio, such that it did not influence the solution for moderately underexpanded jets and its effect increased with increasing strength of the normal shock.

Calculating turbulence is one of the major problems with the pseudo nozzle approximation and it is essential to be able to do this accurately if the mixing and hence downstream properties of the jet are to be predicted correctly and particularly if combustion is to be modelled. Different nozzle diameters and velocities necessitate different absolute value of turbulent kinetic energy and dissipation. These in turn will affect the initial boundary layer thicknesses and spreading rates. Additionally the high velocity gradients, and particularly the Mach disk, lead to high turbulence production rates. Fortunately, it appears that the turbulence levels in the potential core region do not have a significant effect on the overall mixing; it is the levels in the shear layers that are dominant. A further issue to consider is the effect of differencing and numerical dissipation with the pseudo and standard models. Although identical schemes were always employed for equivalent calculations, both the local Mach number dependent pressure correction scheme and TVD convective differencing will result in different schemes locally, since the standard model contains shock cells and hence high velocity gradients, whilst the pseudo model is uniformly at high velocities in the potential core.
3.8 Comparison to Previous Computational Studies

In this section the results obtained in the current work are compared to computations of similar underexpanded jets from the literature. A review of the literature regarding the numerical computations of underexpanded jets was presented in section 1.2.3.

Euler solutions of underexpanded jets were presented by both Sinha et al. [31] and Metha et al. [32]. In both cases inaccurate predictions were obtained not only in the far field region but also the near field shock containing region. Obviously the Euler solutions will be unable to predict the mixing effect in these flows and the shock containing region would continue indefinitely if not for numerical diffusion. Both solutions show errors in the prediction of the location of normal shocks, which have been shown to be predicted accurately in this work (see Figure 3-12). This is more likely to be due to the numerical methods employed rather than the use of an inviscid model, since the flow behaviour in the shock containing regions is dominated by inviscid effects, whilst computational studies employing both inviscid and viscous models [41] have shown little variation in the shock cell location. The inviscid models are also unable to model some of the important flow features of highly underexpanded jets. In particular, the re-acceleration of the subsonic flow immediately downstream of the normal shock due to mixing with the supersonic flow that did not flow through the normal shock is not predicted by the Euler calculations of Metha et al. [32], whilst it is predicted with the Navier-Stokes approach in this work. It is clear that any numerical method to model both the shock containing and far field jet regions must employ the Navier-Stokes equations as its basis.

Chuech [16] employed the PNS code developed by Dash et al. [37] to model the two moderately underexpanded jets (NPR = 2.27 and 2.59) which were studied experimentally in the same work. The PNS method considerably overpredicted the shock cell structure of the two underexpanded sonic jets due to the viscous terms being neglected in the streamwise direction. However, the shock cell wavelength was predicted accurately as, curiously, was the rather odd behaviour observed immediately downstream of the nozzle exit. For NPR = 2.27 the computations appear to show the pressure initially rising from a value below the ambient pressure, whilst for NPR = 2.59 the pressure did initially drop, but from a value considerably below the expected 1.37 bars. The location of the first shock cell was also in error compared to the measurements of Love et al. [1]. The PNS code also overpredicts the potential core region significantly even with the standard $k$-$e$ model, due to the inability of
Chapter 3. Non-Reacting Results

PNS models to represent the rapid mixing in sonic jets. However, downstream \((x/d > 15.0)\) the agreement with the experimental data is reasonable.

The lower pressure ratio case was also computed by Cumber et al. [45], who only presented results for velocity, for which the experimental measurements did not resolve the shock cell structures; no comparison were made to the pressure data. These results appear comparable to those in this thesis, however the shock cell structure is not clearly shown and a direct comparison is not possible. Without any corrections for compressibility the velocity decay was much more rapid than in Figure 3-76, leading to a considerably shorter potential core length. However, with the compressibility correction included similar potential core lengths were predicted. Further downstream the compressibility corrected results showed a similar accuracy to those of the \(k-e-CC\) model.

The overprediction of the potential core length by the PNS model of Chuech [16] was also shown in the fluctuating velocities which increased around five diameters downstream of the rise in the experimental results. However, the peak values were well predicted. The standard turbulence model of Cumber et al. [45] predicted a too rapid a rise in the fluctuating velocity, coinciding with the observed short potential core length, and also an overprediction of the peak value. With the compressibility corrected model the rise occurred around 3 diameters downstream of the experimental data and the peak value was underpredicted. As in the \(k-e-CC\) results, downstream good agreement was found with the experimental data.

A NPR = 3.88 sonic jet was also considered by Cumber et al. [45] and compared to the far field downstream velocity data of Birch et al. [12]. The presented results do not show clearly the resolution of the shock cell structure. In the far field a good agreement was found to the Birch et al. data [12], however the results showed a better agreement with the standard \(k-e\) than with the compressibility corrected model.

Highly underexpanded jets were considered by Cumber at al. [46]. Good agreement is shown for the Mach disk stand-off distance for lower pressure ratios, but this agreement reduces at very high pressure ratios. Little details are given as to the resolution of the shock cell structure, however Mach number contours are shown of the Mach disk structure for NPR = 6.76, showing the typical Mach disk features. For NPR = 6.76 radial profiles are shown at comparable locations to those in Figure 3-92(a-c), compared to the data of Donaldson and Snedeker [6]. Similar agreement is obtained to those in this thesis, although better agreement is found in this work close to the centreline. The computations of Cumber et al. [46] appear
insensitive to corrections for compressibility in the first four nozzle diameters, whilst close to the nozzle the results in this thesis indicate that the compressibility correction has an effect on the mixing at the interface between the subsonic and supersonic flows, immediately downstream of the Mach disk. In the far field region the Cumber et al. [46] computations underpredict the velocities even with a compressibility correction. This underprediction decreases with increasing pressure ratio.

For both moderately and highly underexpanded computations Cumber et al. [45, 46] stated that grid independent results were obtained with a grid spacing of 1/32 diameter; only a 2% change was found between results with this and 1/64 diameters spacing. No other details of the meshes employed for specific calculations were described. However, with a spacing of 1/32d, the 400 diameter domain employed for their downstream mixing data would require 12800 axial mesh points, and assuming a radial grid of at least 10 diameters, would require a mesh size of more than 4 million cells. It is unlikely that this size of mesh was employed, but without further detail of the mesh it is not possible to assess the accuracy. Additionally, no information is given regarding computational run times for the code.

Palacio et al. [41] used a pressure based method to calculate Donaldson and Snedeker's [6] NPR = 6.76 highly underexpanded jet using the Phoenics CFD code [42] and both inviscid and viscous models. The solutions were only obtained for the first four diameter in the axial direction and one diameter in the radial direction and employed a 100x30 cell mesh, with 80 axial cells in the first 3 diameters and 20 cells radially within the nozzle. Both the centreline Mach number and their contours are shown and display many of the typical features of a Mach disk, however, the Mach disk diameter appears much smaller than expected. The authors claim to have predicted two normal shocks, since the centreline Mach number becomes subsonic for the second time at x/d = 4. However, the Mach number contours show no evidence of a second Mach disk. Compared to the data of Donaldson and Snedeker [6] the predicted location of both Mach disks are displaced downstream. The viscous and inviscid models show very little difference upstream of the normal shock. In the subsonic region, behind the normal shock, the inviscid model predicts almost zero velocity compared to a Mach number of 0.75 for the viscous model. The subsonic region also extends further with the inviscid model. This is because without viscous effects the mixing between the supersonic and subsonic streams is much reduced. Calculations in this thesis predicted accurately the location of the first two shock cells for this underexpanded jet. With the compressibility correction employed the Mach number becomes subsonic downstream of
both the first two shock waves and are therefore both normal shocks following the same criteria employed by Palacio et al. [41].

3.9 Closure

The results presented in this chapter demonstrate the ability of the pressure correction model developed in chapter 2 to predict accurately and efficiently both moderately and highly underexpanded jets in both the near field, shock containing region and the far field. Few previous studies have been reported in the literature for the prediction of underexpanded jets and especially highly underexpanded jets. Only one previous study predicted highly underexpanded jets using a pressure based methodology [41] and here only the near nozzle region was modelled using a first order upwind scheme and a very fine mesh to give reasonable shock capturing resolution.

Several numerical issues have been addressed, in particular the effect of the convective differencing scheme. It was shown in section 3.4.1 that developing schemes based on upwinding momentum did not give rise to the desired dissipation term, and in fact in supersonic regions lead to an anti-diffusion flux. This resulted in convective differencing schemes of higher orders of accuracy predicting lower shock cell resolutions than first order schemes, whilst requiring excessive dissipation to be added in the pressure correction equation to obtain stable solutions. Basing the upwinding on velocity gave rise to the correct dissipation terms and resulted in improved accuracy for higher order convective differencing schemes, such as TVD, and a significant reduction in the dissipation required from the pressure correction equation. In fact for NPR less than 3.5 solutions could be obtained applying central differencing in the mass error term of the pressure correction equation and with the stabilising dissipation required to capture the shock cell structure being applied only by the convective differencing scheme.

Several methods of introducing dissipation in the pressure correction term have been assessed. With the modified convective scheme and a new retarded pressure function, solutions were obtained up to NPR=5.0 and a maximum Mach number of around 3.0, compared to a maximum pressure ratio of 3.05 using previous retarded pressure schemes. However, the local Mach number dependent blended differencing scheme developed here was able to predict underexpanded jets up to NPR=30.0 with at least comparable accuracy to the retarded pressure scheme. However, the optimum blend factors required to obtain the
highest accuracy whilst maintaining stability were found to be dependent on the pressure ratio.

Following an assessment of numerical issues the model was validated against the available experimental data for underexpanded jets. Predictions of the distance to the end of the first shock cell in moderately underexpanded jets and the normal shock in highly underexpanded jets showed a very good agreement to experimental data. Prediction of flow properties in the shock containing region generally agreed well with the experimental data, although there was a too rapid a decay in the shock cell strength. Mach disks in highly underexpanded jets displayed the expected features and predictions of the Mach number drop across the normal shock was good. The compressibility correction was found to have no significant effect on the shock cell structure, although in highly underexpanded jet the compressibility correction effected the mixing rate immediately downstream of the normal shock and hence affected the recovered Mach number of the resulting oblique shock cell structure. Downstream of the shock containing region the agreement to the experimental data was good when employing the compressibility corrected turbulence model to reduce the mixing rate.

Compared to limited previous numerical studies of underexpanded jets the results presented here demonstrate at least comparable accuracy, and against many of the studies, especially those not employing turbulent, Navier-Stokes based models, significantly improved results. However, it is not possible to compare the computational resources required for the various models or the required mesh resolutions to obtain accurate results since this information is not generally published.

The pseudo nozzle approximation has been applied to both moderately and highly underexpanded jets with good agreement to predictions employing the standard model. However, as the strength of the normal shock increased with NPR, and hence the total pressure loss across it, the accuracy of the pseudo nozzle approximation decreased, requiring a loss function to improve the accuracy.

In the following chapter the implementation of models for the prediction of reacting underexpanded jets into the model described in chapter 2 and validated here will be described.
3.10 Figures

Figure 3-1. Schematic of Domain and Boundary Conditions

Figure 3-2. 300×105 Computational Mesh

Figure 3-3. Nozzle Region of 300×105 Mesh
Chapter 3. Non-Reacting Results

Figure 3-4. Mach Number Contours, NPR=2.69

Figure 3-5. Mach Number Contours, NPR=3.5
Chapter 3. Non-Reacting Results

Figure 3-6. Centreline Mach Number, NPR=2.69

Figure 3-7. Centreline Mach Number, NPR=3.5
Figure 3-8. Variation of the Focal Point for the First Intercepting Oblique Shocks with NPR for Moderately Underexpanded Jets. Experimental data from Love et al. [1]

Figure 3-9. Mach Number Contours, NPR=6.0
Chapter 3. Non-Reacting Results

Figure 3-10. Mach Number Contours, NPR=30.99

Figure 3-11. Centreline Mach Number, NPR=6.0
Chapter 3. Non-Reacting Results

Figure 3-12. Variation of the Distance to Normal Shock with NPR in Highly underexpanded jets. Experimental data from Love et al. [1]

Figure 3-13. Comparison of the Centreline Mach Number for Hybrid and TVD Convective Schemes
Chapter 3. Non-Reacting Results

Figure 3-14. Comparison of the Centreline Total Pressure for Hybrid and TVD Convective Schemes

Figure 3-15. Effect of Convective Differencing Scheme on the Centreline Mach Number, NPR=2.69
Chapter 3. Non-Reacting Results

Figure 3-16. Comparison of Centreline Mach Number for Hybrid, Upwind and TVD Convective Schemes with Full Upwind Differencing in the Pressure Correction Equation

Figure 3-17. Effect on the Centreline Mach Number of Applying the TVD Convective Scheme to Individual Transport Equations/NPR=3.5
Figure 3-18. Effect on the Centreline Mach Number of Applying the TVD Convective Scheme to Individual Transport Equations, NPR=3.5

Figure 3-19. Comparison of Centreline Mach Number for the QUICK and 50%CD Convective Differencing Schemes to the TVD and Upwind Scheme, NPR=3.5
Chapter 3. Non-Reacting Results

Figure 3-20. Comparison of Centreline Mach Number for the QUICK and 50%CD Convective Differencing Schemes to the TVD and Upwind Scheme, NPR=3.5

Figure 3-21. Comparison of the Centreline Mach Number for Convective Differencing Schemes for Highly Underexpanded Jets, NPR=6.0
Chapter 3. Non-Reacting Results

Figure 3-22. Comparison of Centreline Mach number for $600 \times 210$ and $300 \times 105$ Meshes, NPR=3.5

Figure 3-23. Effect of Axial and Radial Mesh Resolution on the Centreline Mach Number, NPR=3.5
Figure 3-24. Effect on the Centreline Axial Velocity of Applying the TVD Convective Scheme to Individual Transport Equations for a Subsonic Jet

Figure 3-25. Effect on the Centreline Axial Velocity of Applying the TVD Convective Scheme to Individual Transport Equations for a Subsonic Jet
Figure 3-26. Radial Profiles of Axial Velocity, Showing the Effect of Applying the TVD Convective Scheme to Individual Transport Equations for a Subsonic Jet; (a) \(x/d=1.0\), (b) \(x/d=5.0\), (c) \(x/d=10.0\)
Chapter 3. Non-Reacting Results

Figure 3-27. Effect on the Lipline Turbulent Viscosity of Applying the TVD Convective Scheme to Individual Transport Equations for a Subsonic Jet

Figure 3-28. Effect on the Lipline Turbulent Kinetic Energy of Applying the TVD Convective Scheme to Individual Transport Equations for a Subsonic Jet
Figure 3-29. Effect on the Centreline Turbulent Kinetic Energy of Applying the TVD Convective Scheme to Individual Transport Equations for a Subsonic Jet

Figure 3-30. Effect on the Centreline Turbulent Viscosity of Applying the TVD Convective Scheme to Individual Transport Equations for a Subsonic Jet
Figure 3-31. Radial Profiles of Turbulent Kinetic Energy, Showing the Effect of Applying the TVD Convective Scheme to Individual Transport Equations for a Subsonic Jet; (a) $x/d=1.0$, (b) $x/d=5.0$, (c) $x/d=10.0$
Figure 3-32. Centreline Axial Velocity and Density Profiles Through the Oblique Shock Cell Structure of a Moderately Underexpanded Jet

Figure 3-33. Centreline Axial Velocity and Density Profiles Through the Normal and Oblique Shock Cell Structure of a Highly Underexpanded Jet
Chapter 3. Non-Reacting Results

Figure 3-34. Centreline Axial Velocity and Momentum Profiles Through the Oblique Shock Cell Structure of a Moderately Underexpanded Jet

Figure 3-35. Centreline Axial Momentum and Density Profiles Through the Oblique Shock Cell Structure of a Moderately Underexpanded Jet
Figure 3-36. Centreline Axial Velocity and Momentum Profiles Through the Normal and Oblique Shock Cell Structure of a Highly Underexpanded Jet

Figure 3-37. Centreline Turbulent Viscosity for Nozzle Turbulence Specifications Based on 1% and 5% of the Exit Velocity, NPR=3.5
Chapter 3. Non-Reacting Results

Figure 3-38. Centreline Mach Number for Nozzle Turbulence Specifications Based on 1% and 5% of the Exit Velocity, NPR=3.5

Figure 3-39. Comparison of the Centreline Mach Number for Upwind and TVD Convective Scheme, NPR=3.5
Chapter 3. Non-Reacting Results

Figure 3-40. Comparison of the Centreline Mach Number for Upwind and TVD Convective Scheme, NPR=6.0

Figure 3-41. Effect on the Centreline Mach Number of Applying the TVD Convective Scheme to Individual Transport Equations, NPR=3.5
Chapter 3. Non-Reacting Results

Figure 3-42. Effect on the Centreline Mach Number of Applying the TVD Convective Scheme to Individual Transport Equations, NPR=3.5

Figure 3-43. Effect on the Turbulent Kinetic Energy of Applying the TVD Convective Scheme to Individual Transport Equations, NPR=3.5
Figure 3-44. Comparison of the Centreline Mach Number for Various TVD Limiters, NPR=3.5

Figure 3-45. Comparison of the Centreline Mach Number for Various TVD Limiters, NPR=3.5
Chapter 3. Non-Reacting Results

Figure 3-46. Comparison of the Centreline Mach Number for Various TVD Limiters, NPR=6.0

Figure 3-47. Comparison of the Centreline Mach Number for Various TVD Limiters, NPR=6.0
Figure 3-48. Comparison of the Centreline Mach Number for TVD and Upwind Convective Schemes the Retarded Pressure Scheme, NPR=2.69

Figure 3-49. Comparison of the Centreline Mach Number for TVD and Upwind Convective Schemes the Retarded Pressure Scheme, NPR=3.5
Chapter 3. Non-Reacting Results

Figure 3-50. Centreline Mach Numbers Applying the Retarded Pressure Function for NPR=3.5, 4.0 and 5.0

Figure 3-51. Centreline Mach Number with Upwind Differencing for the Pressure Correction Equation, NPR=3.5
Figure 3-52. Centreline Mach Number with 20% Central Differencing and 80% Upwind in the Pressure Correction Equation, NPR=3.5

Figure 3-53. Centreline Mach Number with 20% Central Differencing and 80% Upwind in the Pressure Correction Equation, NPR=3.5; Near Nozzle Region
Chapter 3. Non-Reacting Results

Figure 3-54. Effect on the Centreline Mach number of function $f_1, f_2=0.5$, NPR=3.5

Figure 3-55. Centreline Mach Number With Central Differencing Applied to the Mass Error Term in the Pressure Correction Equation, NPR=2.69
Figure 3-56. Centreline Mach Number With Central Differencing Applied to the Mass Error Term in the Pressure Correction Equation, NPR=3.5

Figure 3-57. Effect of the Blend Factors on the Centreline Mach Number, NPR=3.5
Figure 3-58. Effect on the Centreline Mach number of function $f_1; f_2=0.7$, NPR=6.0

Figure 3-59. Effect on the Centreline Mach number of function $f_1; f_2=0.7$, NPR=6.0; Near Nozzle Region
Chapter 3. Non-Reacting Results

Figure 3-60. Comparison of Centreline Mach Number for Upwind, Central and TVD Differencing Applied to the Differencing of Density in the Pressure Correction Equation, NPR=3.5

Figure 3-61. Comparison of Centreline Mach Number for Upwind, Central and TVD Differencing Applied to the Differencing of Density in the Pressure Correction Equation, NPR=3.5; Near Nozzle Region
Chapter 3. Non-Reacting Results

Figure 3-62. Mach Number Contours for NPR=3.5 with TVD Differencing Applied to the Pressure Correction Equation

Figure 3-63. Comparison of Blended and TVD Differencing for the Mass Error Term in the Pressure Correction Equation, NPR=6.76
Chapter 3. Non-Reacting Results

Figure 3-64. Mach Number Contours for NPR=6.76 with TVD Differencing Applied to the Pressure Correction Equation

Figure 3-65. Comparison of the Centreline Mach Number for the Blended, Upwind and Retarded Pressure Schemes, NPR=3.5
Chapter 3. Non-Reacting Results

Figure 3-66. Comparison of the Centreline Mach Numbers for the Blended, Upwind and Retarded Pressure Schemes, NPR=5.0

Figure 3-67. Comparison of the Centreline Total Pressure for the Blended, Upwind and Retarded Pressure Schemes, NPR=5.0
Chapter 3. Non-Reacting Results

Figure 3-68. Effect of Doubled Axial and Radial Mesh Resolution on the Centreline Mach Number, NPR=3.5

Figure 3-69. Effect of Doubled Axial and Radial Mesh Resolution on the Centreline Turbulent Kinetic Energy, NPR=3.5
Figure 3-70. Effect of Doubled Axial and Radial Mesh Resolution on Radial Mach Number Profiles, NPR=3.5. (a) \(x/d=0.5\), (b) \(x/d=2.3\), (c) \(x/d=15.0\), (d) \(x/d=30.0\)
Figure 3-71. Effect of Axial and Radial Mesh Resolution on the Centreline Mach Number, NPR=3.5

Figure 3-72. Effect of Doubled Axial and Radial Mesh Resolution on the Centreline Mach Number, NPR=5.0
Chapter 3. Non-Reacting Results

Figure 3-73. Effect of the Initial Fluctuating Velocity Component on the Centreline Mach Number, NPR=3.5

Figure 3-74. Effect of the Initial Fluctuating Velocity Component on the Centreline Turbulent Kinetic Energy, NPR=3.5
Chapter 3. Non-Reacting Results

Figure 3-75. Effect of the Initial Fluctuating Velocity Component on the Centreline Turbulent Viscosity, NPR=3.5

Figure 3-76. Centreline Axial Velocity for NPR=2.27, Compared to the Experimental Data of Chuech [16]
Chapter 3. Non-Reacting Results

(a)

(b)
Figure 3-77. Radial Axial Velocity Profiles for NPR=2.27, Compared to the Experimental Data of Chuech [16]. (a) $x/d=5.0$, (b) $x/d=10.0$, (c) $x/d=20.0$

Figure 3-78. Centreline Turbulent Kinetic Energy for NPR=2.27, Compared to the Experimental Data of Chuech [16]
Chapter 3. Non-Reacting Results

(a)

(b)
Figure 3-79. Radial Turbulent Kinetic Energy Profiles for NPR=2.27, Compared to the Experimental Data of Chuech [16]. (a) \(x/d=5.0\), (b) \(x/d=10.0\), (c) \(x/d=20.0\)

Figure 3-80. Centreline Static Pressure for NPR=2.27, Compared to the Experimental Data of Chuech [16]
Chapter 3. *Non-Reacting Results*

![Figure 3-81. Centreline Static Pressure for NPR=2.59, Compared to the Experimental Data of Chuech [16]](image1)

![Figure 3-82. Centreline Static Pressure for NPR=2.27, Compared to the Experimental Data of Chuech [16] with Translated x-coordinate](image2)
Chapter 3. Non-Reacting Results

Figure 3-83. Centreline Static Pressure for NPR=2.59, Compared to the Experimental Data of Chuech [16] with Translated x-coordinate

Figure 3-84. Centreline Mach Number for NPR=2.5, Compared to the Experimental Data of Stickland et al. [7]
Figure 3-85. Centreline Mach Number for NPR=3.5, Compared to the Experimental Data of Stickland et al. [7]
Chapter 3. Non-Reacting Results

(b) 

(c)
Figure 3-86. Radial Mach Number Profiles for NPR=3.5, Compared to the Experimental Data of Stickland et al. [7]. (a) x/d=0.5, (b) x/d=2.3, (c) x/d=15.0, (d) x/d=30.0

Figure 3-87. Centreline Mach Number for NPR=5.0, Compared to the Experimental Data of Stickland et al. [7]
Figure 3-88. Centreline Axial Velocity for NPR=2.69, Compared to the Experimental Data of Donaldson and Snedeker [6]
Figure 3-89. Radial Axial Velocity Profiles for NPR=2.69 Compared to the Experimental Data of Donaldson and Snedeker [6]. (a) \( \chi/d = 1.96 \), (b) \( \chi/d = 7.32 \), (c) \( \chi/d = 23.5 \)
Figure 3-90. Centreline Axial Velocity for NPR=6.76, Compared to the Experimental Data of Donaldson and Snedeker [6]

Figure 3-91. Centreline Axial Velocity for NPR=6.76, Compared to the Experimental Data of Donaldson and Snedeker [6]
Chapter 3. Non-Reacting Results

(a)

(b)
Chapter 3. Non-Reacting Results

Figure 3-92. Radial Axial Velocity Profiles for NPR=6.76 Compared to the Experimental Data of Donaldson and Snedeker [6]. (a) x/d=1.96, (b) x/d=7.32, (c) x/d=11.7

Figure 3-93. Centreline Mach Number for NPR=3.18, Compared to the Experimental Data of Hu and McLaughlin [9]

182
Chapter 3. Non-Reacting Results

Figure 3-94. Centreline Mach Number for NPR=9.15, Compared to the Experimental Data of Hu and McLaughlin [9]
Figure 3-95. Radial Mach Number Profiles for NPR=9.15, Compared to the Experimental Data of Hu and McLaughlin [9]. (a) $x/d=4.06$, (b) $x/d=9.48$, (c) $x/d=13.55$
Chapter 3. Non-Reacting Results

Figure 3-96. Downstream Centreline Axial Velocity for NPR=2.96, Compared to the Experimental Data of Birch et al. [12]

Figure 3-97. Downstream Centreline Axial Velocity for NPR=9.05, Compared to the Experimental Data of Birch et al. [12]
Chapter 3. Non-Reacting Results

Figure 3-98. Downstream Centreline Axial Velocity for NPR=19.07, Compared to the Experimental Data of Birch et al. [12]

Figure 3-99. Downstream Centreline Axial Velocity for NPR=30.99, Compared to the Experimental Data of Birch et al. [12]
Figure 3-100. Centreline Axial Velocity in the Near Nozzle Region for NPR=2.96

Figure 3-101. Comparison of the Centreline Axial Velocity for the Standard and Pseudo Models With and Without the Compressibility Correction to the Experimental Data of Chueh [16], NPR=2.27
Chapter 3. Non-Reacting Results

![Graph (a)](image1)

![Graph (b)](image2)
Chapter 3. *Non-Reacting Results*

Figure 3-102. Comparison of Radial Axial Velocity Profiles for the Standard and Pseudo Models With and Without the Compressibility Correction to the Experimental Data of Chuech [16], NPR=2.27. (a) $x/d=5.0$, (b) $x/d=10.0$, (c) $x/d=20.0$

Figure 3-103. Comparison of the Centreline Turbulent Kinetic Energy for the Standard and Pseudo Models With and Without the Compressibility Correction to the Experimental Data of Chuech [16], NPR=2.27
Chapter 3. Non-Reacting Results
Chapter 3. Non-Reacting Results

Figure 3-104. Comparison of Radial Turbulent Kinetic Energy Profiles for the Standard and Pseudo Models With and Without the Compressibility Correction to the Experimental Data of Chuech [16], NPR=2.27. (a) $x/d=5.0$, (b) $x/d=10.0$, (c) $x/d=20.0$

Figure 3-105. Comparison of the Centreline Mach Number for the Standard and Pseudo Models to the Experimental Data of Stickland et al. [7], NPR=3.5
Chapter 3. Non-Reacting Results

(a)

(b)
Figure 3-106. Comparison of Radial Mach Number Profiles for the Standard and Pseudo Models to the Experimental Data of Stickland et al. [7], NPR=3.5 (a) x/d=0.5, (b) x/d=2.3, (c) x/d=15.0, (d) x/d=30.0
Figure 3-107. Downstream Centreline Axial Velocity for NPR=2.96 with the Standard and Pseudo Models, Compared to the Experimental Data of Birch et al. [12]

Figure 3-108. Downstream Centreline Turbulent Kinetic Energy for NPR=2.96 with the Standard and Pseudo Models
Chapter 3. Non-Reacting Results

Figure 3-109. Downstream Centreline Temperature for NPR=2.96 with the Standard and Pseudo Models

Figure 3-110. Comparison of the Centreline Mach Number for the Standard and Pseudo Models to the Experimental Data of Stickland et al. [7], NPR=5.0
Chapter 3. Non-Reacting Results

Figure 3-111. Comparison of the Centreline Turbulent Kinetic Energy for the Standard and Pseudo Models NPR=5.0

Figure 3-112. Comparison of the Centreline Axial Velocity for the Standard and Pseudo Models to the Experimental Data of Donaldson and Snedeker [6], NPR=6.76
Chapter 3. Non-Reacting Results

(a) k-\varepsilon-CC
 pseudo k-\varepsilon-CC
 Experimental

(b) k-\varepsilon-CC
 pseudo k-\varepsilon-CC
 Experimental
Figure 3-113. Comparison of Radial Axial Velocity Profiles for the Standard and Pseudo Models to the Experimental Data of Donaldson and Snedeker [6], NPR=6.76.
(a) $x/d=1.96$, (b) $x/d=7.32$, (c) $x/d=11.7$, (d) $x/d=39.2$
Figure 3-114. Downstream Centreline Axial Velocity for NPR=9.05 with the Standard and Pseudo Models, Compared to the Experimental Data of Birch et al. [12]

Figure 3-115. Downstream Centreline Turbulent Kinetic Energy for NPR=9.05 with the Standard and Pseudo Models
Figure 3-116. Downstream Centreline Temperature for NPR=9.05 with the Standard and Pseudo Models

Figure 3-117. Downstream Centreline Axial Velocity for NPR=19.07 with the Standard and Pseudo Models, Compared to the Experimental Data of Birch et al. [12]
Figure 3-118. Downstream Centreline Turbulent Kinetic Energy for NPR=19.07 with the Standard and Pseudo Models

Figure 3-119. Downstream Centreline Temperature for NPR=19.07 with the Standard and Pseudo Models
Chapter 3. Non-Reacting Results

Figure 3-120. Downstream Centreline Axial Velocity for NPR=30.99 with the Standard and Pseudo Models, Compared to the Experimental Data of Birch et al. [12]

Figure 3-121. Downstream Centreline Turbulent Kinetic Energy for NPR=30.99 with the Standard and Pseudo Models
Chapter 3. Non-Reacting Results

Figure 3-122. Downstream Centreline Temperature for NPR=30.99 with the Standard and Pseudo Models
Chapter 4. Combustion Methodology

4.1 Introduction

Having developed a computational methodology capable of non-reacting underexpanded sonic jet calculations in chapter 2 and demonstrated its ability to predict accurately both moderately and highly underexpanded jets in chapter 3, this chapter describes the implementation of non-premixed combustion models to allow the computation of combustion in underexpanded sonic jets. Such combustion may result when any high pressure flammable gas is released through an aperture into the atmosphere.

A review of previous studies of combustion in high momentum and underexpanded jets was presented in section 1.3. A review of some of the many methods available in the literature for non-premixed combustion is presented in section 4.2, along with a description of some of the common concepts that are required to model combustion. Section 4.3 then describes issues relating to flame extinction mechanisms and the modelling of lift-off heights. Following this various issues regarding the implementation of combustion modelling into the current pressure correction methodology are described. The employed combustion and extinction models are then described in section 4.5.

4.2 Review of Methods for Non-Premixed Combustion

4.2.1 Chemical Closure - The Need for Combustion Models

There are two important issues to address in order to be able to effectively model combustion. The first relates to the complex chemistry that occurs in the burning of even the most simple fuels, the second is the influence of turbulence on reaction rates.

4.2.1.1 Reaction Mechanisms

It is now well established that, for example, the burning of methane in air:

\[ \text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} \]  

in reality comprises many reaction steps and intermediate species. For example Rogg et al. [180] employed a mechanism with more than 250 reaction steps and 39 species to compute the structure of laminar diffusion flames. Attempting to include all the reactions would introduce severe computational expense, since each reaction requires the calculation of a rate term and each species requires the solution of a transport equation. In addition, although the
detailed mechanism is known for simple fuels such as methane, this is certainly not the case for more complex fuels.

Reduced reaction mechanisms that retain good resemblance to the true chemistry is the subject of much recent work and can produce large savings in computational expense. For example, the reduced mechanism of Peters and Kee [181], uses four reactions and seven scalars:

\[
\begin{align*}
CH_4 + 2H + H_2O &\rightarrow CO + 4H_2 \\
CO + H_2O &\rightarrow CO_2 + H_2 \\
2H + M &\rightarrow H_2 + M \\
O_2 + 3H_2 &\rightarrow 2H + 2H_2O
\end{align*}
\]

4.2.1.2 Chemical Reaction Rates

A one step chemical reaction can be expressed by a stoichiometric equation of the form:

\[
\sum_{i=1}^{N} v_i M_i = \sum_{i=1}^{N} v'_i M_i
\]

where \(v_i\) are the stoichiometric coefficients of the reactants, \(v'_i\) the stoichiometric coefficients of the products, \(N\) the total number of species and \(M_i\) are the species. The reaction rate \((R)\) for the general reaction in eq. 4-3 is expressed as:

\[
R = k \prod_{i=1}^{N} [M_i]^{v_i} \]  

where \(k\) is the reaction rate constant, and \([M_i]\) is the concentration of species \(M_i\).

The reaction rate constant is independent of the species concentrations and is generally calculated using an Arrhenius term:

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

where \(BT^\alpha\) is the collision frequency, and \(E_a\) is the activation energy. The exponential term is the Boltzmann factor and defines the fraction of collisions that have an energy in excess of the activation energy.

Most chemical reactions can proceed in both the forward direction (i.e. reactants forming products with rate term \(k_f\)) and reverse direction (i.e. products reforming the reactants with rate term \(k_b\)) giving a general reversible reaction:
Chapter 4. Combustion Methodology

\[ \sum_{i=1}^{N} v_i M_i \xrightarrow{k_i} \sum_{i=1}^{N} v_i^* M_i \]  

4-6

and rate terms:

\[ R^+ = k_f \prod_{i=1}^{N} [M_{ri}]^{v_i} \]  

4-7

\[ R^- = k_b \prod_{i=1}^{N} [M_{pi}]^{v_i} \]  

4-8

where subscripts \( R \) and \( P \) represent the reactants and products respectively.

For the reaction in eq. 4-6 the overall reaction rate can be expressed as:

\[ \frac{d[M_i]}{dt} = (v_i^* - v_i)k_f \prod_{j=1}^{N} [M_j]^{v_j} + \left( v_i - v_i^* \right) k_b \prod_{j=1}^{N} [M_j]^{v_j} \]  

4-9

At equilibrium there is no net reaction rate and hence the forwards and reverse reaction rates are related through the equilibrium constant \( K_c \):

\[ \frac{k_f}{k_b} = \prod_{j=1}^{N} [M_{j,eq}]^{(v_j^* - v_j)} \equiv K_c \]  

4-10

and therefore eq. 4-9 can be expressed as:

\[ \frac{d[M_i]}{dt} = (v_i^* - v_i)k_f \prod_{j=1}^{N} [M_j]^{v_j} + \left( 1 - \frac{1}{K_c} \right) \prod_{j=1}^{N} [M_j]^{v_j - v_j^*} \]  

4-11

To solve a large system of reactions, eq. 4-11 can be reformulated by introducing partial pressures and mole fractions to obtain equations of the form [62]:

\[ \omega_k = W_i \sum_{i=1}^{NR} (v_{ki}^* - v_{ki}) B_i T^{v_i} \exp \left( \frac{-E_{ai}}{R T} \right) \prod_{j=1}^{N} \left( \frac{X_j P}{R T} \right)^{v_j} \]  

4-12

where \( NR \) is the total number of chemical reactions occurring, and \( X_k \) are the mole fractions which are related to the mass fractions \( Y_k \) by the identity:

\[ X_k = \frac{\sum_{i=1}^{N} Y_i / W_i}{\sum_{j=1}^{N} Y_j / W_j} \]  

4-13

where \( W_k \) is the molecular weight of species \( k \).

Solution of Arrhenius type reaction rates leads to a set of ordinary differential equations, which for complex reaction systems can be very large. This system of ODE's can be solved numerically, however, the broad range of time scales for the chemical reactions can lead to a
stiff system of equations, increasing the computational complexities and expense. In addition, the reaction zone must be resolved adequately by the computational mesh in order to obtain accurate results, which can introduce the requirement for very large computational meshes.

4.2.1.3 Turbulence - Chemistry Interactions

In the preceding section, expressions have been presented for calculating instantaneous reaction rate terms which lead to a set of ODE's which can be solved numerically. In laminar flows these reaction rate terms can be applied directly in species transport equations with the form of eq. 2-4. However, in the case of turbulent flow turbulence - chemistry interactions must be accounted for.

The Favre-averaged equation for the transport of species $Y_k$ was given in eq. 2-31:

$$
\frac{\partial}{\partial t} (\bar{Y}_k) + \sum_j \left( \rho \bar{Y}_k \bar{u}_j \right) - \sum_j \left( \frac{\mu_i}{Sc} \frac{\partial}{\partial x_j} \bar{Y}_k - \rho \bar{Y}_k \bar{u}_j \right) = \bar{\omega}_k
$$

In order to close this equation the standard gradient transport assumptions are applied, requiring only the mean reaction rate to be evaluated. Even for single step reactions conventional Favre averaging of the reaction rate in eq. 4-12, using a series expansion to expand the exponential term, introduces an expanding series of turbulent correlations involving species and temperature fluctuations. Applying a first order truncation of these terms, and hence assuming the fluctuations are negligible and using only the respective mean quantities, gives a very poor representation of the reaction rate, with underprediction typically of an order of magnitude [e.g. 62].

Work has been presented using direct closure for chemical rate terms and usually second order closure of the rate term. This requires additional transport equations for the turbulent correlations and leads to a very complex approach [e.g. 182]. Pfd transport models have also been employed for turbulent non-premixed combustion [e.g. 183] whereby transport equations are solved for the multivariable pdfs such that the reaction rate can be closed directly. However, the solution of these multivariable pdfs requires the Monte-Carlo simulation technique [183].

Direct numerical simulations have also been applied to simple combustion systems with low Reynolds numbers [184]. Here all scales of turbulence are resolved and hence the instantaneous reaction rate terms of the form of eq. 4-12 can be applied directly. However,
the computational expense of such methods prohibits their application to anything approaching practical combustion systems. At the present time their main use is to obtain detailed, statistical information, which can not easily be obtained experimentally, for simple low Reynolds number idealised flows, which aids the development and calibration of both combustion and turbulence models for application to more practical problems.

Much of the work on turbulent combustion is focused on developing models for chemistry - turbulence interactions in order to remove the requirement for solving Arrhenius type reaction rate terms and some of the modelling approaches developed will be discussed in the following sections. These methods involve introducing assumptions in order to detach the chemistry from the turbulent flow field.

4.2.2 Conserved Scalar Approaches

The principle approach to overcome the problem of chemistry - turbulence interactions for non-premixed combustion in practical systems is the conserved scalar approach. Here an assumption is made that the chemical reaction rate is fast compared to the turbulent mixing time and that the combustion is complete as soon as the reactants are mixed. Bilger [149] stated that a turbulent flame can be approximated adequately with the fast chemistry assumption if the chemical reaction time is negligibly small compared to the mixing time. This assumption can be shown to lead to a considerable simplification of the chemical closure problem with the definition of a conserved scalar, since the instantaneous molecular-species concentrations and the temperature can be made to be solely a function of a correctly defined conserved scalar and therefore there is no need to determine the chemical reaction rate. With this approach all chemical reaction is assumed to occur at the stoichiometric contour which can then be viewed as a flamesheet.

A conserved scalar is one that contains no sources. The most commonly used conserved scalar in non-premixed combustion is the mixture fraction which is defined as the sum of the burned and unburned fuel mass fractions, although many others definitions can be employed. In these models unique relationships are derived between the conserved scalar and various other scalar quantities. Thus, with a knowledge of the mean and variance of the conserved scalar the mean and variance of other scalars can be calculated.

The conserved scalar approach leads to a large number of combustion models that vary in both complexity and accuracy, based on how the relationships between the mixture fraction
Chapter 4. Combustion Methodology

and scalars are obtained and also how the influence of turbulent fluctuations and strain are accounted for.

4.2.2.1 Fast chemistry

The most simple conserved scalar combustion model is the fast chemical reacting system (FCRS) and employs the Burke-Schumann fast chemistry limit. Here, the complete thermo-chemical state is derived from the mean mixture fraction using simple algebraic expressions. It is assumed that as soon as the reactants are mixed then combustion is complete. Thus, at all locations at least either all the fuel or all the oxidant are consumed. This method does not take account of turbulent fluctuations in the mixture fraction and relates the Favre averaged scalars to the Favre averaged mixture fraction:

\[ \tilde{\phi} = \phi(\tilde{\tau}) \]  

4-15

4.2.2.2 Presumed Pdf Model

In order to be able to calculate the mean value of scalar quantities in turbulent flows a knowledge of the pdf of the conserved scalar is required. The general approach is to use a presumed shape for this pdf such as a beta function [185] or clipped Gaussian [186], with the parameters obtained from the mean and variance of the conserved scalar. The particular form of the pdf employed has been considered in many studies, with similar conclusions. For example Chen et al. [187] examined the effect of the shape of the pdf on diffusion flames in boundary layers and found that the profiles of mean velocity, enthalpy, mixture fraction and its variance were not significantly affected.

In the presumed pdf model the relationships between the scalar quantities and mixture fraction are in terms of instantaneous values and the Favre averages are obtained by integrating these with the probability density function:

\[ \tilde{\phi} = \int \phi(f)P(f)df \]  

4-16

The form of the function \( \phi(f) \) can be obtained by various means, such as assuming single step reversible or irreversible reactions. The effect of the turbulent fluctuations is to increase the mass fractions of oxidant and fuel around stoichiometric and hence reduce the product mass fraction and temperature. As will be shown in section 4.5.2, these effects only occur when the relationships to the mixture fraction are non-linear.

209
4.2.2.3 Laminar Flamelet Models

The laminar flamelet model is a non-equilibrium extension of the Burke-Schumann limit and assumes that the flame can be represented by a series of laminar flamelets embedded in the turbulent field. Under conditions of one-step reactions with large Damköhler number the laminar flamelet model approaches this limit. Using the properties of laminar flames to represent turbulent flames requires that several condition are met so that the assumption that the instantaneous configuration of the turbulent flame is composed of thin laminar flamelets is valid. Bray and Peters [86] quantified this assumption based on time scales, stating that when the chemical time is less than the Kolmogorov time then combustion is in the flamelet regime. Peters [78] stated that the flamelet approach is valid if the reaction zone is thin in mixture fraction space.

The properties of these flamelets can be described as functions of the imposed turbulent strain rate and other properties such as enthalpy defect [86] to allow for heat loss and pressure gradient effects, and premixedness [180] or reactedness [87] to allow for partial premixing of the flamelets. In the same way as for the presumed pdf model the local, instantaneous scalar properties can be found from the flamelet properties and the mixture fraction. The properties of the laminar flamelets are generally stored in libraries so that their properties do not have to be calculated during the computational run time and can be obtained either by detailed laminar flame calculations [180] or from experimental measurements [188].

The imposed strain rate can be parameterised by various quantities, examples include the scalar dissipation ($\chi$) [78, 85, 189, 190], the strain rate based on the largest eddies ($\varepsilon/k$) [86] and the strain rate based on the smallest or Kolmogorov scale ($\varepsilon/2\nu^{1/4}$) [83]. The most popular is the scalar dissipation, but this must be conditioned a particular mixture fraction since its value is zero at the cold flow boundaries of flames.

To obtain the mean properties of the turbulent flame the laminar flamelet properties are integrated with the relevant pdf. For example using strain rate gives:

$$\bar{\phi} = \int_0^1 \int_0^1 \phi(f; s)P(f, s)dfds$$  \hspace{1cm} 4-17

where $s$ is the strain parameter and $P(f, s)$ the joint pdf of strain rate and mixture fraction.

In the absence of information regarding the joint pdf, it is usual to split it into two separate functions, assuming statistical independence, such that:
Chapter 4. Combustion Methodology

\[ \tilde{P}(f, s) = \tilde{P}(f)\tilde{P}(s) \]

Typically log normal distribution are used with scalar dissipation [85] and a Gaussian form for strain rates [191], whilst a Beta function is often used for the conserved scalar pdf.

Other work has ignored the fluctuations of the strain rate parameter and used flamelet profiles based on the local mean value [81, 86]:

\[ \overline{\phi} = \int_0^1 \phi(f; \bar{s})\tilde{P}(f)df \]

### 4.2.3 Coherent Flame Sheet Models

In a similar manner to the laminar flamelet model, the coherent flamesheet model [192-194] treats the flame front in a turbulent diffusion flame as a collection of thin, one-dimensional laminar diffusion flames embedded in a turbulent field. These laminar flames are considered to be stretched and wrinkled by the turbulent structures. However, this is not a conserved scalar approach and the reaction rate has to be calculated, as the product of the flame surface area per unit volume (\( \Sigma \)) and the reaction rate per unit surface area of the laminar flame. The reaction rate per unit surface area as a function of the local mixture fraction can be obtained by any suitable means, such as one-dimensional laminar flame computations [193]. \( \Sigma \) is obtained by treating the stretched flames as being in steady state and solving its transport equation, where flame growth by stretching balances the local heat and product generation. Growth of the flame sheets is limited by destruction due to the mutual annihilation of adjacent flame sheets and by destruction due to overstretching. When the strain rate based on the largest eddies exceeds a critical value the flamesheet is locally destructed and gives a mechanism for predicting flame extinction and lift-off. The model has been applied to high momentum reacting jets, including the effect of cross flow by Beeri et al. [84]. The results show good agreement with the experimental data.

### 4.2.4 Eddy Dissipation Concept

The eddy dissipation concept (EDC) [88, 195-198] has been applied extensively to many combustion applications, both premixed and non-premixed. The model assumes infinitely fast chemistry, although attempts have been made to include some finite rate effects [197] to allow soot and pollutant formation to be predicted. The eddy dissipation concept is related to the eddy break-up (EBU) model for premixed combustion of Spalding [199].
The model, applied to non-premixed combustion, assumes that initially the fuel and oxidant are separated and that bulk mixing occurs by the action of large eddies. It is further assumed that the chemical reaction rate is sufficiently large such that the reaction rate is completely determined by the rate of mixing of the large eddies of fuel and oxidant on a molecular scale. Thus, the reaction rate is dependent on the dissipation of large eddies. The mixing of the large eddies is obviously an intermittent process and the mixing will therefore be dependent on the fluctuating oxygen and fuel fields. However, Magnussen and Hjertager [195] proposed that there must be a relationship between the fluctuating and mean concentrations of each species and therefore the reaction rate was assumed to be proportional to the mean fuel mass fraction. In fuel rich regions it is the rate of dissipation oxidant eddies that is the rate limiting factor and hence the model takes the minimum of the dissipation of fuel and oxidant.

In the application to premixed combustion the fuel and oxidant are already mixed to a molecular level and hence eddies will contain both fuel and oxidant. In this case the rate limiting factor is the transfer of heat from the burned to unburned eddies to initiate reaction, which is also assumed to be due to the dissipation of large eddies. This process is assumed to be proportional to the mean concentration of products, which for low speed flows is proportional to the temperature. This is also applied to the non-premixed model and thus the reaction rate is proportional to the minimum concentrations of fuel, oxidant and products. The model can be extended to multi-step reactions by applying a separate rate term for each reaction. The model has been shown to have good accuracy for non-premixed, partially premixed and premixed flames [197, 198].

The EDC model has more recently undergone modifications to incorporate a number of important effects. Gran et al. [198] described an extension of the model to include the effects of non-premixedness and extinction due to high local strain rates [196]. The model was applied to combustor flows and compared to a stretched laminar flamelet model. The models were found to give similar levels of accuracy, and therefore the EDC model was preferred due to the considerable savings in computational expense that could be obtained, the reduced complexity of its formulation and the elimination of the need to calculate fluctuating scalar quantities.
4.2.5 Choice of Combustion Model

Many studies have been performed which compare various combustion models. However, it is essential to have a knowledge of the required results in order to select the most appropriate models. For the current application the main interest is the calculation of flame geometry and temperatures. Much of the requirement for complex models is the need to predict species concentrations accurately which is particularly important for many applications in terms of predicting pollutants; this is not a requirement in the current application. However, they may become important should soot or radiation modelling be required. Much evidence exist in the literature regarding the relative performance of various combustion models.

Fairweather et al. [81] employed a laminar flamelet model for the calculation of lifted turbulent hydrocarbon flames, employing flamelets with three strain rates. They found that employing different strain rates had little effect on the fluid dynamical aspects of the flow because density was not a strong function of strain rate. However, significant differences were found in the prediction of certain species, in particular carbon monoxide. Recognising that the mean temperature and density are not strong functions of the strain rate, many studies use only one reacting flamelet and hence neglect the influence of strain. For example Sanders and Lamers [83] employed only one reacting flamelet calculated at one strain rate for their predictions of lifted diffusion flames. The strain rate was only employed to determine whether burning would occur locally, and in non-reacting regions an isothermal flamelet was applied. Liew et al. [189] also used only two flamelets, one of which was the non-burning flamelet, the other was the undisturbed flamelet ($\chi = 0$).

Lau [200] compared a pdf transport methodology and the eddy dissipation model applied to a propane diffusion flame. The pdf transport equation was solved using the Monte Carlo method and a four step reduced chemical scheme was assumed. The EDC model also contained some dependence on the chemical kinetics in the reaction rate by employing empirical kinetic rate expressions and taking the minimum rate of this and the EDC rate for each of the four reaction steps. The results using the two methods are comparable for mean mixture fraction and unburned hydrocarbon concentrations. However, the carbon monoxide, carbon dioxide and nitrogen oxide mass fractions were predicted more accurately with the pdf model.

Bai and Fuchs [201] compared several combustion models for application to diffusion flames in gas turbine combustors. The EDC, fast chemistry with presumed pdf, and two
version of the laminar flamelet model were compared. They found that mean unburned fuel concentrations, temperature and velocity were insensitive to the choice of model and also the model parameters. However, detailed species concentrations such as carbon monoxide were much more sensitive. The presumed pdf model was found to be inadequate for flows with high turbulent intensity because it had no mechanism to account for local flame quenching effects due to strain. The EDC model gave good agreement to the experimental data for many cases, however, the model was more sensitive than the other models to the choice of model constants.

Gran and Magnussen [202] compared the EDC, presumed β-pdf and pdf transport models for the computation of bluff body stabilised diffusion flames. The EDC model was employed with both the fast chemistry assumption and also with complex chemistry included. The authors found that the choice of turbulence model was more important than the combustion model in determining accurately the flame properties. In the cases assuming fast chemistry the choice between EDC, β-pdf and pdf transport had a much smaller effect than the turbulence model. However, in the case of bluff body stabilised flames, the flame is anchored in the recirculation region behind the bluff body, which must be successfully modelled if the subsequent flame is to be modelled accurately and thus the sensitivity to the turbulence model is more significant than in the free jet case. Both the β-pdf and EDC models overpredicted the axial decay of the jet, with better results obtained with the transported pdf model. Radial profiles were comparable for the β-pdf and EDC models, although the EDC overpredicted the maximum temperature close to the stoichiometric contour more than with the β-pdf model. Janicka [203] developed a Reynolds-Stress model for predicting diffusion flames, arguing that the turbulence model was more important the combustion model.

Since there is no requirement in the current work to predict species concentrations, no account is made of chemical kinetic effects and one step chemistry is assumed, recognising that the overall heat release rate and flame shape are relatively insensitive to kinetic effects. It should also be noted that schemes involving complex chemistry, such as pdf transport models, are very computationally expensive and are generally only applied to simple flows and not to practical applications. In addition, the influence of high speed compressible flow is not clear within these models. Therefore the EDC models are employed along with the FRCS model and the presumed pdf model. The presumed pdf model employs the relationship for single step irreversible reactions and a laminar flamelet approach is not
pursued. This is because the effect of strain and chemical kinetics on the mean fluid dynamic properties is small.

4.3 Extinction Phenomena

The previous section discussed the various combustion models applied to turbulent diffusion flames. Whilst the effects of strain on the fluid dynamical properties of the flame may be small, its effects in terms of causing the flame to lift from the nozzle and blow-out are not. Thus, the important phenomena of finite chemistry that causes flame extinction cannot be neglected. Much work has been done in this area, but considerable work is still required to fully understand the complex interaction of chemistry and turbulence.

The classical theory of jet lift-off was first presented by Vanquickenborne and Van Tiglen [204] and assumes that the flow is premixed at the flame base. This allows stabilisation theories of premixed flames to be applied in this region and a turbulent burning velocity, based on the local turbulence structure, to be calculated. When the flow velocity is greater than the flame speed the flame travels back towards the nozzle and blow-out may occur due to a flashback type phenomena. When the flow velocity is less than the flame speed then the flame travels away from the nozzle and blow-off may again occur. Flame stabilisation occurs at the position where the time averaged velocity along the stoichiometric contour is equal to the burning velocity. When this occurs away from the nozzle the jet flame is said to be detached and lift-off has occurred. Following on from work applied to premixed combustion, the turbulent burning velocity can be calculated as a function of the laminar burning velocity and the local turbulent Reynolds number [e.g. 205].

Various experimental studies have been performed that support this theory for flame lift-off. Vanquickenborne and Van Tigelen [204] measured both reacting and non-reacting turbulent jets of methane for several diameters and velocities. The result indicated that the flame is initiated along the stoichiometric contour, where the local flame speed is a maximum. Kalghatgi [28] used the premixed theory of lift-off to correlate his experimental measurements. Eickhoff et al. [206] found that the local flow is 50% premixed at the base of the lifted flame.

The premixed model of flame stabilisation is not collaborated by the observations of Pitts [207]. The intermittent behaviour of the mixture fraction in isothermal jets was studied and large concentration gradients were found along the boundaries of the large scale structures. This indicated that these structures were ejected from the high mixture fraction jet core into
the ambient. Analysing the instantaneous mixture fraction data at the radial location of jet stabilisation showed that the flow was highly intermittent and for a large proportion of the time the flow was completely air.

This classical theory has more recently been challenged by several workers such as Peters and Williams [85]. They argued that a turbulent burning velocity could not be calculated because the local flow was not premixed to a molecular level. Instead, the extinction processes that occur in turbulent flames were assumed to determine the location of flame stabilisation. This was then incorporated into a laminar flamelet model as a means of modelling lifted flames. When the parameter characterising the local flame stretch (in this case the scalar dissipation) exceeded a particular value then the laminar flamelet was locally extinguished forming a hole in the flamesheet. Lift-off was assumed to occur when enough flamelets became extinguished to prevent a connected flamesheet forming back to the nozzle lip. Stabilisation occurred where the strain rate decreased sufficiently to allow a connected flamesheet to form. Since all reaction is assumed to occur at the stoichiometric contour of diffusion flamelets, the characterising strain rate is that at the location of the stoichiometric contour.

The effect of fluctuations in the scalar dissipation at the stoichiometric contour was included by employing the PDF of the scalar dissipation rate along the stoichiometric contour, \( P(\chi | f = f_n) \). The probability that the flamesheet was not occupied by holes, which can also be interpreted as the probability of burning (\( P_b \)), was then calculated as:

\[
P_b = \int_{\chi_q}^{\chi_i} P(\chi | f = f_n) d\chi
\]

The theory of continuum percolation in two-dimensions (pertaining to the analysis of electrical conductivity of sheets of conductors with random holes) was employed to determine the likelihood of a local flame being stabilised for a particular proportion of the flamesheet not containing holes and a critical value, \( P_c \), was found to be in the range of 0.6 to 0.7. In the absence of any experimental data, \( P(\chi | f = f_n) \) was computed assuming a log-normal form. Applying this, along with an assumption that \( P_c = 0.63 \) leads to the condition for flame stabilisation:

\[
\bar{\chi}_n = \chi_q
\]

where \( \chi_q \) is the quenching value of the scalar dissipation.
Thus, their statistical analysis concluded that for practical calculations of lift-off heights there was no need to include the effect of variation of the scalar dissipation and that the flame is stabilised at the location where the mean scalar dissipation on the stoichiometric contour equals a critical value.

Sander and Lamers [83] employed a similar analysis to that of Peters and Williams [86], but found that the strain rate of the smallest eddies provided better agreement to experimental data than the scalar dissipation as a measure of the likelihood of local flame extinction. A quasi Gaussian pdf was employed for strain rate leading to the following condition for the location of flame stabilisation:

\[ \tilde{s}_n = \frac{s_s}{P_c \pi^{1/2}} \]  

where \( P_c \) was also assumed to be 0.63. The fluctuation of the location of the flamebase was included into this model by introducing \( P_L \), the probability that a particular location is downstream of the flame stabilisation location. The form of this PDF was stated to be triangular, around the lift-off height, and with a five diameter width. Only one reacting flamelet was employed and the mean scalar was obtained from:

\[ \tilde{\phi} = P_L P_s \int_0^1 \phi_b(f)\tilde{P}(f)df + [(1-P_s)P_L + (1-P_c)] \int_0^1 \phi_u(f)\tilde{P}(f)df \]  

where \( \phi_b \) represents the burning flamelet and \( \phi_u \) the isothermal flamelet. The probability of burning was calculated using the local strain rate, and not that at the stoichiometric contour as employed when determining the lift-off height:

\[ P_b = \int_0^s P(s)ds \]  

Therefore, in this model a lift-off plane was defined as the location where the mean strain rate on the stoichiometric contour decreases below a critical value. Upstream of this point no reaction occurs. Downstream of the lift-off point the flame is assumed to still be experiencing local extinction based on the local strain rate, but insufficient to prevent a connected flamesheet forming.

Fairweather et al. [81] performed predictions of lifted turbulent reacting jets in a cross-flow with a flamelet model approach. Lift-off was assumed to occur at the location where a critical value of the large scale strain rate was exceeded by the centreline value.

Pitts [208] has assessed some of the theories for lift-off in diffusion flames. He stated that the laminar flamelet model cannot describe the features of flame stability because experimental
work has shown that some premixing of fuel and oxidant takes place prior to combustion, whereas the laminar flamelet models assume this not to be the case. Peters [209] and Bradley et al. [87] have developed models that take into account some degree of premixing. Peters [209] describes the application of partially premixed diffusion flamelets to non-premixed turbulent combustion. It was found that partial premixing made the laminar flamelets more susceptible to the effects of stretching and that for non-premixed reactants it is the flamelet quenching that appeared to be the dominant mechanism for flame stabilisation.

Bradley et al. [87] employed a mixedness-reactedness laminar flamelet model to predict the lift-off heights of methane flames in order to incorporate the effects of premixing in the flamebase upstream of the stabilisation plane. In this model the unstrained turbulent heat release rate is calculated as the product of the laminar heat release rate as a function of mixedness and reactedness and the joint pdf of mixedness and reactedness. This is similar to the approach used for premixed flames, in which case the mixedness is usually constant and the reactedness is often expressed in terms of a reaction progress variable. In this case the reactedness is calculated based on temperature. The effect of strain on the laminar heat release rate is not included in this model, with flame quench due to strain modelled by assuming that the distribution of strain rates is uncorrelated with other variables and takes a quasi-Gaussian form. The joint pdf of mixedness and reactedness is obtained as the product of the separated pdfs by assuming that the pdfs are uncorrelated. The laminar heat release rate is obtained from an algebraic approximation to computed heat release data.

With this model no threshold behaviour is included; the lift-off height is determined as the location of the onset of heat release. The model was applied to calculate lift-off heights in subsonic methane flames, compared to the experimental data of Kalghatgi [28] and a good agreement was obtained. The authors concluded that the lift-off height was a complex function of convection, turbulent mixing, heat release under strain and thermal expansion.

An extinction model based on large scale structures was presented by Broadwell et al. [210]. This model assumed that flame stabilisation occurs as the result of re-entrainment of hot gases which were previously expelled from the reacting region by large scale structures, which cause the ignition of non-reacting eddies in the jet. Miake-Lye and Hammer [211] also developed a model based on extinction in the large scale structures and found good agreement with the available experimental data. They also found that the observations of
fluctuations in the location of the flamebase was consistent with extinction in the large scale structures.

Kaplan et al. [212] performed computations of lifted jet diffusion flames and found that their results corroborated some aspects of both premixed and extinction lift-off theories. The flame was stabilised on an inner shear layer vortical structure, located on the stoichiometric surface at a height where local flow velocity was approximately equal to the local turbulent burning velocity. The flame base was found to move upwards with the vortical structure to which it was attached and then jump down to attach to a new lower vortex. This resulted in an oscillation of the flame base.

Various terms have been used to represent finite rate terms, examples include the scalar dissipation ($\chi$)[78, 85, 189, 190], the strain rate based on the largest eddies ($\varepsilon/\kappa$)[81, 86] and the strain rate based on the smallest or Kolmogorov scale ($\varepsilon/2\nu_\kappa$)[83]. The most popular is the scalar dissipation. Measurement of the scalar dissipation have been made in turbulent jets. Dibble et al. [70] presented the first measurements and found that the scalar dissipation was a crucial parameter in the calculation of non-equilibrium effects in turbulent non-premixed combustion.

Bray and Peters [86] employed the strain rate based on the largest turbulent structures ($\varepsilon/\kappa$) on the grounds that the scalar dissipation rate contains the influence of two terms; the turbulent time scale represented by $\varepsilon/\kappa$ and the influence of scalar fluctuations. However, the chemistry is not dependent on the mixture fraction variance unless these variations enter the reaction zone, and is only affected by the time scale. Basing the strain parameter on $\varepsilon/\kappa$ was found to give the experimentally observed dependence of lift-off heights on exit velocity and nozzle diameters, not obtained with the scalar dissipation at the stoichiometric contour.

Sanders and Lamers [83] argued that the strain rate based on the smallest eddies should be used, since the scalar dissipation gives poor agreement to the experimental data for lift-off heights. They present several argument to support the use of strain rates, including the inconsistencies involved when calculating the mean scalar dissipation. They also use experimental laminar flame data for the boundaries of quenching flames stating that using scalar dissipation predicts an increase in the critical value as the fuel mass fraction decreases, whilst experimental data suggests the opposite. Strain rates are also preferred since a specific location is not required. Since the scalar dissipation reduces to zero on the cold flow boundaries, the stoichiometric contour value is usually used. Strain rate can be taken from
any point in the flame. Finally Sanders and Lamers [83] stated that for constant flame thickness the mean scalar dissipation reduces to the strain rate of the largest eddies anyway. No arguments are put forward to support the use of the strain rate of the smallest eddies over that of the largest eddies, although the computational results appear to support the use of the small scale eddies.

A model for extinction is described with the EDC model [88, 198] employing the strain rate of the turbulent fine scale structures to characterise the strain field. A characteristic time is identified for the fine structures as:

\[ \tau^* = 0.41 \left( \frac{V}{\varepsilon} \right)^{1/3} \]

When \( \tau^* \) is less than the characteristic chemical time scale (\( \tau_{chem} \)) extinction is predicted and the reaction rate is set to zero. Due to the assumption of finite rate chemistry, calculating \( \tau_{chem} \) based on the local temperature is not possible. Therefore the authors used experimental data based on their setup to obtain \( \tau_{chem} \) with which to equate \( \tau^* \). Initially, this extinction method was applied to gas turbine combustors and the strain rate was not conditioned on a particular value of mixture fraction. In this way extinction can be modelled without specifying a threshold and flame stabilisation need not occur at the stoichiometric contour. Byggstoyl and Magnussen [88] employed the model based on the small scale structures to predict lift-off heights in diffusion flames and found an excellent agreement with the available experimental data. Calculations were performed for jet flows and the critical quenching time scale was derived by comparison with experimental data. By employing a quenching time scale the increase of lift-off height with increasing jet velocity was reproduced accurately. However, the quenching time was found to vary with nozzle diameter.

Conserved scalar models assume that the flamesheet is thin and that all reaction occurs at the stoichiometric contour. Thus, extinction is defined on the conditions at the stoichiometric contour, which leads to the definition of a threshold upstream of which no reaction can occur. Models such as the EDC models are not conserved scalar approaches and do not assume that all chemical reaction occurs at the stoichiometric contour such that the model is applicable to premixed, partially-premixed and non-premixed combustion regimes. Therefore, extinction conditions do not have to be based on those conditions at the stoichiometric contour. It will be further demonstrated in section 5.4.5 that employing
extinction based on local strain rates not conditioned on the stoichiometric contour can not be applied accurately within a conserved scalar approach without the inclusion of an additional parameter to define reactedness. The laminar flamelet model of Bradley et al. [87] does include additional parameters and does not define a threshold; lift-off was predicted on a local basis. However, Sanders and Lamers [83] state that this model is questionable because no threshold behaviour is included, which was stated to be a characteristic feature of a lifting flame. However, no evidence, experimental or otherwise, is presented to support this statement.

In this work several models for predicting lift-off behaviour will be applied to underexpanded jet diffusion flames and the specific details and implementation of each model described in section 4.5.4. Both local and threshold extinction models are tested and models based on both small and large scale turbulence are assessed, within the context of the EDC and conserved scalar combustion models.

4.4 Numerical Implementation

4.4.1 Conserved Scalar

A general one step chemical reaction can be written as:

\[
\{I \text{ kg Fuel}\} + \{r \text{ kg Oxidant}\} + \{\text{diluent}\} \rightarrow \{(I + r) \text{ kg Products}\} + \{\text{diluent}\}
\]

In the case of a methane and oxygen (or air) reaction then \( r = 4.0 \).

With this definition the following conserved scalars can be defined, often referred to as the Shvab-Zel’dovich coupling parameters:

\[
\beta_{FP} = Y_F + \frac{Y_F}{r+1}
\]

\[
\beta_{RO} = Y_F - \frac{Y_O}{r}
\]

\[
\beta_{OP} = Y_O + \frac{rY_F}{r+1}
\]

The following relations between the reaction rates of each species exist:

\[
\dot{\omega}_F = \frac{1}{r} \dot{\omega}_O = -\frac{1}{1+r} \dot{\omega}_P
\]
Throughout this thesis the conserved scalar employed is the mixture fraction, \( f \), that is the mass fraction of burned and unburned fuel, which is equivalent to \( \beta_{FP} \) in eq. 4-26. The transport equation for \( f \) is:

\[
\frac{\partial}{\partial t} \left( \bar{\rho} f \right) + \frac{\partial}{\partial x_j} \left( \bar{\rho} \bar{u}_j f \right) - \frac{\partial}{\partial x_j} \left( \mu_i \frac{\partial f}{\partial x_j} \bar{u}_j \right) = 0
\]

where:

\[
\bar{\rho} f \bar{u}_j = \frac{\mu_i}{\sigma_f} \frac{\partial f}{\partial x_j}
\]

For a reacting system with the fuel stream consisting entirely of fuel and the ambient stream containing both oxygen and diluent then:

\[
Y_D = Y_{D,A}(1 - f)
\]

\[
Y_O = Y_{O,A}(1 - f) - \frac{r}{r+1} Y_P
\]

where the subscript \( A \) refers to the ambient stream. \( Y_P \) is related to \( f \) by:

\[
Y_P = (f - Y_F)(r + 1)
\]

and therefore \( Y_O \) can be obtained from:

\[
Y_O = Y_{O,A}(1 - f) - (f - Y_F)r
\]

and it follows that the mixture fraction in terms of \( Y_O \) and \( Y_F \) is:

\[
f = \frac{rY_F - Y_O + Y_{O,A}}{r + Y_{O,A}}
\]

At the stoichiometric mixture fraction, neither fuel or air are present and therefore:

\[
f_n = \frac{Y_{O,A}}{r + Y_{O,A}}
\]

### 4.4.2 Energy Equation

The energy equation can be cast into many forms, but for the case of high speed flows an equation for total enthalpy (\( H \)) has been found to be the most convenient. Neglecting body forces this can be expressed as:

\[
\frac{\partial}{\partial t} \rho H + \frac{\partial}{\partial x_j} \rho \bar{u}_j H - \frac{\partial}{\partial t} P = \frac{\partial}{\partial x_j} \bar{u}_j \tau_y + \dot{Q} - \frac{\partial}{\partial x_j} q
\]
where

\[ H = h + \frac{\mu \nu_i}{2} \]  
4-39

\[ h = \sum_{i=1}^{N} h_i Y_i = e + \frac{P}{\rho} \]  
4-40

\[ h_i = \Delta h_{f,i}^0 + \int_{T_i}^{T_f} C_{p,i} dT \]  
4-41

\[ q_j = -\lambda \frac{\partial T}{\partial x_j} + \rho \sum_{i=1}^{N} h_i Y_i + R^0 T \sum_{i=1}^{N} \sum_{k=1}^{N} \left( \frac{X_i \alpha_i}{W_i D_{ij}} \right) (V_i - V_j) \]  
4-42

and \( V_i \) is the mass diffusion velocity of species \( i \) and \( D_{ij} \) is the binary diffusivity for species \( i \) and \( j \). Applying Fick’s law of diffusion allows the mass flux of species \( i \) to be calculated as:

\[ \rho_i V_i = -\rho D_{ij} \frac{\partial}{\partial x_j} Y_i \]  
4-43

Introducing the dimensionless quantities, Prandtl number and Schmidt number (\( \sigma \) and \( Sc \)):

\[ \sigma = \frac{C_p \mu}{\lambda} \]  
4-44

\[ Sc = \frac{\mu}{\rho D} \]  
4-45

and neglecting the Dufour effect, gives the following expression for the heat flux:

\[ q_j = -\frac{\mu}{\sigma} \frac{\partial H}{\partial x_j} - \frac{\mu}{\sigma} \left( \frac{1}{Sc} - \frac{1}{\sigma} \right) \sum_{i=1}^{N} h_i \frac{\partial}{\partial x_j} Y_i \]  
4-46

If the assumption is made of equal Prandtl and Schmidt numbers, that is the rate of energy transport is equal to the rate of mass transport and therefore the Lewis number is unity, then eq. 4-46 simplifies to:

\[ q_j = -\frac{\mu}{\sigma} \frac{\partial H}{\partial x_j} \]  
4-47

This assumption is not entirely desirable and may lead to considerable inaccuracies for some applications. However, its incorporation simplifies combustion models and allows the adoption of a single conserved scalar for non-premixed combustion.

The equation for total enthalpy has to be cast into Favre averaged quantities. Substituting eq. 2-11, eq. 2-15 and eq. 2-20 into eq. 2-3 gives:
\[
\frac{\partial}{\partial t} (\rho \tilde{H} + \rho H') + \frac{\partial}{\partial x_j} \left( \rho \tilde{H} \tilde{u}_j + \rho H' \tilde{u}_j + \rho \tilde{u}' \tilde{H} + \rho \tilde{u}' H' \right) = \frac{\partial}{\partial t} (\tilde{P} + P') + \frac{\partial}{\partial x_j} (u_j \tau_{ij} - q_j) + \dot{Q}
\]

4-48

Time averaging gives:
\[
\frac{\partial}{\partial t} \bar{H} + \frac{\partial}{\partial x_j} \bar{H} \bar{u}_j = \frac{\partial}{\partial t} \bar{P} + \frac{\partial}{\partial x_j} \bar{u}_j \tau_{ij} - \frac{\partial}{\partial x_j} q_j - \frac{\partial}{\partial x_j} \rho H' u_j' + \dot{Q}
\]

4-49

where:
\[
\bar{p} \bar{H} = \overline{\rho \left( \tilde{H} + \frac{1}{2} \tilde{u}_k \tilde{u}_k + \tilde{k} \right)}
\]

4-50

4.4.3 Conserved Scalar for Enthalpy

Assuming a unity Lewis number and neglecting the viscous terms reduces eq. 4-49 to:
\[
\frac{\partial}{\partial t} \bar{H} + \frac{\partial}{\partial x_j} \bar{H} \bar{u}_j - \frac{\partial}{\partial x_j} \left( \frac{\mu_l}{\sigma} \frac{\partial}{\partial x_j} \bar{H} - \bar{H} \mu_l \sigma \frac{\partial}{\partial x_j} u_j' \right) = 0
\]

4-51

This is equivalent to the conserved scalar equation for mixture fraction (eq. 4-30) if the turbulent transport coefficients are equivalent in each case:

Therefore, the conserved scalar treatment can be applied to the conservation of total enthalpy such that:
\[
f = \frac{H - H_A}{H_f - H_A}
\]

4-52

where \(H_A\) and \(H_f\) represent the total enthalpy of the ambient and fuel streams respectively. In order to employ this conserved scalar approach the total enthalpy of both the ambient and fuel streams must remain constant, both spatially and temporally. This is achieved here since the total temperature of both streams is constant, and although both the static temperatures and velocities may change the total enthalpy does not. Therefore:

\[
H_A = T_{0_A} \sum_{i=1}^{N} Y_{i,A} C_{p,i}
\]

4-53

The temperature is then derived in an identical manner to that with a transport equation for total enthalpy.
4.4.4 Thermo-Chemistry

Once the total enthalpy has been calculated, either by solving its transport equation or by employing the conserved scalar approach, the temperature and density have to be derived. For most applications it is sufficiently accurate to approximate the species enthalpy (eq. 4-40) by [213]:

\[
    h = C_p T + \sum_{i=1}^{N} Y_i \Delta H_i
    \tag{4-54}
\]

where:

\[
    C_p = \sum_{i=1}^{N} Y_i C_{p,i}
    \tag{4-55}
\]

and \( \Delta H_i \) is a constant selected to approximate the chemical heat release rate. In the case of a combustion system containing only two reactants and one product, eq. 4-54 can be further simplified, noting the since \( H \) does not appear as an undifferentiated term in the conservation equations, to give:

\[
    h = C_p T - \frac{Y_p}{r+1} \Delta H_{\text{comb}}
    \tag{4-56}
\]

where \( \Delta H_{\text{comb}} \) is the heat of combustion. Thus we have:

\[
    T = \frac{H + \frac{Y_p}{r+1} \Delta H_{\text{comb}} - \frac{1}{2} u_k u_k}{C_p}
    \tag{4-57}
\]

However, it was shown in section 2.7.3 that rearranging the equation state produces a more robust numerical scheme and therefore density is calculated as:

\[
    \rho = \frac{1}{H + \frac{Y_p}{r+1} \Delta H_{\text{comb}}} \left[ P \left( \frac{\gamma}{\gamma-1} \right) + \frac{1}{2} \rho u_k u_k \right]
    \tag{4-58}
\]

Temperature then follows from the equation of state:

\[
    T = \frac{PW_m}{R \rho}
    \tag{4-59}
\]

where:

\[
    W_m = \sum_{i=1}^{N} Y_i W_i
    \tag{4-60}
\]
4.4.5 Calculation of Thermodynamic Properties

In order to obtain closure of the system of equations, $C_p$ must be obtained as a function of both mixture composition and temperature. The mixture $C_p$ is obtained from:

$$ C_p(Y_i, T) = \sum_{i=1}^{N} Y_i C_{p,i}(T) $$

where $C_{p,i}$ are obtained as a function of temperature from Table 4-1 [214] and the molecular mass. During rapidly developing flow it is necessary to iterate the calculation of thermodynamic properties and temperature in order to aid convergence and prevent the generation of spuriously high temperatures.

<table>
<thead>
<tr>
<th>Gas</th>
<th>$C_{p0}$ (kJ kmol$^{-1}$ K)</th>
<th>Range (K)</th>
<th>Max. Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N$_2$</td>
<td>$39.060 - 512.799 T^{-1.5} + 1072.7 T^{-2} - 820.409 T^{-3}$</td>
<td>300-3500</td>
<td>0.43</td>
</tr>
<tr>
<td>O$_2$</td>
<td>$37.432 + 0.0201029 T^{1.5} - 178.570 T^{-1.5} + 236.880 T^{-2}$</td>
<td>300-3500</td>
<td>0.30</td>
</tr>
<tr>
<td>H$_2$O</td>
<td>$143.05 - 183.540 T^{0.25} + 82.7519 T^{0.5} - 3.69899$</td>
<td>300-3500</td>
<td>0.43</td>
</tr>
<tr>
<td>CO$_2$</td>
<td>$-3.7357 + 30.5290 T^{0.25} - 4.10340 + 0.0241980 T^{2}$</td>
<td>300-3500</td>
<td>0.19</td>
</tr>
<tr>
<td>CH$_4$</td>
<td>$-672.8 + 439.740 T^{0.25} - 24.8750 T^{0.75} + 323.880 T^{-0.5}$</td>
<td>300-2000</td>
<td>0.15</td>
</tr>
</tbody>
</table>

Table 4-1. Constant-Pressure Specific Heats

In order to maintain uniform total enthalpy across the inlets $C_p$ must not be a function of static temperature at inflow boundaries, since this would make $C_p$ and hence the total enthalpy a function of the varying inlet velocities. Noting that the static temperature at the inlets is always below the stagnation temperature (usually 288K), and below 300K the values in Table 4-1 are not accurate, $C_p$ is set to the value at 300K for $T \leq 300K$.

Finally, $\gamma$ for the mixture is obtained via:

$$ \gamma = \frac{C_p}{C_p - R_0/W_m} $$

4.4.6 Numerical Treatment of Energy and Scalar Transport Equations

The inclusion of a transport equation for energy (or similar) is known to be extremely problematic for compressible pressure based methodologies, and often an assumption of total enthalpy is assumed and a transport equation is not solved, thus neglecting viscous forces, as
was the case for the non-reacting flows in chapter 3. However, such an assumption is not valid if fluid streams of different total temperatures, as in heated jets, or combustion are to be modelled, unless assumptions of the type shown in section 4.4.3 are included. In these cases a full energy equation must be solved.

Energy equations are numerically unstable due to strong, non-linear linking to momentum, through velocity and density and to pressure via the mass equation. The energy equation will amplify any instabilities in the momentum or pressure solutions, transferring these to density. In turn, these will be amplified again by the momentum and mass equations. Hence, numerical instabilities can rapidly grow and lead to numerical failure. It is therefore important to construct a scheme for the energy equation that is as robust and stable as possible. It is for these reasons that energy conservation is expressed as an equation for constant total enthalpy. The choice of constant enthalpy for the energy equation is made since in the absence of heat sources, conduction and viscous effects the total enthalpy is a conserved quantity. It is not dependent on the local flow velocity or pressure. In this way a stable scheme can be constructed that will provide the required stability by breaking up the non-linear linkage between pressure, momentum and energy.

The first requirement for the enthalpy discretisation is that it must be able to conserve enthalpy:

\[ \frac{\partial}{\partial t} \rho H + \frac{\partial}{\partial x_j} \rho u_j H = 0 \tag{4-63} \]

To achieve this several issues must be addressed. The first is the use of density weighted or primitive variables. In the case of the momentum equations the density weighted variable is conserved. However, for both scalar transport and total enthalpy this is not the case. In incompressible flow it is not important, but for compressible flow it is essential that the primitive variables for scalars and enthalpy are used if stability is to be attained. If the density based variables are used for the constant total enthalpy, then this quantity is no longer conserved in the presence of a density gradient, such as a shock wave, and the transport equation must capture the shock because of the density change. In this way the loop of strong linkages is reformed. In addition, it was shown in section 3.4.1.2 that upwinding based on density weighted variables leads to anti-diffusive first order terms instead of dissipative terms. It is then possible to find over or undershoots around the shock wave leading to numerical instabilities. In addition, any lack of conservation or instability in the density solution would be included implicitly in the density weighted variable.
Chapter 4. Combustion Methodology

Using primitive variables requires evaluation of the face mass flux \((p_u)\). In order to avoid oscillations across discontinuities when solving the total enthalpy equation it is essential that the face mass flux is the converged solution for mass flux. Therefore, the mass flux formulation used for the convective terms of the enthalpy equation must be identical to that used in the mass error term of the pressure correction equation (eq. 2-130); no other mass flux can guarantee conservation and in the region of shock waves almost certainly will not. If the mass flux employed is not conserved, then neither will the enthalpy and this leads to numerical instabilities and in many cases failure of the numerical scheme.

The same requirements must also be applied to scalar equations. However, it is not as critical with this equation as with the enthalpy equation, since it does not have the same linkages to the mass and momentum equations. Failure to use the primitive variable \((Y_k)\) or the correct converged mass flux gives rise to spurious errors around shock waves and mixture fractions can be calculated outside the range \(0 < f < 1\).

4.5 Combustion Models

In the following sections the detailed implementation of each of the combustion models will be described.

4.5.1 Fast Chemical Reacting System

The mixed is burned model assumes that complete reaction has taken place wherever fuel and oxidant are mixing. Thus, at every location either all the fuel or all the oxygen are consumed. For \(f < f_s\) all the fuel is consumed and for \(f > f_s\) all the oxygen is consumed. For \(f = f_s\) all the fuel and oxygen are consumed. Figure 4-1 shows the mass fractions of various species for varying mixture fraction with the mixed is burned model.

No account of mixture fraction variations are included in the FCRS model and the assumption is made that the mean values of scalars are equivalent to the instantaneous values based on the mean mixture fraction.
Chapter 4. Combustion Methodology

1.0

Figure 4-1. Mass Fraction of Fuel, Oxidant, Diluent and Combustion Products for Varying Mixture Fractions for the Fast Chemical Reacting System

The relationship between the mean mixture fraction and each of the mean product species can be obtained by substituting either $Y_F = 0$ or $Y_O = 0$ into eq. 4-34 and eq. 4-35. The resultant relationships are shown in Table 4-2.

<table>
<thead>
<tr>
<th>$\bar{f} &lt; f_n$</th>
<th>$\bar{f} \geq f_n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\bar{Y}_F = 0$</td>
<td>$\bar{Y}_F = \bar{f} - f_n$</td>
</tr>
<tr>
<td>$\bar{Y}<em>O = \left[ f_n - \bar{f} \right] Y</em>{O,A}$</td>
<td>$\bar{Y}_O = 0$</td>
</tr>
<tr>
<td>$\bar{Y}<em>D = \bar{f} Y</em>{D,F} + (1 - \bar{f}) Y_{D,A}$</td>
<td>$\bar{Y}<em>D = \bar{f} Y</em>{D,F} + (1 - \bar{f}) Y_{D,A}$</td>
</tr>
<tr>
<td>$\bar{Y}_P = 1 - \bar{Y}_O - \bar{Y}_D$</td>
<td>$\bar{Y}_P = 1 - \bar{Y}_F - \bar{Y}_D$</td>
</tr>
</tbody>
</table>

Table 4-2. Relationships between Mixture Fraction and Mass Fractions of Fuel, Oxidant, Diluent and Combustion Products for the Mixed is Burned Model
Chapter 4. Combustion Methodology

The system is closed by employing eq. 4-52 to determine the total enthalpy and eq. 4-58 and eq. 4-59 to derive the temperature and density respectively, and again assuming that instantaneous values are equivalent to mean values.

The mixed is burned model is the simplest combustion model available and requires the addition of only one extra conservation equation to the non-reacting methodology and is therefore computationally inexpensive. However, many aspects of the physics and combustion chemistry are ignored and lead to major inaccuracies for many systems.

4.5.2 Presumed PDF Model

The presumed PDF model is an extension of the mixed is burned model to include the effects of variance of the mixture fraction when calculating the mean scalar quantities. Thus the Favre average of any scalar, \( \phi \), which is a function of mixture fraction is obtained from:

\[
\bar{\phi} = \int_{0}^{1} \phi(f) \bar{f}(f) df
\]

where \( \bar{f}(f) \) is the Favre averaged PDF of mixture fraction.

The PDF can be either prescribed or obtained via transport equations. However, in view of the high computational expense of transporting the PDF and recognising that the exact form of the PDF has little effect on the computed mean and variances [187], only a prescribed PDF will be employed here. The form chosen for this PDF is a two variable Beta function:

\[
\bar{f}(f) = \frac{f^{a-1}(1-f)^{b-1}}{\beta(a,b)}
\]

where the beta function, \( \beta(a,b) \), is defined as:

\[
\beta(a,b) = \int_{0}^{1} f^{a-1}(1-f)^{b-1} df
\]

and \( a \) and \( b \) are:

\[
a = \bar{f} \left( \bar{f} \left( 1 - \bar{f} \right) / \bar{f}^{*2} - 1 \right)
\]

\[
b = \left( 1 - \bar{f} \right) \left( \bar{f} \left( 1 - \bar{f} \right) / \bar{f}^{*2} - 1 \right)
\]

The mixture fraction variance is obtained from the following transport equation:

\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{f}^{*2}) + \frac{\partial}{\partial x_j} \left( \bar{\rho} u_j \bar{f}^{*2} \right) = -\frac{\partial}{\partial x_j} \left( \bar{\rho} u_j \bar{f}^2 \right) - 2 \bar{\rho} u_j \bar{f} \frac{\partial \bar{f}}{\partial x_j} - \bar{\rho} \bar{\chi}
\]

where the scalar dissipation is defined as:
and the mean scalar dissipation is modelled as:

\[ \bar{\chi} = c_x \frac{\bar{\varepsilon}}{k} \bar{f}^2 \]

where \( c_x \) is a model constant and is assumed to be 2.0. Employing the standard gradient diffusion approximations leads to:

\[ \overline{\rho u_j f^2} = -\overline{\rho \mu_s \frac{\partial f}{\partial x_j}} \]

and

\[ \overline{\rho u_j f^2 \bar{f}^2} = -\overline{\rho \mu_s \frac{\partial \bar{f}^2}{\partial x_j}} \]

Relizability theory imposes a limit on the mixture fraction variance such that:

\[ \bar{f}^2 \leq \bar{f}(1 - \bar{f}) \]

This also ensures that \( a \geq 0 \) and \( b \geq 0 \), which is a condition of the beta function. Other limits are imposed to ensure that the Favre averaged quantities tend to the instantaneous values as the mixture fraction variance tends to zero. In addition, when the mean mixture fraction approaches zero or one then no integration of the PDF is required since \( \overline{\phi} = \phi(f) \). This reduces the computational requirements in regions where mixing has not occurred.

The number of PDF integrations required can be reduced significantly by considering the various functions.

For example the Favre averaged total enthalpy is defined as:

\[ \bar{H} = \int_0^1 H(f) \bar{\rho}(f) df \]

and therefore:

\[ \bar{H} = \frac{\int_0^1 (f(H_f - H_A) + H_A)f^{a-1}(1-f)^{b-1} df}{\beta(a,b)} \]

which can be expanded to give:

\[ \bar{H} = \frac{1}{\beta(a,b)} \left[ \int_0^1 (H_f - H_A)f^{a}(1-f)^{b-1} df + \int_0^1 H_A f^{a-1}(1-f)^{b-1} df \right] \]

and therefore:
Chapter 4. Combustion Methodology

\[ \bar{H} = \frac{1}{\beta(a,b)} \left[ (H_f - H_A)\beta(a+1,b) + H_A\beta(a,b) \right] \] 4-78

By definition of the PDF, the Favre averaged mixture fraction can be expressed as:

\[ \bar{f} = \frac{\beta(a+1,b)}{\beta(a,b)} \] 4-79

which gives:

\[ \bar{H} = \bar{f}(H_f - H_A) + H_A \] 4-80

and hence no integration of the PDF is required.

This is the case for any linear function of \( f \):

\[ \bar{\phi} = \int_0^1 \phi(f)\bar{P}(f)\,df = \phi(\bar{f}) \] 4-81

Thus, conserved scalars such as enthalpy and diluent mass fraction do not need to be integrated with the PDF. In addition, for non-reacting flow regions the fuel and oxidant mass fractions can also be obtained without integrating the PDF, since they too are linear function of \( f \). Therefore, the only integrations that are required are for the fuel and oxidant mass fraction in reacting flow regions.

The mean fuel mass fraction is obtained from:

\[ \bar{Y}_f = \int_0^1 \max\left((f - f_u), 0\right) f^{a-1}(1-f)^{b-1} \,df \] 4-82

For \( f \leq f_u \), \( Y_f \) is zero and therefore the integral need only be performed from \( f_u < f \leq 1 \):

\[ \bar{Y}_f = \int_{f_u}^1 (f - f_u) f^{a-1}(1-f)^{b-1} \,df \] 4-83

Defining the incomplete beta function \( I_x \) as:

\[ I_x(a,b) = \int_0^x f^{a-1}(1-f)^{b-1} \,df \] 4-84

and recognising that:

\[ \int_0^1 (f - f_u) f^{a-1}(1-f)^{b-1} \,df = \int_0^1 (f - f_u) f^{a-1}(1-f)^{b-1} \,df - \int_0^{f_u} (f - f_u) f^{a-1}(1-f)^{b-1} \,df \] 4-85

gives:

\[ 232 \]
\[
\int_{f_{st}}^{f} (f - f_{st}) \frac{1}{f} (1 - f)^{n-1} df = \beta(a, b) \left[ \frac{\beta(a + 1, b)}{\beta(a, b)} \right]^{f_{st}} - \beta(a + 1, b) + f_{st} I_{f_{st}}(a, b) \] 4-86

Therefore the mean fuel mass fraction can be evaluated as:

\[
\overline{Y}_f = \frac{1}{(1 - f_{st})} \left( \frac{\beta(a + 1, b)}{\beta(a, b)} \right) - \frac{f_{st} I_{f_{st}}(a, b)}{(1 - f_{st}) (\beta(a + 1, b) + f_{st} I_{f_{st}}(a, b))} \] 4-87

Similarly, the Favre averaged oxidant mass fraction is obtained as:

\[
\overline{Y}_o = \frac{Y_{o,u}(f_{st} I_{f_{st}}(a, b) - I_{f_{st}}(a + 1, b))}{f_{st}} \] 4-88

With these simplifications only one beta function and two incomplete beta functions need to be evaluated for each node, where the mean mixture fraction is away from its bounds, the mixture fraction variance is non-zero and reaction is occurring.

Temperature and density must also be calculated with the effect of mixture fraction variance included via the presumed pdf. Temperature is obtained as a function of the mixture fraction and also velocity, noting that the total enthalpy may come from a transport equation or a conserved scalar relationship:

\[
T = \frac{H(f) - \frac{1}{2} \mu_k u_k + Y_p(f) \Delta H_{\text{comb}}}{Cp(f, T)} \] 4-89

Applying the pdf for the mixture fraction gives:

\[
\bar{T} = \int_{0}^{1} \left[ \frac{H(f) + Y_p(f) \Delta H_{\text{comb}} - \frac{1}{2} \mu_k u_k - \bar{k}}{Cp(f, T)} \right] \overline{p}(f) df \] 4-90

Temperature and specific heat capacity as a function of mixture fraction for stagnating flows such that \( u \) and \( k \) are zero, are shown in Figure 4-2 and Figure 4-3.
Figure 4-2. Temperature as a Function of Instantaneous Mixture Fraction for the Fast Chemical Reacting System

Figure 4-3. Specific Heat Capacity at Constant Pressure as a Function of Instantaneous Mixture Fraction for the Fast Chemical Reacting System
In this case both the temperature and mixture fraction are unique functions of mixture fraction. However, in the case of high speed flows this is not the case; both quantities are also a function of the local flow speed. In this situation eq. 4-90 would require numerical integration and iteration to evaluate. This is a computationally expensive option. Therefore, the specific heat capacity of the local fluid is evaluated based on the Favre averaged mass fractions which are already known, and using the latest guess of the Favre averaged temperature. Thus:

$$\overline{C}_p = \sum_{i=1}^{\nu} \overline{Y}_i C_{p,i}(\overline{T})$$  \hspace{1cm} 4-91$$

and

$$\overline{T} = \frac{1}{C_p(\overline{Y}, \overline{T})} \left[ \int_0^1 H(f) + \frac{\overline{Y}_p(f)}{r+1} \Delta H_{comb} \overline{P}(f) df - \frac{1}{2} \overline{u}_k \overline{u}_k - \overline{k} \right]$$  \hspace{1cm} 4-92$$

which can be further simplified to give:

$$\overline{T} = \frac{1}{C_p(\overline{Y}, \overline{T})} \left[ \overline{H} + \frac{\overline{Y}_p}{r+1} \Delta H_{comb} - \frac{1}{2} \overline{u}_k \overline{u}_k - \overline{k} \right]$$  \hspace{1cm} 4-93$$

Note that this is not equivalent to $\overline{T} = T(\overline{f})$ as is the case with the FCRS, since the effect of mixture fraction fluctuations are included because the mass fraction of products is evaluated by integration with the pdf and $C_p$ is calculated using the correctly Favre averaged mass fractions. In effect this assumes that the instantaneous specific heat capacity is based on the mean temperature and composition and that essentially it does not vary significantly over the range of mixture fractions where the pdf is non-zero known.

Density is obtained from the Favre averaged pdf and the instantaneous density as:

$$\frac{1}{\overline{\rho}} = \frac{1}{\rho} \overline{P}(f) df$$  \hspace{1cm} 4-94$$

which gives:

$$\frac{1}{\overline{\rho}} = \frac{1}{\rho} R^0 T(f) \overline{P}(f) df$$  \hspace{1cm} 4-95$$

Assuming that pressure fluctuations are thermo-chemically unimportant [215] and again assuming that thermo-chemical properties can be evaluated based on the mean species mass fractions gives:
4.5.2.1 Numerical Implementation

The beta functions need to be computed efficiently and this can be best achieved by replacing them with gamma functions [216]:

\[ \beta(a, b) = \frac{\Gamma(a) \Gamma(b)}{\Gamma(a + b)} \]

where:

\[ \Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt \]

and the gamma function is calculated using a standard approximation method [217]. Standard methods are also available for incomplete beta functions. In this case a continued fraction representation is employed [216].

4.5.3 EDC Model

For this model two additional scalar transport equations are required. Any combination of fuel, oxidant, product or diluent mass fractions could be chosen. In this case the fuel mass fraction and mixture fraction are chosen:

The remaining species are then obtained via eq. 4-32, eq. 4-34 and eq. 4-35.

The advantage of employing the conserved scalar mixture fraction is to allow the total enthalpy to be derived from this. Closure can be achieved by either assuming \( H \) to be a conserved scalar and employing eq. 4-52, or by solving a transport equation for \( H \). A comparison of solutions employing both methods is shown in section 5.3.

All that is now required is an expression for the reaction rate. In the basic form of the EDC model the reaction rate is found as the minimum of the normalised fuel, oxidant and product mass fractions, scaled by a rate term based on the time scale of the largest eddies:
The model constants are assigned values suggested by [195] as \( C_1 = 4.0 \), \( C_2 = 4.0 \) and \( C_3 = 1.0 \).

The extended form of the EDC model [198] is implemented in an almost identical manner to the basic EDC model. The only difference appears in the reaction rate and the extinction mechanism.

Here a more complex reaction rate term is employed such that:

\[
\tilde{\omega}_F = -C_o \kappa \frac{\tilde{\varepsilon}}{k} \min \left[ \left( \tilde{Y}_r - \frac{\tilde{Y}_o}{r} \right), \left( \frac{\tilde{Y}_o}{1+r} + \frac{\tilde{Y}_p}{1+r} \right) \right]
\]

where:

\[
\tilde{Y}_{\text{min}} = \min \left[ \tilde{Y}_r, \frac{\tilde{Y}_o}{r} \right]
\]

and \( \gamma \) is the mass fraction occupied by the turbulent fine structure region:

\[
\gamma = \frac{C_\gamma}{k^2} \left( \frac{\tilde{Y}_o}{r} \right)^\gamma
\]

\( \kappa \), the correlation parameter for non-premixedness, is defined as:

\[
\kappa = \frac{\left( \frac{\tilde{Y}_o}{1+r} + \frac{\tilde{Y}_p}{1+r} \right)}{\left( \frac{\tilde{Y}_r}{1+r} + \frac{\tilde{Y}_o}{1+r} + \frac{\tilde{Y}_p}{1+r} \right)}
\]

Values for the constants are given as [198] \( C_o = 11.1 \) and \( C_\gamma = 2.1 \).

With the EDC models an ignition procedure is required since initially \( Y_F = 0.0 \) throughout the whole of the domain. This is achieved by calculating the reaction rate only on the fuel and oxidant mass fractions during a short ignition period.

Throughout the rest of this thesis the EDC models employing the source term as specified by eq. 4-101 will be referred to as the EDC1 model, whilst that employing the reaction rate in eq. 4-102 will be the EDC2 model.
4.5.4 Extinction Mechanisms

In the current work several different lift-off theories are compared. The theory developed by Peters and Williams [86] is applied, such that a lift-off plane is determined based on the location where the strain rate on the stoichiometric contour is equal to some critical value. This plane can also be determined from the cold flow, prior to ignition. Previous work [83, 86] has shown that the strain rate should be used as the strain rate parameter and not the scalar dissipation rate and will therefore be used here. For the strain rate, both the small and large scale strain are compared. This application of the quenching conditions will be referred to as threshold quenching.

The lift-off theory of Byggstoyl and Magnussen [88] differs from that of Peters and Williams [85] only in the method of application of the critical strain rate. Here, if the local strain rate exceeds the critical value of strain then the local reaction rate is set to zero, and therefore no threshold is defined. In this case the lift-off height is determined from the location where significant heat release begins to occur. Both large and small scale rates of strains are employed and the results compared. This method can not be applied accurately within single conserved scalar approaches.

Implementation of threshold quenching involves locating the point where the critical strain rate and stoichiometric mixture fraction contours intersect. Then, at axial locations upstream of this point the flow is assumed to be non-reacting, whilst downstream the flow is assumed to be fully reacted. This plane could be defined based on the cold flow prior to ignition. However, as will be shown in chapter 5, more accurate results were obtained by allowing the stabilisation plane to move due to the effects of heat release on the flow. However, in order to improve stability and convergence it was found beneficial to fix the location of the lift-off plane during the initial period after ignition to prevent large oscillations occurring in the flamebase location. After this initial period the location of the flamebase was calculated in each computation cycle based on the reacting flow mixture fraction and strain rate fields.

Employing this kind of switch between the non-reacting and reacting regions leads to numerical difficulties, particularly for FCRS type models. Generally, the flow will have undergone an amount of mixing upstream of the lift-off location and the local mixture fraction will be such that the FCRS model will predict high temperatures. In fact, the definition of the lift-off height requires that at some point on the lift-off plane the stoichiometric contour is present. This means that at the lift-off plane the flow jumps from the unburned to the burned state and hence a very large temperature gradient occurs. To
overcome this problem a blending of the two states has been applied around the lift-off plane using a pdf approach similar to that of Sanders and Lamers [83]. The form of the pdf was taken to be triangular, centred around the mean lift-off height determined by any suitable method and with a width of five nozzle diameters.

Employing this type of method results in a linear combination of the reacting and non-reacting states in the region close to the lift-off plane:

\[ \phi = \alpha \phi_r + (1-\alpha) \phi_{nr} \]

Threshold quenching is implemented into the EDC models by setting the reaction rate to zero at axial locations upstream of the defined lift-off plane. The EDC models do not exhibit numerical instabilities at the lift-off threshold because the reaction rate terms predict a gradual increase in temperature at the location of flame stabilisation. This occurs because, in the case of the EDC model, the reaction rate is calculated as the minimum of normalised fuel, oxidant and product mass fractions. Near to the flame stabilisation point the rate limit term is that of the products which ensures an exponential increase in temperature.

Local quenching is implemented by assuming a critical rate of strain \( (q_s) \) on a local basis. Thus for EDC models, at each node no reaction occurs if the strain rate exceeds the critical value, otherwise the standard reaction rate term is employed:

\[ \bar{\omega} = 0 \quad \text{for} \quad \varepsilon/k > s_q \]

For the FCRS and pdf models the non-reacting conserved scalar relations (see section 4.4.1) were employed for nodes where the strain rate exceeded the critical value, whilst for values lower than critical the reacting relationships (Table 4-2) were employed. However, this again leads to a jump condition in temperature and density across the critical strain rate contour for the FCRS and pdf models and to prevent this, reaction was initiated in a linear manner over a small range of strain rates.

4.6 Closure

This chapter has discussed some of the issues involved with the implementation of a methodology for predicting underexpanded, jet diffusion flames into the non-reacting...
methodology described in chapter 2. The following chapter describes the results obtained using the various models presented here.
Chapter 5. Reacting Results

5.1 Introduction

This chapter presents the results obtained for underexpanded jet diffusion flames employing the methods developed in the previous chapters. Initially, the results for non-reacting underexpanded jet calculations including mixture fraction transport are presented and compared to the available experimental data. Following this, results employing a transport equation for total enthalpy are compared to calculations employing the constant total enthalpy assumption. Section 5.4 presents calculations for subsonic, lifted, diffusion flames in order to calibrate the critical strain rate for lift-off calculations and to demonstrate the modelling accuracy compared to experimental data and previous numerical predictions. Section 5.5 then presents the underexpanded jet diffusion flame calculations, comparing various models and assessing the accuracy in terms of the limited experimental data. Reacting calculations employing the pseudo nozzle approximation are presented in section 5.6, whilst section 5.7 discusses some of the results presented in this chapter.

5.2 Mixing Calculations

Computations have been performed for underexpanded releases of methane into quiescent air, as studied experimentally by Birch et al. [13]. This requires minor modifications to the inlet boundary conditions in order to correctly specify the thermodynamic properties at the nozzle. Computations have also been performed for the air-air experiments of Chuech [16], which employed a tracer to track the flow originating from the nozzle and measure the mixing properties of the release and is simulated by a passive scalar.

5.2.1 Effect of TVD scheme

The effect of applying TVD differencing to the convective terms in the mixture fraction transport equation are shown in Figure 5-1 for a methane-air underexpanded with NPR = 3.5. As expected the TVD scheme predicts a small increase in the potential core length and a reduction in the mixing rate due to the reduced numerical dissipation. However, the effect of this variation in the mixture fraction on the other flow properties is very small.
5.2.2 Comparison to Experimental Data

Two sources of experimental data regarding mixing rates of underexpanded jets have been found in the literature. Chuech [16] provided axial data and radial data for two axial locations for the underexpanded jet studied in section 3.5.1, with NPR = 2.27. The mixing data was for air-air jets and was obtained using LIF and an iodine seed. Comparison of predicted and experimental results with and without the compressibility correction are shown in Figure 5-2. Clearly, the mixing rate is underpredicted leading to an overprediction of the potential core length. Since mixing rates are already underpredicted with the standard k-ε, employing the compressibility correction leads to a further underprediction of the mixing rate. The corresponding axial velocity and turbulence profiles were shown in Figure 3-76 and Figure 3-78, which showed better agreement to the experimental data outside the shock containing region than is found for the mixture fraction and for the axial velocity the k-ε-CC model predictions were the most accurate. Radial profiles of mixture fraction, normalised by the centreline value are presented in Figure 5-3 at \( \frac{x}{d} = 10.0 \) and \( \frac{x}{d} = 20.0 \). These show that the mixing profiles are correctly predicted with the k-ε-CC model, even though the overall mixing rate is slightly underpredicted.

The maximum experimental error for the LIF measurements was found by the author to be 20% and was due to uncertainties with flow conditions and errors due to the detector operation. It is also possible that the iodine seed had an effect on the mixing rate of the jet. Computations of this case were performed by the Chuech [16] using a PNS code, with significantly larger differences predicted between the experimental and computational data than that shown in Figure 5-2. However, a subsonic and a sonic perfectly expanded jet were also predicted and measured using the same experimental procedures and a much better agreement was obtained. Calculations have been performed here for this sonic jet and the centreline mixture fraction profiles are shown in Figure 5-4. In this case a similar level of agreement is found between the experimental and computational data to that of Chuech [16].

The second source of experimental data for mixing in highly underexpanded jets is that of Birch et al. [13], who presented data for underexpanded jets of natural gas. As with their velocity data [12], the data was presented in the form of a hyperbolic function based on a pseudo diameter:

\[
 f = \frac{\lambda d_{en}}{x-a} \left( \frac{\rho_{enb}}{\rho_{gas}} \right)^{0.5}
\]

5-1
where $\rho_{amb}$ and $\rho_{gas}$ are the densities of the ambient and gas streams at STP and the pseudo diameter ($d_{ps}$) was calculated as:

$$\frac{d_{ps}}{d} = \left[ C_D \left( \frac{P_o}{P_{amb}} \frac{\gamma + 1}{\gamma + 1} \right)^{\frac{y+1}{2\gamma-2}} \right]^{0.5}$$  \hspace{1cm} 5-2$$

where $C_D$ is the discharge coefficient for the nozzle. This gives the following expression for the mixture fraction decay:

$$f = \frac{\lambda d}{x/d - a/d} \left( C_D \left( \frac{P_o}{P_{amb}} \frac{\rho_{amb}}{\rho_{gas}} \frac{2}{\gamma + 1} \right)^{\frac{y+1}{2\gamma-2}} \right)^{0.5}$$  \hspace{1cm} 5-3$$

Values for the constants $a$ and $\lambda$ for underexpanded jets were obtained from a series of experiments and were found for natural gas to be $-0.1$ and $4.9$ respectively and the discharge coefficient was taken to be $0.89$. Eq. 5-3 was stated to be valid over the range $29 \leq x/d_{ps} \leq 100$.

Centreline mixture fraction profiles are compared to data calculated using eq. 5-3 in Figures 5-5 to 5-7 for NPR = 5.415, 10.519 and 28.115 respectively. With the $k-\varepsilon$ model the mixing rate is always underpredicted for all pressure ratios. Prediction with the $k-\varepsilon$-$CC$ model show better agreement in the initial mixing region, downstream of the potential core. However, with increasing axial displacement this agreement decreases and the centreline mixture fraction is underpredicted in the far field. These results are the opposite to those presented for NPR = 2.27.

Velocity data was not measured for these test cases, however velocity data was obtained for similar air-air jets and comparisons of these to the computations were made in section 3.5, where a better agreement was made for the velocity than for those of mixture fraction shown here.

The results for mixture fraction presented here can be optimised by several factors. Firstly, since the mixing rate is principally dependent on turbulent mixing, this can be significantly effected by the turbulent Schmidt number, $\sigma_T$. This value was set to 0.7, as is typically found in the literature. However, increasing this to 0.9 leads to an increase in the potential core length and a decrease in the downstream mixing rate. Figure 5-8 compares the centreline mixture fraction with $\sigma_T$ set to 0.9 and 0.7 for NPR = 2.27. The reduced mixing decreases the
correlation between experimental and predicted values. However, reducing the mixing rate would have a beneficial effect on the results presented in Figures 5-5 to 5-7 compared to the experimental data of Birch et al. [13]. Modifying $\sigma_f$ has no effect on the velocity field in the case of air-air jets, and only a minor effect on natural gas-air jets, due to density differences. The mixing rate can also be affected by the nozzle turbulence parameters. As shown in section 3.4.5, increasing the effective turbulent viscosity in the nozzle increases overall jet mixing rates and hence that of the mixture fraction.

Cumber et al. [45, 46] found similar inaccuracies in comparison to the data of Birch et al. [13]. No comparisons were made to the mixture fraction data of Chuech [16], although velocity data was presented. A more elaborate compressibility correction was considered, which included pressure-dilatation terms as well as those for compressible dilatation, modelled in this work, in an attempt to improve the agreement for highly underexpanded jets [46]. However, this was found to deteriorate the agreement with experimental data compared to the compressibility corrected $k$-$\varepsilon$ model. It is well known that the $k$-$\varepsilon$ turbulence model tends to overpredict mixing rates in axisymmetric jets and several corrections have been suggested to improve this. One of these corrections, which modifies the model constants for the $k$-$\varepsilon$ model, was employed by Cumber et al. [46], but this was found to reduce significantly the agreement between computational and experimental results.

Since comparisons to the available experimental data is inconclusive as to the whether the computations over or underpredict the mixing rates, standard values have been employed for $\sigma_f$ and the initial turbulence parameters and no additional turbulence model corrections have been employed. Clearly, this is an area in which more work needs to be done, but this can only be achieved if better and more extensive experimental data is available. Whilst the data of Chuech [16] provides radial and axial, mean and fluctuating velocities and mixture fractions, there is some question over its accuracy, especially in shock containing regions and is limited in that it only provides this data for one pressure ratio (NPR = 2.27). The data of Birch et al. [12, 13] does provide data over a wider range of pressure ratios, however this data is limited since it only covers centreline velocities for air-air jets and centreline mixture fraction for natural gas-air jets. In addition, this data is only presented as hyperbolic decay functions which are only valid in the far field region.
5.2.3 Pseudo Source Calculations

Extension of the pseudo nozzle approximation (see section 3.7) to include mixture fraction transport requires no further modifications to the boundary conditions. Since mass is conserved in the nozzle between the true and pseudo conditions, then applying the true mixture fractions for the pseudo nozzle conserves the correct fuel and air flow rates into the computational domain.

Calculations employing the pseudo nozzle approximation for two cases, an air-air jet with NPR = 2.27 and a natural gas jet with NPR = 28.115, are shown in Figure 5-9 and Figure 5-10 respectively. For NPR = 2.27, with both the $k$-$\varepsilon$ and $k$-$\varepsilon$-CC models the pseudo model tends to smooth off the end of the potential core and have a more gradual mixing. Downstream of 10 diameters the agreement between the standard and pseudo models is very good. This behaviour was also observed for velocity (Figure 3-101). For NPR = 28.115, the overprediction of the centreline Mach number (Figure 5-11) due to the total pressure loss across the strong normal shock leads to an increase in the potential core length and a reduction in the mixing in the first 150 diameters. Downstream of 150 diameters the agreement is good.

5.3 Energy Calculations

5.3.1 Comparison to Constant Enthalpy Assumption Solution

All the computational results presented in chapter 3 employed the assumption of constant total enthalpy described in section 2.2.3. The implementation of a transport equation for total enthalpy was described in section 4.4.2. Comparison of the results using the two approaches are shown in Figure 5-12 and Figure 5-13 for an air-air jet with NPR = 3.5. The centreline Mach number shows a slight reduction in the shock capturing resolution. This is due to losses in the total enthalpy due to viscous effects. The centreline temperature also shows the reduction in the shock resolution, and an increased temperature in the far field regions.

5.3.2 Effect of TVD scheme

The application of TVD differencing to the total enthalpy equation has little effect on either the centreline Mach number or temperature. This is expected since there is little change in the total enthalpy over the solution. Figure 5-14 and Figure 5-15 show the effect of applying the TVD scheme to the energy equation on the centreline Mach number and temperature for NPR = 3.5.
Chapter 5. Reacting Results

5.4 Reacting Subsonic Jets

A small number of reacting subsonic jet calculations have been performed in order to validate and calibrate the lift-off height calculations. A relative coarse mesh has been employed since there is no shock structure to resolve. The obtained lift-off heights are compared to the experimental data of Kalghatgi [28] and previous computational studies.

The calculations presented here employ only the EDC2 model with local quenching based on the strain rate of the large scale structures (\(\varepsilon/\kappa\)). In addition, the lift-off heights obtained from the cold flow as the location of the intersection of the critical strain and stoichiometric contours are also presented.

5.4.1 Computational Setup

The domain size for the subsonic, lifted, diffusion flame calculations was 80x35 diameters employing a 80x50 cell mesh. The axial mesh had constant spacing, whilst the radial mesh was expanded to give the highest resolution on the nozzle lip line and six cells within the nozzle. The nozzle diameter was 8mm. The boundary conditions were the same as those applied for subsonic non-reacting computations (see section 3.4.1.1), with additional specifications for mixture fraction and fuel mass fractions. In all cases the nozzle was assumed to consist of entirely methane and therefore the mixture and fuel mass fractions were 1.0, whilst the ambient stream had mixture and fuel mass fractions of 0.0. The oxygen mass fraction in the ambient was 0.233 and the nitrogen mass fraction was 0.767. The thermodynamics properties were calculated based on the local static temperature and gas composition. As discussed in chapter 4, in order to apply the conserved scalar approximation to the total enthalpy the thermodynamic properties had to be calculated at a single static temperature for each reactant feed. This was achieved by assuming the static temperature to be 300K when calculating the thermodynamic properties.

Initially a converged non-reacting solution was obtained in order to allow the cold flow properties to be obtained, taking 5000 cycles with CFL = 5.0. Ignition was then initiated over a short period by calculating reaction rates assuming that the product mass fraction was not the rate limiting factor and converged solutions were obtained in around 4000 cycles with CFL = 2.0. With the reduced mesh the computational expense was small, taking around 150 seconds for 1000 cycles, and requiring around 25 minutes to obtain converged solutions on an SGI R10000 processor.
5.4.2 Results

Contours of temperature for subsonic methane jet computations with exit velocities ranging from 40-100ms\(^{-1}\) are shown in Figure 5-16. These calculations employ the EDC2 model with local quenching based on the strain rate of the largest turbulent eddies with a critical value of 100s\(^{-1}\). The value of the critical strain rate was calibrated by performing calculations for the 60ms\(^{-1}\) case with varying strain rates in order to match the experimental lift-off height to the data of Kalghatgi [28]. The predicted lift-off height was obtained as the location where appreciable reaction commences; this was taken as the location of the 600K temperature contour. Taking different temperature contours requires an adjustment to the critical strain rate to give equivalent agreement to the experimental data. The same critical strain rate was then applied to all other calculations, both subsonic and supersonic.

In each case the flame was predicted to be lifted from the nozzle rim between 15 and 32 diameters, with the lift-off height increasing with velocity. The flame stabilised in the shear layer at a radial location displaced from the axis, where mixing results in near stoichiometric mixture fractions and the strain rate is below the critical value. The displacement from the axis increased as the jet velocity increased.

Experimental studies of lift-heights as a function of jet exit velocity have been performed in several studies [28, 67, 218]. Figure 5-17 compares the predicted lift-off heights to the experimental data of Kalghatgi [28]. The predicted lift-off heights show very good agreement with the experimental data, within the experimentally measured variation. The experimental data was obtained for various nozzle exit diameters by analysing three photographs of the flame with an exposure of 1/30s and taking the lift-off height as the mean measured distance to the base of the visible flame. The results were found to be independent of the diameter.

Cold flow lift-off height predictions have also been obtained for the subsonic cases. Figure 5-18 shows the lift-off heights as function of jet velocity for the cold flow simulations with critical strain rates of 100s\(^{-1}\) and 140s\(^{-1}\) compared to the EDC2 predictions and the experimental data of Kalghatgi [28]. With a strain rate of 100s\(^{-1}\) the lift-off heights are overpredicted, whilst increasing the strain rate to 140s\(^{-1}\) provides a better agreement to the experimental data. For jet velocities of 20ms\(^{-1}\) and 40ms\(^{-1}\) the cold flow simulations with \(S_q = 140\text{s}^{-1}\) and the EDC2 model predict the same lift-off heights, however as the jet velocity is increased further the EDC2 models predicts larger lift-off heights due to the effect of heat release and expansion on the jet.
The effect of the critical strain rate on the cold flow lift-off heights for five jet velocities is shown in Figure 5-19. Increasing the critical strain rate leads to a significant decrease in the predicted lift-off height. However, the relationship between the lift-off and velocity is not affected by the critical strain rate. The predicted lift-off heights are also found to be a function of the initial specification of the turbulence parameter in the nozzle. The mixing properties of the jet are dependent on the turbulent viscosity in the nozzle, whilst the initial specification of strain rate also has an effect. With different specification of the nozzle turbulence parameters a good agreement to the experimental data could still be obtained if the critical strain rate was recalibrated.

Predictions of subsonic lift-off heights have been reported in several previous studies. Sanders and Lamers [83] presented lift-off heights for cold flow calculations with quenching based on either the small or large scale turbulent structures and a threshold basis. The critical strain rate was calibrated using the solution for a nozzle exit velocity of 71ms\(^{-1}\). For the large scale turbulent structures a value of 88.3s\(^{-1}\) was employed, whilst 4870.7s\(^{-1}\) was employed for the small scale turbulence. For these cold flow computations the small scale turbulence gave the best agreement to the experimental data. Results for reacting computations also specified a stabilisation threshold and were only presented with the small scale turbulence with a critical strain rate of 2092.6s\(^{-1}\). A similar agreement to the cold flow results of this work was obtained. Bradley et al. [87] employed a partially premixed flamelet model without specifying a threshold on which reaction was initiated, taking the lift-off height as the location where the onset of reaction occurs. Quenching was based on the small scale turbulence and a Gaussian pdf was assumed for the distribution of flame straining. The results for the lift-off height showed a good agreement to the data of Kalghatgi [28].

Contours of temperature are shown by both Bradley et al. [87] and Sanders and Lamers [83] for a single case. Sander and Lamers [83] predict a much more rapid temperature rise close to the axis than either the current work or that of Bradley et al. [87] and this results in a significant increase in the jet spread rate, whilst the predictions of Bradley et al. [87] indicate a slower increase in temperature along the centreline than the current work. However, no experimental data is available to determine which of the predictions are most accurate.

The grid independence of the lift-off height predictions has been assessed by performing calculations applying meshes of 160×50 and 120×75 to the subsonic diffusion flame with the same domain dimensions (80×35 diameters). Figure 5-20 compares the lift-off heights obtained from the cold flow with the different meshes as a function of the critical strain rate.
whilst Figure 5-21 compares the centreline temperatures. Clearly, the results obtained with the 80x50 mesh are not significantly different from the higher resolution meshes and can therefore be seen as mesh independent. The centreline temperature rise becomes slightly more rapid with increasing axial mesh resolution, however this does not effect the solution further downstream. The lift-off height observed for reacting flow using the EDC2 model are within 0.5 diameters for each of the meshes.

5.5 Reacting Underexpanded Jets

This section describes the results obtained for computations of underexpanded reacting jets. Initially the different modelling methods employed are compared and a sample of the obtained results presented. A comparisons to the limited experimental data is then presented.

5.5.1 Computational Setup

For the calculation of reacting underexpanded jets much larger computational domains are required than for the non-reacting and the reacting subsonic jet calculations. Experimental results indicate that lift-off heights can be in excess of 50 diameters [90], whilst flame length can exceed 250 diameters [29]. Thus, an extended domain is employed of 250x40 diameters for the reacting underexpanded jet calculations.

In order to satisfactorily compute the shock structure an order of resolution similar to that for the non-reacting calculations is employed close to the nozzle. Away from the nozzle region the mesh is expanded to reduce the computational requirements, resulting in a computational mesh of 400x130 cells. This gives a similar resolution in the far field to that employed for the subsonic calculations which was shown in section 5.4.2 to be sufficient for essentially mesh independent results.

The boundary conditions are identical to those employed for the non-reacting calculations (see section 3-2). Mixture fraction boundary conditions and issues arising with respect to the thermodynamic properties were previously described in regard to subsonic reacting jets (see section 5.4.1). The mixture fraction variance, required for the pdf model, is set to zero at all inlet boundaries.

Each of the computations were performed by initially obtaining a converged solution for the non-reacting flow using local time stepping with CFL = 3.0. Ignition was then initiated in a manner dependent on the particular model. For EDC models the reaction rate was assumed to be independent of the product mass fractions for a short period. For the FCRS model the
only required action was to switch from the relationship between the mixture fraction and scalar properties for non-reacting flow to those for reacting flow. In the case of the pdf model, the flame was initially developed using the FCRS model before applying the pdf, in order to reduce the required number of calculations of the computationally expensive pdf. Reacting parts of the calculations required that the CFL number be reduced to 0.5 in order to prevent numerical instabilities. The above procedures were found to be the most efficient in order to obtain converged solutions. However, igniting the flow prior to obtaining a converged non-reacting solution and using smaller CFL numbers also resulted in the same converged solution, independent of the steps taken to achieve it.

Runtimes for the reacting calculations increase significantly from those for non-reacting calculations. This is partly due to the increased computational time per node per time step and also the number of steps required for convergence. All the models require that mixture fraction is transported during the whole runtime, including the non-reacting jet development. In addition, during the reacting phase, the EDC models require a transport equation for fuel mass fraction, whilst the pdf model requires an equation for mixture fraction variance and also one beta function and two incomplete beta functions in the source term for each node at each timestep. Each computation required around 15000 cycles to obtain a converged non-reacting solution on the enlarged domain. A further 15000 cycles were then also required in order to compute the reacting flow. This results in total runtime of around 20 hours for each computation on an SGI R10000 processor. This represents an increase of around 20% per node per timestep over the non-reacting computations. Calculation employing the pdf combustion model required on average double the computational time per cycle per node as the EDC calculations, although this time was dependent on the number of iterations required to converge the beta and incomplete beta functions and also the number of nodes where conditions required that the pdf was solved.

5.5.2 Energy Equation

The majority of computations in this chapter calculate the total enthalpy by assuming it is a conserved scalar. To ensure that the assumptions employed in doing this are valid computations have also been employed with a transport equation for total enthalpy, details of which were given in section 4.4.2. Figure 5-22 compares the centreline temperature obtained with the conserved scalar approximation and the transport equation for total enthalpy for an NPR = 5.415 underexpanded jet flame. Downstream of 50 diameters the centreline temperature is insensitive to the method of calculating the total enthalpy. In the supersonic
region viscous dissipation effects, neglected with the conserved scalar approach, lead to some variation in solutions. Radial profiles of the temperature are shown in Figure 5-23. Again this shows that downstream of the supersonic region the temperature is dominated by the heat release due to combustion and that the viscous effects are negligible. Therefore, all subsequent computations in this chapter will assume that total enthalpy is a conserved scalar. This is equivalent to using the constant total enthalpy assumption for the non-reacting cases with the mixture fraction, and hence the total enthalpy, constant. Removing the need to solve a transport equation for energy has beneficial effects in reducing computational expense. In addition, the implementation of energy equations in compressible, pressure based methodologies has been known to cause numerical stability problems which can be avoided by a conserved scalar approach.

5.5.3 EDC Models

The various combustion models employed in this work have been compared for the solution of an underexpanded jet with NPR = 5.415 and a nozzle diameter of 50.6mm. This case was studied experimentally by Birch and Hargrave [90] who measured the lift-off height to be 1.709m (33.77 diameters). Temperature contours for the whole computational domain are shown for the different models in Figure 5-24, whilst Figure 5-25 shows the near lift-off region in more detail, including the stoichiometric and critical strain rate contours for four of the models. All temperature contours in this chapter employ the same colour contour range and this is shown in Figure 5-24.

Figure 5-24(a) shows the predicted temperature contours for this case applying the EDC2 model. Flame quenching was achieved by setting the reaction rate to zero on a local basis wherever the strain rate for the large scale structures (ε/k) exceeded a critical value, in this case 100s⁻¹. This value was obtained from the subsonic computations described in section 5.4.2. In the supersonic region, upstream of around 20 diameters, the flow is unaffected by the subsequent reaction. Here the strain rate exceeds the critical value in all regions where some degree of mixing of the fuel and air has occurred, as can be seen in Figure 5-25(a) which shows the temperature contours in the lift-off region with the stoichiometric and critical strain rate contours. From around 20 diameters a slight increase in the temperature occurs as some mixing is now occurring in regions with lower strain rate. However, the temperature rise is still small because the flow close to stoichiometric is still quenched. Downstream of around 30 diameters more rapid reaction occurs and the flame temperature increases significantly. By around 36 diameters the temperature has increased to 600K, and
at 40 diameters the strain rate at the stoichiometric contour drops below the critical strain rate. However, even though the mixture fraction is stoichiometric the temperature is still some way below the maximum flame temperature observed further downstream on the stoichiometric contour, because the mass fraction of the products and the fluid dynamics close to the stabilisation point combine to limit the reaction rate.

Temperature contours for the same case employing the EDC1 model are shown in Figure 5-24(b). The results appear to show no significant differences to those with the EDC2 model. The centreline temperatures are shown in Figure 5-26, with close agreement between the two models. However, radial profiles shown in Figure 5-27 indicate that the reaction rates with the two models differ close to the stabilisation plane. At $x/d = 25.0$, the EDC1 model predicts the highest temperature, whilst by $x/d = 50.0$ the EDC2 model predicts the highest temperature. The reaction rate terms for each of the models are shown along the centreline in Figure 5-28 and the radial profiles in Figure 5-29. Clearly, the predicted reaction rate varies considerably between the two EDC models. However, the far field temperatures, downstream of 100 diameters, are very similar indicating that the rate of heat release occurring upstream is not important here. This is because far enough downstream both models predict that either almost all the fuel or oxidant have been consumed locally. Therefore, assuming that the rate of heat release does not effect the entrainment processes significantly, the total fuel burned and hence the total heat released will be equivalent downstream and the overall jet expansion will be dependent on this total heat released and not its rate.

The centreline reaction rates shows that both models have an equivalent initial rise in the reaction rate once the strain rate has decreased below critical, however the EDC2 reaction rate continues to rise to more than double the EDC1 rate. The important factor here is the product of the reaction rate constant ($C_0$) and the premixedness correlation ($\kappa$) for the EDC2 model compared to reaction rate constant $C_1$ for the EDC1 model. In both the EDC2 and EDC1 models the rate limiting term in this region is the normalised mass fraction of product. Figure 5-30 and Figure 5-31 show the centreline and radial profiles respectively of the minimum normalised mass fraction of fuel and oxidant ($Y_{\text{min}} = \min[Y_F, Y_O/r]$) and the normalised mass fraction of products ($Y_p/(1+r)$). Axial and radial profiles of the small scale structure mass fraction are shown in Figure 5-32 and Figure 5-33(a) respectively, showing that in all areas where reaction is occurring, the value is approximately 0.1. Therefore, the additional term for the EDC2 model based on the mass fraction of the small scale structures
will not be the limiting factor. Axial and radial profiles of the non-premixedness correlation are shown in Figure 5-34 and Figure 5-33(b) respectively. Around the start of reaction, on the centreline, \( K \) is around 0.3 and therefore the product of \( K \) and \( \chi_{u} \) is approximately three times the value of \( C_{1} \) and this is shown in the reaction rate terms. However, the reaction rate for the EDC2 model decreases more rapidly as the small scale term becomes the rate limiting factor. When the minimum normalised mass fractions of fuel, oxidant and species are all present in sufficient quantities, the additional small scale EDC2 term is the rate limiting factor.

5.5.4 FCRS Model

Temperature contours for the NPR = 5.415 reacting underexpanded jet employing the FCRS are shown in Figure 5-24(c). The temperature gradients are much larger where combustion is initiated with the FCRS than the EDC model (see Figure 5-24(a)), since at any location where the strain rate is below critical either all the fuel, or all the oxidant will be consumed; there is no dependence on the temperature, through the product mass fraction or the turbulent time scale, as in the EDC models. As described in section 4.5.4, the reaction had to be initiated over a range of strain rates with the FCRS and pdf models to prevent a jump in conditions, and particularly density, over the critical strain rate contour leading to numerical instabilities. In this case a linear combination of the reacting and non-reacting states was applied when \( 100 < \epsilon/k < 150 \). Figure 5-25(c) shows the temperature contours along with the stoichiometric mixture fraction and strain rate contours, representing the region over which reaction is initiated. Even with the inclusion of this measure, the temperature rise close to the flame lift-off height is still larger than with the EDC models. By \( x/d = 25.0 \) the temperature has already exceeded 600K with the FCRS model, which does not occur until 37 diameters for the EDC2 model. The centreline temperatures for the two models are compared in Figure 5-35, showing the difference in the predicted temperature rise.

Figure 5-36 compares the radial profiles of temperature for the EDC and FCRS models. The more rapid increase in temperature in the shear layer where stabilisation occurs can be seen at \( x/d = 25.0 \). Here, the rate of increase of temperature for the FCRS model is controlled by the method of switching between the burned and unburned states and hence the strain rate, whilst the maximum temperature is purely a function of the local mixture fraction. The decrease in temperature on the outside of the flame is controlled by mixing processes reducing the mixture fraction such that the flame temperature reduces. With the EDC models the reaction rate in this region is governed by the product mass fraction.
The more rapid initial reaction rate leads to an abrupt increase in the flame width, which continues downstream. Even by $x/d = 200.0$ the flame width and maximum temperatures are still larger with the FCRS model. However, the shape of the temperature profiles become similar downstream.

### 5.5.5 PDF Model

The presumed pdf model introduces the effect of mixture fraction variance to the FCRS model such that the mean species mass fractions are evaluated as a function of the instantaneous mixture fraction and the probability density of the mixture fraction.

Figure 5-37 and Figure 5-38 show the relationship between the mean mixture fraction and the mean species mass fractions for $\bar{\phi^2} = 0.01$ and $\bar{\phi^2} = 0.001$ respectively. Compared to the instantaneous relations (see Figure 4-1), employed for the mean value in the FCRS, the inclusion of the pdf leads to an increase in the Favre averages mass fractions of fuel and oxidant around the stoichiometric contour. The instantaneous relations require either the mass fraction of air or fuel to be zero at all locations, and both to be zero at stoichiometric. With the pdf model both fuel and air are present at stoichiometric and over a wide range of mixture fractions. This means that, since the diluent mass fraction is independent of the pdf, the mass fraction of products and hence the temperature must decrease at the stoichiometric contour. In addition, the location of the peak temperature is shifted to the fuel rich side of the flame. As the mixture fraction variance increases then the influence of the pdf increases. Figure 5-39 shows the effect of increasing the mixture fraction variance on the product mass fraction. For very low mixture fraction variance the mean product mass fraction tends to the instantaneous value based on the mean mixture fraction. For high mixture fraction variance the peak product mass fraction is significantly reduced and occurs in fuel rich regions.

The temperature contours for a reacting underexpanded jet with NPR $= 5.415$ employing the pdf model are shown in Figure 5-24(d). Compared to the FCRS model (Figure 5-24(c)), the pdf model does not appear to alter the jet structure significantly. However, the temperatures are lower and therefore the expansion rate is reduced. The effect of the pdf model on the centreline temperature is not significant (see Figure 5-40), since the mixture fraction variance is relatively low here. However the radial profiles indicate that the pdf has a significant effect on the flame structure. Figure 5-41 compares the radial profiles for the EDC, FCRS and pdf models. The peak temperature observed at the stoichiometric mixture fraction and the high temperature gradients around this point with the FCRS model are
reduced with the pdf model, and the peak temperature moves nearer to the axis due to both the reduced expansion and the movement of peak heat release to the fuel rich side of the flame. Compared to the EDC models, the pdf model initially predicts higher temperatures and jet spread for the same reasons as the FCRS model. However, by $x/d = 150.0$ the pdf and EDC models predict similar temperature profiles and by $x/d = 200.0$ the pdf model predicts a lower spread rate compared to the EDC models and a maximum temperature closer to the jet centreline. In the far field the pdf model predicts the lowest temperature of any of the models, significantly lower than the FCRS model.

5.5.6 Extinction Models

Computations employing quenching based on the local large and small scale turbulence structures have been compared. Temperature contours employing the small scale turbulence are shown in Figure 5-24(e) with a critical time scale of $1.0 \times 10^{-5}$s. This value was obtained using the method employed by Gran et al. [198]. The results obtained are similar to those with the large scale structures (Figure 5-24(a)). The centreline temperatures are compared in Figure 5-42, where the temperature rise occurs earlier with the large scale structures. However, downstream of 100 diameters the results are very similar.

All the preceding calculations have employed quenching based on the local strain rate. However, most previous work on lift-off heights has treated lift-off as a threshold phenomena, whereby the strain parameter conditioned on a particular mixture fraction is employed to determine a stabilisation plane. Calculations have also been performed here applying threshold quenching.

Computations employing threshold quenching based on the large scale strain rate have been performed with the EDC, FCRS and PDF models and the temperature contours are shown in Figure 5-24(f-h) respectively. Applying quenching in this manner changes the flame structure close to the lift-off point. Quenching on a local basis effectively leads to a point source for the initiation of combustion, at a location close to the intersection of the stoichiometric and critical strain rate contours. However, using quenching on a threshold basis leads to a distributed line source centred on the intersection of the stoichiometric and critical strain rate contours and therefore there is a more rapid expansion of the flame immediately downstream of the stabilisation point. This can be clearly seen in Figure 5-25 which compares the near field temperature contours and stoichiometric and critical strain rate contours for the EDC and FCRS models with both local and threshold quenching. The
initial rate of temperature increase with threshold quenching is controlled by the flamebase fluctuation pdf rather than the specific combustion model. This prevents a discontinuity in density and temperature such that the temperature rise occurs over 5 nozzle diameters and results in similar temperature profiles for the EDC and FCRS models.

Figure 5-43 and Figure 5-44 compare the centreline temperature and mixture fraction for the two quenching methods with the FCRS model. The temperature remains at that of the unburned jet for a further 20 diameters downstream with the local scheme since the strain rate on the centreline is still too high for reaction to occur (Figure 5-25(c)). However, since the strain rate on the stoichiometric contour is low enough for reaction to occur (Figure 5-25(d)), the threshold scheme predicts a temperature increases to around 1000K. When the temperature begins to rise for the local quenching scheme, the temperature rapidly exceeds that with threshold quenching, because the mixture fraction is closer to stoichiometric on the centreline due to more entrainment (see Figure 5-44). Radial temperature and mixture fraction profiles close to the stabilisation plane are compared in Figure 5-45. The increased initial flame expansion with the threshold method can be clearly observed. Expansion reduces the entrainment of air into the core of the fuel jet; this behaviour has been observed experimentally [219]. By 75 diameters downstream of the nozzle the solutions are becoming similar.

Centreline temperature profiles comparing the EDC2 and FCRS models with threshold quenching are shown in Figure 5-46. Here, very similar temperature profiles are obtained, with the only significant differences occurring immediately downstream of the stabilisation plane. The temperature contours (Figure 5-24(f-g)) are also very similar. The rate term of the EDC2 models with threshold quenching is not dependent on the product mass fraction and therefore the temperature increase is similar to that with the FCRS model. This is because the line source is able to produce sufficient mass fraction of products to overcome the effects of convection and sustain sufficiently high concentrations of products, compared to the point source for local quenching. Centreline temperature profiles for the EDC2 model comparing local and threshold quenching are shown in Figure 5-47, whilst temperature contours are shown in Figure 5-24(a,f).

Radial temperature profiles comparing the EDC2, FCRS and pdf model with threshold quenching are shown in Figure 5-48. In all cases no reaction occurs upstream of the stabilisation location and therefore at $x/d = 25.0$ the temperature is that of the non-reacting flow. Throughout the remaining flow field the EDC and FCRS models predict very similar
solutions. This further indicates that the limiting factor in the EDC reaction rate term is not the product mass fraction and that all fuel is rapidly consumed upstream of the threshold with the EDC model. The FCRS model must consume all the fuel immediately. The pdf model predicts a lower peak temperature occurring on the fuel rich side of the flame.

Figure 5-49 compares the radial temperature profiles for the EDC2 and pdf models with local and threshold quenching. In regions close to the stabilisation location the temperature profiles are very different, due to the different reaction rates of the models. Without any suitable experimental data available, it is not possible to determine which model provides the most accurate predictions. However, by x/d = 200.0 the radial profiles are all very similar. Here, the flow is mainly a function of the total heat released and is not a strong function of the model used to determine the rate of burning.

With all the models oxidant is entrained into regions where quenching is preventing reaction occurring, resulting in regions containing both fuel and air, and hence a degree of premixing occurs. In the case of local quenching and the EDC models this fuel is then burned in a partially premixed manner with the reaction rate dependent on the product mass fraction, which can be viewed as a measure of temperature or reaction progress. This gives a finite reaction rate, dependent on the local turbulence properties and the species concentrations and a relatively slow increase in temperature. With the FCRS model, once in the burning region, the fuel and oxidant are assumed to have burned upstream at stoichiometric conditions and an infinite reaction rate is assumed and the temperature increase is accordingly rapid. With the threshold model the FCRS model again assumes that all flow through the stabilisation plane has already reacted and a large temperature gradient also occurs. However, with threshold quenching the EDC model also exhibits a rapid rise in temperature because the line source produces sufficient reaction product not to limit the reaction rate. Note that the temperature gradients are similar in both cases because the pdf for the fluctuation of the flame base dictates that the flame is distributed a minimum of five nozzle diameters.

These type of effects are dependent on the pressure ratio. Figure 5-50 and Figure 5-51 show the temperature contours with the stoichiometric mixture fraction and critical strain rate contour for a jet with NPR = 28.115 and both local and threshold quenching with the EDC2 model. In this case although the temperature rise is more rapid with threshold quenching, because the shear layer is less well mixed and the flow velocity considerably higher at the flame stabilisation plane than with NPR = 5.415, the initial temperature field shows more resemblance to that with local quenching than for the lower pressure ratio.
Figure 5-25(a) shows the temperature contours in the initial 100 diameters of the domain, along with the stoichiometric and critical strain rate contours for the EDC2 model and local quenching. The temperature is greater than the jet stagnation temperature in some regions where the strain rate exceeds critical. This is due to the reaction products generated in regions with lower strain rates convecting into the higher strain region and mixing with the unburned reactants. In the case of the FCRS model (Figure 5-25(c)) this can not happen; for strain rates higher than critical the temperature is always equal to or below the stagnation temperature. This occurs because, assuming low speed flow, the local temperature of the fluid is determined entirely by the mixture fraction. If a portion of the burned gas is convected into a region where no reaction is occurring due to extinction phenomena then the FCRS model assumes that the gas is unburned and applies the non-reacting relationships between the scalar and mass fractions. Thus, there can be no product mass fraction and the flow has no knowledge that this fluid has previously reacted and that the local temperature should be above that of the unreacted flow.

This can not easily be remedied since there is no longer a unique relationship between the mixture fraction and the other scalars and a measure of the reactedness of the fluid must be included. This could take the form of a reaction progress variable, as is frequently employed in premixed combustion problems [220] or a transport equation for one of the species mass fractions. Although this is relatively straightforward within the FCRS framework, including this in the pdf model leads to a considerable increase in the complexity of the model, since there is a requirement for the joint pdf of mixture fraction and progress variable.

This also applies to other models employing relations between conserved scalars and the mixture fraction, including the laminar flamelet model. On the other hand, the EDC models are not conserved scalar approaches and do not assume a unique relationship between the mixture fraction and other scalars, but include a transport equation for the fuel mass fraction and therefore a knowledge of the reactedness is available, which allows quenching to occur on a local basis. Note, however, that the mixture fraction transport equation is solved in both the EDC models, but this is for convenience and could be replaced by, for example, the oxidant mass fraction; other scalars are not obtained as functions of mixture fraction. The application of the conserved scalar to total enthalpy is not affected by the flame quenching mechanism and retains a unique linear relationship with mixture fraction and can therefore be employed.
Previous studies of lifted diffusion flames employing a conserved scalar approach have
avoided this problem by using a threshold criteria for the stabilisation location [81, 83].
Here, the location of flame stabilisation is assumed to occur where the stoichiometric
mixture fraction and critical strain rate contours intersect. For axial locations upstream of
this point the flow was assumed to be non-reacting, whilst downstream the flow was
assumed to be fully reacted. In order for the conserved scalar approach to remain valid in
this case, it must be assumed that no reacted flow re-circulates back into the non-reacted
region. This is generally valid for high momentum free jets. However, this may not always
be the case for other applications of interest to safety in the chemical industry.

The use of single conserved scalar approaches with flame quenching also raises other
questions. In particularly these models assume that reaction occurs at the stoichiometric
contour. This is the case in flows without quenching, or sufficiently downstream of the
quenching location. However, when the flow that has mixed in quenched regions passes
through the stabilisation plane, complete reaction is assumed to have occurred upstream at
stoichiometric conditions. Clearly, some degree of premixing has occurred and a better
treatment of the behaviour close to the stabilisation plane is desirable. The EDC model can
be used for premixed, partially premixed and non-premixed combustion and accordingly is
more applicable to predictions in regions close to lift-off. Partially premixed flamelet models
are also capable of modelling all these regimes of combustion and offer improved accuracy.

5.5.7 Comparison to Experimental Data

Only limited experimental data is available for underexpanded jet diffusion flames with
which to validate the models. The combustion models have previously been validated for
application to subsonic hydrocarbon diffusion flame. Therefore, no further validation is
presented here. For the quenching mechanism validation for subsonic methane jet flames
was shown in section 5.4.2 for the EDC model with local quenching and for cold flow
predictions employing a threshold mechanism.

5.5.7.1 Lift-Off Height Predictions

Predictions of subsonic jet lift-off heights using the EDC model with local quenching were
presented in section 5.4.2, where the critical strain rate value was calibrated and the ability to
predict accurately lift-off heights demonstrated. Here, the predicted lift-off heights for
underexpanded jet flames are compared to the available experimental data. The lift-off
heights of underexpanded reacting jets of natural gas were studied by Birch and Hargrave
Chapter 5. Reacting Results

[90] over a range of pressure ratios. Computations have been performed for a number of these test cases and the results obtained with different combustion and quenching models are compared in this section. The experimental measurements were obtained from natural gas jets (92.6% CH₄). For unconditionally stable underexpanded flames \((d > 30\text{mm})\) steady state experiments were performed with the flames stabilised for a minimum period of 25 seconds. The lift-off heights were obtained from video recordings of the flames over the period during which a stabilised flame was sustained, taken at a single angular location and both mean and rms lift-off heights were presented.

In all computations a mean lift-off height was obtained since the computations were stable around the lift-off height. For cases employing local quenching no unique value for the lift-off height was obtained from the computations and as such the lift-off height was taken to be the location where significant increase in heat release occurs, and for the results presented here the lift-off height was assumed to be the shortest axial distance from the nozzle rim to the location where the temperature exceeds 600K. With threshold quenching methods the lift-off height was taken as the axial distance from the nozzle lip to the intersection of the stoichiometric mixture fraction and the critical strain rate contours as employed during the computations. Note that the temperature does begin to increase before the lift-off height, since the model for the fluctuations of the lift-off height results in the lift-off plane being distributed over 5 diameters.

Figure 5-52 compares the predicted lift-off heights obtained using the EDC2 model and local quenching based on the strain rate of the largest eddies to the experimental data of Birch and Hargrave [90] for the unconditionally stable nozzle diameter of 50.6mm. The results show a very good agreement between the computational and experimental results; the maximum error was 11% for NPR = 10.519 and indicates that quenching based on the local large scale strain rate can predict the increase in lift-off height with pressure ratio for underexpanded jet flames.

Two of the cases have also been computed employing a quench criteria based on the small scale turbulence. Figure 5-53 compares the results employing large and small scale strain rates. The predicted lift-off heights were not found to vary significantly between the two models, but more accurate predictions were obtained with the large scale strain rate. Thus, all remaining computations employ the large scale strain rate.

Lift-off height predictions employing threshold quenching based on the strain rate of the largest eddies are compared to the experimental data and prediction using local quenching in
Figure 5-54. For these computations a critical strain rate of 100s\(^{-1}\) is employed, identical to that employed with local quenching. The predicted lift-off heights show a similar level of agreement to the experimental data as that for local quenching. This is perhaps somewhat surprising since the critical strain rate was calibrated for local quenching methods and the temperature profiles close to the stabilisation location are considerably different with the two models.

Predictions of the lift-off height of subsonic diffusion flames based on cold flow simulations were presented in section 5.4.2. This demonstrated that the lift-off heights could be predicted accurately using the cold flow. However, as the jet velocity grew, the cold flow computations predicted shorter lift-off heights than the reacting flow computations. Increasing the critical strain rate gave a better agreement between the cold and reacting flow computations at large velocities, but not at lower velocities. Figure 5-55 compares the cold flow predictions employing critical strain rates of 100s\(^{-1}\) and 140s\(^{-1}\) to the reacting flow predictions and the experimental measurements. At most pressure ratios, the lift-off height is underpredicted with cold flow computations and \(S_q = 140\text{ms}^{-1}\), whilst for computations with \(S_q = 100\text{ms}^{-1}\) the lift-off heights are generally overpredicted. The critical strain rate for cold flow computations can be varied to give better agreement for part of the experimental data. However, the reacting flow predictions with \(S_q = 100\text{ms}^{-1}\) give the best agreement with the experimental data over the whole range of pressure ratios.

In almost all cases the reacting flow computations predict a shorter lift-off height compared to the cold flow computations for the same critical strain rate. This is due to jet expansion caused by the decreased density in the reacting flow. Figure 5-56 shows the velocity contours for an NPR = 5.415 underexpanded jet flame, along with the stoichiometric and strain rate contours, for the cold flow and solutions with three combinations of combustion and extinction models. For the cold flow (Figure 5-56(a)) the lift-off height is predicted to be 42.3 diameters with \(S_q = 100\text{ms}^{-1}\). However, for the reacting flow the lift-off height reduces to 32 diameters, with threshold quenching and the FCRS model (Figure 5-56(b)). The jet can be seen to expanded abruptly around the lift-off height and this leads to a shift in the location of flame stabilisation. With the EDC model and local quenching (Figure 5-56(c)) the expansion occurs much more gradually due to the slower initial reaction rate. In this case the intersection of the stoichiometric and critical strain rate contours moves upstream by around one diameter compared to the cold flow. However, with this model the lift-off height is based on the location where appreciable temperature rise occurs and this was found to be around 37 diameters (Figure 5-25(a)). The velocity contours for the reacting flow using
threshold quenching and the EDC2 model are shown in Figure 5-56(d). The same lift-off height is predicted as for the FCRS. However, the velocity fields differ in the stabilisation region.

Centreline profiles of mixture fraction and velocity are shown for this case in Figure 5-57 and Figure 5-58 respectively. The effect of heat release is to reduce entrainment and hence increase the mixture fraction on the jet axis. In addition, the onset of heat release and the resulting density decrease causes an increase in velocity. In cases with threshold quenching this occurs over a short distance and a large velocity gradient results. With local quenching the velocity gradient is lower.

Several factors must be considered when comparing the computational and experimental lift-off heights. The experimental data plotted in Figures 5-52 to 5-55 is the mean observed lift-off height and significant variations were observed in the measurements due to fluctuations of the flamebase. For NPR = 28.115 a time history of the lift-off height was presented by Birch and Hargrave [90]. The recorded lift-off height varied from 42 to 65 diameters and the RMS of the fluctuations was found to be 3.7 diameters. The lift-off height varied in a periodic manner and this was caused by the propagation of helical vortices. Statistical analysis showed the variation to be Gaussian.

The lift-off height has been observed to reach a limiting value at high NPR, with further increases in pressure not increasing the lift-off height. This behaviour is shown in the experimental data in Figures 5-52 to 5-55 and the computational results also appear to predict this feature.

The experimental data of Birch and Hargrave [90] measured an abrupt change in the lift-off height for pressure ratios between 3 and 5 for a nozzle diameter of 50.6mm, whilst between pressure ratios of 3 and 4 the transient data showed a decrease in lift-off height with increasing pressure ratio. This was not observed in the computational results. For the 112.2mm nozzle there was insufficient experimental data to determine whether this behaviour also occurred. This was attributed to the type of orifice being employed, since it was thought that the nozzle flow did not become fully choked until the stagnation pressure was several bars in excess of the critical pressure and the sudden change in lift-off height corresponded to the flow becoming fully choked. If this was the case, the computations will not predict this, since the jet boundary conditions assume fully choked flow whenever the pressure ratio exceeds critical. Another possible explanation could be that at around this pressure ratio normal shocks form as the jet becomes highly underexpanded. However, the
predictions show that the change from moderately to highly unexpanded jets has little effect on the downstream structure and the resulting flame. Alternatively, the unsteady behaviour of the jet may be important. A brief review of unsteady effects was presented in section 1.2.4. It may be that this change in lift-off height coincides with a change in mode of the unsteady behaviour.

Unlike for subsonic jets, a strong dependence of the lift-off height on the nozzle diameter was found by Birch and Hargrave [90] for underexpanded jet flames. This behaviour can be accounted for by considering the relative locations of the shock containing potential core and the lift-off height as the diameter varies. The potential core length is proportional to the nozzle diameter, whilst the lift-off height in subsonic jets is not dependent on the nozzle diameter. Thus, for larger diameters combustion would be stabilised nearer to the potential core and eventually in it. However, in underexpanded jets the mixing rate and decay in turbulent strain rate are reduced close to the shock containing region prohibiting the stabilisation of a flame in this region. Therefore, the lift-off height must increase in order that stabilisation occurs sufficiently downstream of the potential core region. Hence, the flame stabilisation location is a function of diameter for underexpanded jets. This behaviour has been tested in the computational model by predicting the lift-off height for two cases with a nozzle diameter of 111.2mm (NPR = 5.597 and NPR = 9.794). For NPR = 5.597 the measured lift-off height was 2.879m ($x/d = 25.89$) compared to around 1.7m ($x/d = 34.0$) for a nozzle diameter of 50.6mm. The computations predict a lift-off height of 2.685m ($x/d = 24.15$) for this case, indicating that the effect of nozzle diameter is predicted accurately.

Table 5-1 compares the results obtained for NPR = 9.794 to those for NPR = 10.519 and $d = 50.6$mm. Note that at these pressure ratios the lift-off height does not vary strongly with NPR, as the asymptotic lift-off height is being approached, and therefore the difference between the results are due predominately to the effect of the nozzle diameter and not the variation in NPR. For the reacting flow computations, both quenching methodologies predict the correct trend and show reasonable quantitative agreement to the experimental data with, for this pressure, threshold quenching the most accurate. However, the cold flow predictions do not predict the correct trend and in this case do not model the increase in lift-off height with diameter.
Table 5-1. Effect of Diameter on the Predicted and Measured Lift-Off Heights. Experimental data from Birch and Hargrave [90]

<table>
<thead>
<tr>
<th>$d$ (mm)</th>
<th>NPR</th>
<th>experimental (m)</th>
<th>predictions</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>local (m)</td>
</tr>
<tr>
<td>50.6</td>
<td>10.519</td>
<td>2.513</td>
<td>2.24</td>
</tr>
<tr>
<td>111.2</td>
<td>9.794</td>
<td>3.100</td>
<td>2.78</td>
</tr>
</tbody>
</table>

5.5.7.2 Downstream Data

The only known measurements of properties in underexpanded jet diffusion flames are those due to Gore et al. [29]. They measured the centreline temperature for seven underexpanded natural gas (95% methane) diffusion flame test cases. Two nozzle diameters, 76mm and 102mm, were employed giving either approximately 100MW or 200MW flames respectively. In each case the pressure ratio was determined by measuring the stagnation pressure upstream of the orifice and varied between 2.87 and 4.24 bar. The range of ambient wind speed was measured for each case and this varied from 0.2 to 2.1ms$^{-1}$. The results are grouped for each of the two flame sizes and the variation in precise initial conditions within each was not found to alter significantly the results. However, the effect of the ambient wind speed was thought to be more significant. The conditions for the experimental test cases are given in Table 5-2.

<table>
<thead>
<tr>
<th>Case</th>
<th>$d$ (mm)</th>
<th>$Q$ (MW)</th>
<th>$T_o$ (K)</th>
<th>$P_o$ (bar)</th>
<th>$u_{ao}$ (ms$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>76</td>
<td>147</td>
<td>242</td>
<td>4.18</td>
<td>0.8-0.9</td>
</tr>
<tr>
<td>1b</td>
<td>76</td>
<td>135</td>
<td>259</td>
<td>4.24</td>
<td>0.9-2.0</td>
</tr>
<tr>
<td>2a</td>
<td>102</td>
<td>192</td>
<td>272</td>
<td>3.31</td>
<td>0.4-0.5</td>
</tr>
<tr>
<td>2b</td>
<td>102</td>
<td>187</td>
<td>263</td>
<td>3.06</td>
<td>0.2-0.5</td>
</tr>
<tr>
<td>2c</td>
<td>102</td>
<td>174</td>
<td>252</td>
<td>2.87</td>
<td>0.6-0.7</td>
</tr>
<tr>
<td>2d</td>
<td>102</td>
<td>210</td>
<td>249</td>
<td>3.52</td>
<td>1.1-2.1</td>
</tr>
<tr>
<td>2e</td>
<td>102</td>
<td>207</td>
<td>256</td>
<td>3.49</td>
<td>1.3-1.8</td>
</tr>
</tbody>
</table>

Table 5-2. Initial Conditions for the Experimental Test of Gore et al. [29]
Computations were performed for the two flame sizes by Gore et al. [29]. Detailed analysis of the shock containing region was avoided by employing a pseudo nozzle approximation and assuming a supersonic, perfectly expanded jet on the grounds that the external expansion region had not been studied very much and the capability to treat this flow was limited. A laminar flamelet model was employed, but no details were given of this and no mechanism for modelling flame lifting phenomena was applied.

Figure 5-59 compares predicted centreline temperature to the measurement of Gore et al. [29] for the 100MW cases. The predictions employ the pdf model with threshold quenching and the EDC2 model with both local and threshold quenching. The experimental data shows large variations in the measured temperatures between the two 100MW flames; more than 1000K at $x/d = 250.0$. However, the conditions for these two cases do not vary significantly, with a difference in stagnation pressure of 0.06bar and stagnation temperature of 17K.

Computations have been performed with these variation in conditions with almost identical results obtained. The significant difference here is the maximum ambient wind speed, which is significantly larger in case 1b. It is likely, therefore, that the lower measured temperatures for case 1b were the results of an increase in wind speed and that the results for case 1a were also affected by the ambient wind speed, which although lower than case 1b was still significant. It was reported by Gore et al. [29] that wind disturbances deflected the flame from the axis and caused the measured temperatures to be too low. Also cited as a source of experimental error were thermocouple radiation errors.

The agreement between the predicted and measured temperatures is reasonable in the first 100 diameters. The rate and location of the initial temperature rise is well predicted and the peak temperatures obtained at $x/d = 100$ are within 20%. Further downstream the predicted temperature continues to rise, up to a peak of approximately 2100K at $x/d = 200$, whilst the measured temperatures decrease downstream of $x/d = 100$, to around 1500K for case 1a and 800K for case 1b at $x/d = 200$. Clearly, the effect of the wind is significant in this region for both cases.

The predicted centreline temperatures for the 200MW flames are shown in Figure 5-60, compared to the three experimental tests with the lowest ambient wind speed (2a-c). For case 2 the initial conditions vary more significantly than for case 1, however only computational results employing the conditions of case 2c are shown. The agreement obtained in this case is similar to that found for case 1, with both models overpredicting the temperature. No measure of the flame length can be determined from the experimental data, since the
measurement are not taken sufficiently far downstream. In the region immediately upstream of the flame stabilisation point more detailed measurements are required in order to determine which model is most accurate.

Figure 5-61 compares the predicted and measured centreline temperatures for the two flame sizes against normalised axial displacement, showing that this normalisation is not enough to collapse the data. Similarly, Figure 5-62 shows the same data, but without normalisation of the axial displacement and the results are dependent on diameter. Normalising the experimental data by diameter appears to be sufficient to correlate the data for the two flame sizes.

The agreement between the measured and predicted temperatures are as good as can be expected considering the many uncertainties in the experimental data, especially with respect to the ambient wind speed and the complexities of the problem. Compared to test 1b the temperature is overpredicted by around 300K, but the flame length appears to be reasonable. The overpredicted temperature could be due to chemical kinetic effects and heat loss due radiation, as well as the uncertainties in the experimental data. The initial temperature rise close to the nozzle is predicted most accurately by the pdf model with threshold extinction. However, since the initial rate of temperature rise close to the centreline is similar for the three models, increasing the critical strain rate would lead to the EDC model predicting the best agreement.

The computations of Gore et al. [29] do not appear to show any closer resemblance to the experimental data than in the current work. This is to be expected since the model assumes that the flame is attached to the burner rim; the experimental observations state that the flame was generally lifted by 15-20 nozzle diameters.

5.6 Pseudo Calculations

Calculations of underexpanded jet diffusion flames employing the pseudo nozzle approximation are presented in this section. Details of the pseudo source approximation and the results obtained for non-reacting underexpanded jets were presented in section 3.7, whilst its application to mixing calculations was described in section 5.2.3.

Figure 5-63 shows the temperature contours for pseudo nozzle approximations of a jet with NPR = 5.415, whilst Figure 5-64 shows the critical strain and stoichiometric contours in the near lift-off region. Centreline temperature profiles are compared in Figure 5-65 for the standard and pseudo models using the FCRS with threshold quenching and EDC with local
quenching. The results clearly show that the pseudo nozzle approximation can represent accurately this underexpanded reacting jet. In both cases the temperature rise occurs a few diameters downstream with the pseudo model. This is because the pseudo model does not account for the loss of total pressure in the normal shock which leads to an overprediction of the potential core. Centreline mixture fraction profiles are shown in Figure 5-66. The radial temperatures, shown in Figure 5-67, again show good agreement between the pseudo and standard models.

Predicted lift-off heights with the pseudo model are shown in Table 5-3. For NPR = 5.415 each of the quenching methods overpredicts the standard model by around 10%. This is because total pressure losses in the normal shock are not accounted for. For NPR = 28.115 the difference in the results is much larger; around 30% for the EDC and cold flow models. However, for the FCRS the difference is only 12%. The increased difference between results is expected as the total pressure loss in the normal shock increases. The reason for the smaller difference with the FCRS model is not clear.

<table>
<thead>
<tr>
<th>NPR</th>
<th>exp</th>
<th>EDC, local</th>
<th>FCRS, threshold</th>
<th>cold flow</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>standard</td>
<td>pseudo</td>
<td>standard</td>
</tr>
<tr>
<td>5.415</td>
<td>33.7</td>
<td>36.9</td>
<td>40.4</td>
<td>31.96</td>
</tr>
<tr>
<td>28.115</td>
<td>52.8</td>
<td>53.36</td>
<td>68.9</td>
<td>57.66</td>
</tr>
</tbody>
</table>

Table 5-3. Effect of pseudo nozzle approximation on lift-off heights (V/d)

Figure 5-68 shows the temperature contours for NPR = 28.115 with the pseudo nozzle approximation and the EDC2 model with local quenching. The lift-off height in this case is 68.9 diameters, obtained as the distance to the 600K contour. Equivalent results without the pseudo nozzle approximation were shown in Figure 5-50, where the lift-off height was 53.4 diameters. Although the pseudo nozzle results predict a larger lift-off height, it predicts that the first rise in temperature is closer to the nozzle; the initial rise in temperature along the stoichiometric contour is slower. The predicted spread rate of the jet prior to ignition is lower with the pseudo model as shown in Figure 5-10 and this results in the cold flow calculations predicting an increased lift-off height. This can also be seen with the strain rate which decays below the critical value further downstream with the pseudo calculations. A narrower flame is predicted with the pseudo model, located closer to the jet axis, again due to the lower mixing rate and narrower shear layers.
The results presented here have shown that the pseudo nozzle approximation can be employed for lower pressure ratio cases. However, for higher pressure ratio cases, work needs to be done to determine the total pressure loss across the normal shock for a particular pressure ratio and included into the pseudo nozzle approximation conditions.

5.7 Closure

The results presented in the preceding sections represent the first known numerical, whole-field computations of underexpanded jet flames and the first predictions of lift-off heights in underexpanded jets. Without any suitable experimental data, extensive validation of the model can not be achieved. However, the various components of the calculations have been validated with the available data. Chapters 2 and 3 described the extensive validation of the non-reacting underexpanded jet flow over a wide range of pressure ratios. In particular, the downstream velocity decay compared accurately to the data of Birch et al. [12] (see section 3-6) and the mixing properties to the data of Birch et al. [13] (see section 5.2.2). The EDC and presumed $\beta$-pdf are standard combustion models that have previously been applied to attached subsonic jet diffusion flames and successfully predicted the fluid dynamic features of these jets. The models for flame extinction have also been validated. Local quenching based on the strain rate of the large scale structures was validated for subsonic jet calculations in section 5.4.2 and predicted accurately the underexpanded jet lift-off heights reported by Birch and Hargrave [90]. Both cold and reacting flow predictions based on a threshold criteria and the strain rate of the large scale turbulent structures have also shown good agreement to the experimental data for underexpanded jets and were previously applied to subsonic jets [83].

A single critical large scale strain rate, calibrated for subsonic, lifted diffusion flames, has been employed for both local and threshold quenching and also for the cold flow simulations. The value of $100\,\text{s}^{-1}$ is close to the value of $88.3\,\text{s}^{-1}$ used by Sanders and Lamers [83] for cold flow computations employing threshold quenching based on the large scale structures. Reacting calculations only used the small scale strain rate with $4870.6\,\text{s}^{-1}$ for the cold flow and $2092.6\,\text{s}^{-1}$ for the reacting flow. For the cold flow calculations a value of $140\,\text{s}^{-1}$ was found to give the most accurate predictions. Fairweather et al. [81] employed a value of $200\,\text{s}^{-1}$ for the critical strain rate based on the large scale turbulent structures, but here quenching was assumed to occur when the strain rate on the centreline decayed below this value.
Several uncertainties, however, still remain. As shown in for example Figure 5-47, applying lift-off heights via local and threshold phenomena give significantly different temperature profiles in the region close to the stabilisation point even though in both cases the predicted and measured lift-off heights agree well. Threshold quenching gives rise to a much more rapid increase in temperature initiated as a line source, whereas the increase in temperature is more gradual with local quenching, initiated as a point source.

There is little experimental data to support either local or threshold quenching. As discussed in section 5.4.2, contours of temperature for subsonic diffusion flames presented by Bradley et al. [87] and Sanders and Lamers [83] differ significantly, but it is not clear which are most realistic. Fairweather et al. [81] found that the employing a threshold lift-off criteria based on the value $e/k$ on the jet centreline improved results for lifted jets in across flow compared to computations assuming that the flame was rim stabilised. However, their results indicated that this lift-off criteria leads to an overexpansion of the flow in the region close to flame stabilisation. Sanders and Lamers [83] employed threshold quenching based on the strain rate of the smallest turbulent structures at the stoichiometric contour and compared the predicted centreline velocity to experimental data for a subsonic, 71ms$^{-1}$ lifted diffusion flame. The predicted velocity gradient at lift-off was steep. This behaviour was not observed in the experimental data. Local quenching does not predict this sudden increase for either subsonic or underexpanded flames.

Schefer et al. [219] measured CH and CH$_4$ concentrations in a lifted, 21ms$^{-1}$ methane diffusion flame. CH is a good tracer of the flame zone since it is a reaction intermediate that occurs only in the presence of intense combustion. The results showed that the reaction takes place around the stoichiometric contour and displaced from the jet axis. Contours of CH$_4$ concentration do not show a rapid expansion of the jet flow around the lift-off height as shown in Figure 5-56(b) for threshold quenching. This experimental data appears to support the results presented employing local quenching.

Threshold quenching has been employed in most studies of lifted diffusion flames, however it is not clear whether this is as a numerical convenience. When employing a conserved scalar approach it has the advantage of not requiring a measure for reactedness. In addition, the chemical reaction terms need be calculated in a smaller number of cells since for all axial locations upstream of the stabilisation plane the flow is known to be non-reacting. In the case of local quenching the combustion model must be applied to all locations with strain rates
above the critical value. Depending on the design of the computational mesh this can increase the computational requirements significantly.

In the current work numerical problems were found when employing threshold quenching with the FCRS or pdf models since the temperature at the stabilisation plane increased from the non-reacting jet temperature to the stoichiometric temperature across a single cell. This meant that the density could decrease by a factor of more than 6. The numerical method was not able to compute this jump condition satisfactorily. Additional difficulties occurred because any instabilities generated caused the turbulence properties to vary which often caused the stabilisation plane to fluctuate, generating spurious large scale structures, shed from the lift-off plane and convecting downstream.

The laminar (diffusion) flamelet model proposes that the flamesheet is the ensemble of laminar flamelets located at the instantaneous stoichiometric contour. If this flamesheet becomes too stretched then flamelets maybe quenched, and if too many of these quenching events occur then the flamesheet may no longer be connected to the rim and lift-off occurs. It therefore follows that it is the strain rate at the instantaneous stoichiometric contour that should be the critical describer of the lift-off phenomena. Both Peters and Williams [85] and Sanders and Lamers [83] employ the strain rate at the stoichiometric contour. The model of Bradley et al. [87] employs a laminar flamelet approach but in this case the flamelets are partially premixed, that is the flame is not assumed to be located at the instantaneous mixture fraction location and the model is similar to a premixed flamelet model. In this case reaction can occur in any region, within the flammability limits of the fuel. This model supports the use of local quenching, such that reaction can occur at a particular axial location even when the stoichiometric contour is experiencing a strain rate above critical.

Finally, a number of the assumptions imposed remain a source of uncertainty. In particular the assumption of unity Lewis number may neglect some important physical effects. This is however an assumption made in the vast majority of combustion models applied to diffusion flames. Single step, fast chemistry has been assumed throughout this work and was justified in section 4.2.5. The effect of neglecting viscous effects was examined and found to be small. No account was made of the heat loss due to radiation. This will act to reduce the temperature in flames. As with the non-reacting calculations, various factors affect the solution, notably the initial turbulence conditions in the nozzle, and possibly the profiles of velocity at the nozzle exit. Grid independence was shown for both the non-reacting underexpanded jets and also for subsonic reacting jets.
5.8 Figures

Figure 5-1. Effect of TVD for the Mixture Fraction Transport Equation on its Centreline Value, NPR=3.5

Figure 5-2. Comparison of Centreline Mixture Fraction Profiles for NPR=2.27 with and without the Compressibility Correction, Experimental Data from Chuech [16]
Figure 5-3. Comparison of Radial Mixture Fraction Profiles for NPR=2.27 with and without the Compressibility Correction, Experimental Data from Chuech [16]. (a) $x/d=10.0$, (b) $x/d=20.0$
Chapter 5. Reacting Results

Figure 5-4. Comparison of Centreline Mixture Fraction Profiles with and without the Compressibility Correction for a Perfectly Expanded Sonic Jet. Experimental Data from Chuech [16]

Figure 5-5. Centreline Mixture Fraction Profiles for NPR=5.415, Comparing the Standard and Compressibility Corrected $k$-$\varepsilon$ Model, Experimental Data Birch et al. [13]
Chapter 5. Reacting Results

Figure 5-6. Centreline Mixture Fraction Profiles for NPR=10.519, Comparing the Standard and Compressibility Corrected $k$-$\varepsilon$ Model, Experimental Data Birch et al. [13]

Figure 5-7. Centreline Mixture Fraction Profiles for NPR=28.115, Comparing the Standard and Compressibility Corrected $k$-$\varepsilon$ Model, Experimental Data Birch et al. [13]
Chapter 5. Reacting Results

Figure 5-8. Effect of $\sigma_f$ on the Centreline Mixture Fraction Profiles with and without the Compressibility Correction for NPR=2.27, Experimental Data Chuech [16]

Figure 5-9. Comparison of Centreline Mixture Fraction Profiles with the Pseudo and Standard Models for NPR=2.27. Experimental Data from Chuech [16]
Chapter 5. Reacting Results

Figure 5-10. Comparison of Centreline Mixture Fraction Profiles with the Pseudo and Standard Models for NPR=28.115, Experimental Data Birch et al. [13]

Figure 5-11. Comparison of Centreline Mach Number Profiles with the Pseudo and Standard Models for NPR=28.115
Chapter 5. Reacting Results

Figure 5-12. Comparison of Centreline Mach Number with the Constant Total Enthalpy Assumption and the Full Energy Equation, NPR=3.5

Figure 5-13. Comparison of Centreline Temperature with the Constant Total Enthalpy Assumption and the Full Energy Equation, NPR=3.5
Figure 5-14. Effect of TVD for the Energy Equation on the Centreline Mach Number, NPR=3.5

Figure 5-15. Effect of TVD for the Energy Equation on the Centreline Temperature, NPR=3.5
Figure 5-16. Temperature Contours for Subsonic Jet Flames with (a) \( u_* = 40 \text{ms}^{-1} \), (b) \( u_* = 60 \text{ms}^{-1} \), (c) \( u_* = 80 \text{ms}^{-1} \) and (d) \( u_* = 100 \text{ms}^{-1} \).
Figure 5-17. Lift-Off Heights for Subsonic Methane Jet Flames with the EDC 2 model and local quenching. Experimental Data of Kalghatgi [28]

Figure 5-18. Lift-Off Heights for Subsonic Methane Jet Flames with the EDC 2 model and local quenching compared to the cold flow solution. Experimental Data of Kalghatgi [28]
Figure 5-19. Effect of Critical Strain Rate ($S_q$) on the Lift-Off Heights of Subsonic Methane Jet Flames Derived from Cold Flow Computations with Varying Jet Velocities

Figure 5-20. Effect of Critical Strain Rate on the Lift-Off Heights of Subsonic Methane Jet Flames Derived from Cold Flow Computations Showing the Effect of Mesh Resolution for a Jet Velocity of 60 ms$^{-1}$
Chapter 5. Reacting Results

Figure 5-21. Centreline Temperature for a 60ms\(^{-1}\) Methane Jet Diffusion Flame, Showing the Effect of Mesh Resolution

Figure 5-22. Centreline Temperature Profile for the EDC 1 Model Comparing Solutions with \(H\) Calculated as a Conserved Scalar and via a Transport equation, NPR=5.415
Figure 5-23. Radial Temperature Profiles for the EDC 1 Model Comparing Solutions with $H$ Calculated as a Conserved Scalar and via a Transport equation, NPR=5.415. (a) $x/d=25.0$, (b) $x/d=50.0$, (c) $x/d=75.0$, (d) $x/d=100.0$, (e) $x/d=150.0$, (f) $x/d=200.0$
Figure 5-24(a-b). Contours of Temperature for an Underexpanded Jet Diffusion Flame, NPR=5.415 with Various Combustion Models
Figure 5-24 (c-e). Contours of Temperature for an Underexpanded Jet Diffusion Flame, NPR=5.415 with Various Combustion Models.
Figure 5-24 (f-h). Contours of Temperature for an Underexpanded Jet Diffusion Flame, NPR=5.415 with Various Combustion Models
Figure 5-25. Contours of Temperature Showing the Critical Strain Rate (---) and Stoichiometric Contours (----) for an Underexpanded Jet Diffusion Flame, NPR=5.415, With Various Combustion Models
Figure 5-26. Comparison of Centreline Temperatures for the EDC 1 and EDC 2 Models, with Local Extinction Based on the Large Scale Structures
Figure 5-27. Comparison of the Radial Temperature Profiles for the EDC 1 and EDC 2 models. (a) $x/d=25.0$, (b) $x/d=50.0$, (c) $x/d=75.0$, (d) $x/d=100.0$, (e) $x/d=150.0$, (f) $x/d=200.0$
Figure 5-28. Centreline Reaction Rates Profiles for the EDC 1 and EDC 2 Models, NPR=5.415
Figure 5-29. Radial Profiles of Reaction Rates for the EDC 1 and EDC 2 Models, NPR=5.415. (a) $x/d=25.0$, (b) $x/d=50.0$, (c) $x/d=75.0$, (d) $x/d=100.0$, (e) $x/d=150.0$, (f) $x/d=200.0$
Chapter 5. Reacting Results

Figure 5-30. Centreline Plots of $Y_{\min}$ and $Y_p/(r+1)$ for the EDC 1 and EDC 2 Models

Figure 5-31. Radial Profiles of $Y_{\min}$ and $Y_p/(r+1)$ for the EDC 1 and EDC 2 Models. (a) $x/d=25.0$, (b) $x/d=50.0$, (c) $x/d=75.0$, (d) $x/d=100.0

292
Figure 5-32. Centreline Plot of the Mass Fraction of the Fine Scale Structures for the EDC 2 Model

Figure 5-33. Radial Profiles of (a) the Mass Fraction of the Fine Scale Structure and (b) the Premixedness Correlation at $x/d=50.0$
Figure 5-34. Centreline Profile of the Premixedness Correlation for the EDC 2 Model

Figure 5-35. Comparison of Centreline Temperature for the EDC 2 and FCRS Models with Local Extinction Based on the Large Scale Structures, NPR=5.415
Figure 5-36. Comparison of Radial Temperature Profiles for the EDC 2 and FCRS Models with Local Extinction Based on the Large Scale Structures, NPR=5.415. (a) \(x/d=25.0\), (b) \(x/d=50.0\), (c) \(x/d=75.0\), (d) \(x/d=100.0\), (e) \(x/d=150.0\), (f) \(x/d=200.0\).
Figure 5-37. Favre Averaged Species Mass Fractions as a Function of the Mean Mixture Fraction with $\bar{f}^{*2} = 0.01$

Figure 5-38. Favre Averaged Species Mass Fractions as a Function of the Mean Mixture Fraction with $\bar{f}^{*2} = 0.001$

Chapter 5. Reacting Results
Figure 5-39. Favre Averaged Product Mass Fractions as a Function of the Mean Mixture Fraction for Varying $\tilde{f}^{*2}$

Figure 5-40. Comparison of Centreline Temperatures for the FCRS and PDF models With Local Extinction Based on the Large Scale Structures
Figure 5-41. Comparison of EDC1, EDC2, FCRS and pdf with local extinction based on the large scale structures. (a) \(x/d=25.0\), (b) \(x/d=50.0\), (c) \(x/d=75.0\), (d) \(x/d=100.0\), (e) \(x/d=150.0\), (f) \(x/d=200.0\)
Chapter 5. Reacting Results

Figure 5-42. Centreline Temperature for the EDC 2 Model, Comparing Local Extinction Based on the Large and Small Scale Structures
Figure 5-43. FCRS Model, Comparing Centreline Temperature for Local and Threshold Extinction Based on the Large Scale Structures

Figure 5-44. FCRS Model, Comparing Centreline Mixture Fraction for Local and Threshold Extinction Based on the Large Scale Structures
Figure 5-45. Temperature and mixture fraction profiles close to the lift-off plane for the FCRS model with local and threshold extinction models.
Figure 5-46. Comparison of Centreline Temperature for EDC 2 and FCRS with Threshold Extinction Based on the Large Scale Structures

Figure 5-47. Centreline Temperature for the EDC 2 Model, Comparing Local and Threshold Extinction Based on the Large Scale Structures
Figure 5-48. Comparison of Radial Temperature Profiles for the EDC2, FCRS and PDF Models with Threshold Extinction Based on the Large Scale Structures. (a) \(x/d=25.0\), (b) \(x/d=50.0\), (c) \(x/d=75.0\), (d) \(x/d=100.0\), (e) \(x/d=150.0\), (f) \(x/d=200.0\)
Chapter 5. Reacting Results

Figure 5-49. Comparison of EDC2 and PDF Models with Local and Threshold Extinction Based on the Large Scale Structures. (a) $x/d=25.0$, (b) $x/d=50.0$, (c) $x/d=75.0$, (d) $x/d=100.0$, (e) $x/d=150.0$, (f) $x/d=200.0$.

Key: (1) EDC, Local Quenching; (2) EDC, Threshold Quenching; (3) Pdf, Local Quenching; (4) Pdf, Threshold Quenching

304
Figure 5-50. Temperature Contours in the Lift-off Region for NPR=28.115 with the EDC 2 Model and Local Quenching Based on the Large Scale Structures

Figure 5-51. Temperature Contours in the Lift-off Region for NPR=28.115 with the EDC 2 Model and Threshold Quenching Based on the Large Scale Structures
Figure 5-52. Lift-Off Height as a Function of NPR, Employing the EDC2 Model with Local Quenching Based on the Strain Rate of the Large Scale Structures. Experimental data from Birch and Hargrave [90]

Figure 5-53. Lift-Off Heights as a Function of NPR, Comparing the EDC2 Model with Local Quenching Based on the Large and Small Scale Strain Rate. Experimental data from Birch and Hargrave [90]
Figure 5-54. Lift-Off Height as a Function of NPR, Comparing Local and Threshold Quenching. Experimental data from Birch and Hargrave [90]

Figure 5-55. Lift-Off Height as a Function of NPR, Comparing the Results from Cold Flow Reacting Flow Computations. Experimental data from Birch and Hargrave [90]
Figure 5-56. Velocity Contours Showing Stoichiometric (----) and Strain Rate Contours (—) for NPR=5.415 Comparing the Cold Flow Solution to the Reacting Solution with EDC and FCRS Combustion Models
Chapter 5. Reacting Results

Figure 5-57 Centreline Mixture Fraction Profiles, Comparing Cold Flow Prediction with those Employing Various Combustion Models, NPR=5.415

Figure 5-58. Centreline Axial Velocity Profiles, Comparing Cold Flow Prediction with those Employing Various Combustion Models, NPR=5.415
Figure 5-59. Centreline Temperature for 100MW Jet with EDC and PDF Models, Compared to the Experimental Data of Gore et al. [29]

Figure 5-60. Centreline Temperature for 200MW Jet with EDC and PDF Models Compared to the Experimental Data of Gore et al. [29]
Figure 5-61. Centreline Temperature against Axial Displacement, Normalised by Nozzle Diameter for 100MW and 200MW Flames, Experimental Data Gore et al. [29]

Figure 5-62. Centreline Temperature against Axial Displacement for 100MW and 200MW Flames, Experimental Data Gore et al. [29]
Figure 5-63. Contours of Temperature for an Underexpanded Jet Diffusion Flame, NPR=5.415, with the Pseudo Nozzle Approximation
Figure 5-64. Contours of Temperature Showing the Critical Strain (-----) and Stoichiometric Contours (----) for an Underexpanded Jet Diffusion Flame, NPR=5.415, with the Pseudo Nozzle Approximation.
Figure 5-65. Effect of Pseudo Nozzle Approximation on the Centreline Temperature with the EDC2 and FCRS Models, NPR=5.415

Figure 5-66. Effect of Pseudo Nozzle Approximation on the Centreline Mixture Fraction with the EDC2 and FCRS Models, NPR=5.415
Figure 5-67. Effect of Pseudo Nozzle Approximation on the Radial Temperature Profiles with the EDC2 and FCRS models, NPR=5.415. (a) x/d=25.0, (b) x/d=50.0, (c) x/d=75.0, (d) x/d=100.0, (e) x/d=150.0, (f) x/d=200.0
Figure 5-68. Temperature Contours Showing Stoichiometric (----) and Critical Strain Rate Contours (-----) for NPR=28.115, Employing the Pseudo Nozzle Approximation and the EDC 2 Model with Local Quenching
Chapter 6. Conclusions

The principal aim of this study was to develop an accurate and efficient non-reacting pressure based methodology applicable to all Mach numbers and then extend this to allow the computation of underexpanded jet diffusion flames. This chapter presents the main conclusion drawn from this study.

1) The developed pressure correction methodology can predict accurately the flow features of both moderately and highly underexpanded sonic jets. In particular, both the oblique shock cell structure of moderately underexpanded and the Mach disk structure of highly underexpanded jets were predicted. This represents one of the few studies of highly underexpanded jets reported in the literature and the first employing a pressure based methodology to predict both the near field shock containing region and the far field.

2) Pressure based methods can compute highly underexpanded jet flows accurately and efficiently only if the differencing of the mass error terms is treated correctly in the pressure correction equation. Upwinding density in the mass error term of the pressure correction equation leads to a very robust scheme, but at the expense of a very smeared shock cell structure, whilst the previously used retarded pressure scheme has good shock capturing performance, but is unstable at high Mach numbers. The Mach number dependent blended differencing scheme developed in this study attained the same resolution of shock capturing found with previous retarded pressure schemes, whilst extending the range of application to much higher pressure ratios. However, the blend factors which describe the proportions in which central and upwind differencing are combined are dependent on the pressure ratio in order to obtain the most accurate results without any loss of robustness.

3) The accuracy of the scheme can be improved by applying higher order differencing schemes to the convective differencing. Second order total variation diminishing schemes gave improved shock capturing capabilities compared to upwind and hybrid schemes. However, this upwinding must be based on primitive and not density weighted variables, as is common practice in compressible pressure based schemes. Applying upwind differencing to the density weighted variables in supersonic flow regions actually results in a dissipation term opposite in sign to the physical viscous terms, which leads to an increase in shock capturing resolution. However, in order to obtain a stable solution, such practices require that large dissipation terms are added in the pressure correction equation.
Upwinding based on velocity, on the other hand, gives the desired dissipation terms and allows jets with NPR less than 3.5 to be computed without the need for any explicit dissipation in the pressure correction scheme.

4) The methodology has been validated by comparison to available experimental data and generally the agreement obtained was good. The location of the first shock interaction in moderately underexpanded jets and the normal shock in highly underexpanded jets agrees very well with experimental data. Detailed velocity and Mach number measurements show good agreement in the first few shock cells, however the subsequent shock cell structure is dissipated too rapidly. Downstream of the shock containing region good agreement with experimental velocity data is obtained when a compressibility correction is employed within the $k$-$\varepsilon$ model for turbulence. This compressibility correction only influenced downstream regions and had no significant affect in the shock containing region, apart from reducing the recovered Mach number downstream of the normal shock in highly underexpanded jets.

5) Following development and validation of the non-reacting methodology several combustion models have been implemented, along with transport equations for scalar transport and total enthalpy and models for flame extinction. Downstream mixture fraction profiles are predicted accurately. Comparing solutions employing a transport equation for energy to those employing an assumption of total enthalpy confirm that this assumption is valid for non-reacting flows.

6) Following calibration of the critical strain rate, the lift-off heights of subsonic, methane diffusion flames were predicted using an extinction mechanism based on the strain rate of the large scale turbulent structures on a local basis, with the lift-off height obtained as the location where significant heat release begins. Excellent agreement was obtained compared to experimental data.

7) The results presented for underexpanded jet diffusion flames represent the first known numerical, whole-field computations of such flames and the first predictions of lift-off heights in underexpanded jets. The lift-off heights showed very good agreement to the available experimental data using a quench methodology based on either a local or threshold methodology and employing the same critical strain rate. A threshold criteria for lift-off using the cold flow has also been applied to both subsonic and underexpanded jet diffusion flame lift-off heights with a reduced accuracy and an increased critical strain rate.
8) The EDC, FCRS and presumed pdf models have all been applied to the prediction of underexpanded jet flames using both local and threshold quenching, although the conserved scalar models (FCRS and pdf) can not be applied accurately with local quenching. Each of the models gives some variation in the predicted temperature fields as does the particular extinction model employed, but without better experimental data it is not possible to assess which is most realistic. However, far enough downstream of the lift-off plane the solutions become similar.

9) A pseudo nozzle approximation has been developed which replaces an underexpanded sonic jet with a perfectly expanded supersonic jet of increased diameter by assuming an isentropic expansion to ambient conditions and hence eliminating the need to predict a shock cell structure. This pseudo nozzle approximation has been applied to both reacting and non-reacting jets. For non-reacting jets the agreement to the standard computations is very good downstream of the shock containing region, although for highly underexpanded jets the total pressure loss in the normal shock is not accounted for and leads to an increasing overprediction of the potential core length as the pressure ratio increases. For reacting jets, failure to account for total pressure losses in the normal shock leads to an overprediction of the lift-off height.
Appendix A. Staggered Grid

The need for staggered mesh can be demonstrated by considering a finite difference discretisation of the one-dimension momentum equation. Neglecting the viscous and non-linear convection terms this can be approximated by:

\[
\frac{\partial u}{\partial t} = -\frac{\partial P}{\partial x} \tag{A-1}
\]

In finite difference terms, with an explicit time-integration and central spatial discretisation this becomes:

\[
(u_i^{n+1} - u_i^n) \frac{1}{\Delta t} = \frac{1}{2\Delta x} (p_{i+1}^{n+1} - p_{i-1}^{n+1}) \tag{A-2}
\]

The steady-state continuity equation in one-dimension is:

\[
\frac{\partial u}{\partial x} = 0 \tag{A-3}
\]

which can be written as:

\[
\frac{\partial}{\partial x} [u_i^{n+1} - u_i^n] = -\frac{\partial}{\partial x} u^n \tag{A-4}
\]

Substituting from the momentum equation:

\[
(u_i^{n+1} - u_i^n) \frac{1}{\Delta t} = \frac{\partial}{\partial x} p^{n+1} \tag{A-5}
\]

gives a Poisson equation for pressure:

\[
\frac{\partial^2 p^{n+1}}{\partial x^2} = -\frac{1}{\Delta t} \frac{\partial u^n}{\partial x} \tag{A-6}
\]

In finite difference form this becomes:

\[
p_{i+1}^{n+1} - 2p_i^{n+1} + p_{i-1}^{n+1} = \frac{\Delta x}{2\Delta t} (u_i^n - u_{i+1}^n) \tag{A-7}
\]

Hence, the pressure at point \(i\) is not influenced by the velocity at point \(i\), and similarly the velocity at point \(i\) is not affected by the pressure at point \(i\). In this way the pressure and velocity become decoupled. In compressible flow this problem does not exist since density changes will couple together the velocity and pressure. Although the current application here is compressible, the incompressible regions embedded in the flow will suffer from
decoupling and therefore the problem must be addressed. Prevent this decoupling to be taken. The common way to overcome this problem for incompressible flow is to use a staggered grid, where the state variables \( (P, \rho, T \text{ etc.}) \) are stored at the centre of control volumes, whilst the velocities (either \( u \) or \( \rho u \)) are displaced in the relevant direction such that they are located on the main control volume faces, as shown in fig 2-1. This prevents the checkerboard problem since the derivatives can now be calculated over a single control volume. For example:

\[
\left( \frac{\partial u}{\partial x} \right) = \frac{1}{\Delta x} \left( u_{i+\frac{1}{2}} - u_{i-\frac{1}{2}} \right) \tag{A-8}
\]

The momentum equations are now solved over the displaced control volumes such that:

\[
\left( \frac{\partial u}{\partial t} \right)_{i+\frac{1}{2}} = \left( -\frac{\partial P}{\partial x} \right)_{i+\frac{1}{2}} \tag{A-9}
\]

becomes:

\[
\left( u_{i+\frac{1}{2}}^n - u_{i+\frac{1}{2}}^{n+1} \right) \frac{1}{\Delta t} = \frac{1}{\Delta x} \left( P_{i+1}^{n+1} - P_i^{n+1} \right) \tag{A-10}
\]

and

\[
\frac{\partial^2 P^{n+1}}{\partial x^2} = -\frac{1}{\Delta t} \frac{\partial u^n}{\partial x} \tag{A-11}
\]

becomes

\[
P_{i+1}^{n+1} - 2P_i^{n+1} + P_{i-1}^{n+1} = \frac{\Delta x}{2\Delta t} \left( u_{i+\frac{1}{2}}^n - u_{i-\frac{1}{2}}^n \right) \tag{A-12}
\]

Hence there are no decoupling problems since the pressure at point \( i \) is coupled to the velocity at all neighbouring points.
Appendix B. Numerical Diffusion

B.1 Convective Differencing

Two types of convective differencing, central and upwind, are employed for the convective differencing in both the hybrid and TVD schemes. The particular scheme defines how the two type of differencing are combined. In order to understand their accuracy, it is important to assess their numerical properties.

Taylor expansions of the face flux terms gives:

\[
(u\phi)_{+,Y} = (u\phi)_i + \frac{\Delta x}{2} \frac{\partial}{\partial x} (u\phi) + \frac{\Delta x^2}{8} \frac{\partial^2}{\partial x^2} (u\phi) + \frac{\Delta x^3}{48} \frac{\partial^3}{\partial x^3} (u\phi) + \frac{\Delta x^4}{384} \frac{\partial^4}{\partial x^4} (u\phi) + O\Delta x^5 \tag{B-13}
\]

\[
(u\phi)_{-,Y} = (u\phi)_i - \frac{\Delta x}{2} \frac{\partial}{\partial x} (u\phi) + \frac{\Delta x^2}{8} \frac{\partial^2}{\partial x^2} (u\phi) - \frac{\Delta x^3}{48} \frac{\partial^3}{\partial x^3} (u\phi) + \frac{\Delta x^4}{384} \frac{\partial^4}{\partial x^4} (u\phi) + O\Delta x^5 \tag{B-14}
\]

and therefore the central difference operator is:

\[
\frac{(u\phi)_{+,Y} - (u\phi)_{-,Y}}{\Delta x} = \frac{\partial}{\partial x} (u\phi)_i + \frac{\Delta x^2}{24} \frac{\partial^3}{\partial x^3} (u\phi)_i + O\Delta x^4 \tag{B-15}
\]

Hence, central differencing is second order accurate, giving rise only to dispersive truncation errors (odd derivatives), and no dissipative terms (even derivatives).

Subtracting the face flux with central differencing from that with upwind differencing gives:

\[
[UP] - [CD] = \left[ u_{i+Y}^+ \phi_i + u_{i+Y}^- \phi_{i+1} \right] - \left[ \left( u_{i+Y}^+ + u_{i+Y}^- \right) \left( \frac{\phi_i + \phi_{i+1}}{2} \right) \right] = \frac{u_{i+Y}^-}{2} \left( \phi_i - \phi_{i+1} \right) + \frac{u_{i+Y}^+}{2} \left( \phi_{i+1} - \phi_i \right) \tag{B-16}
\]

\[
= -\frac{\Delta x}{2} \left[ u_{i+Y} \left( \frac{\partial}{\partial x} \phi \right) \right]_{i+Y}
\]

and hence the x-direction convective term is:

\[
\frac{(u_{i+Y}^+ \phi_i + u_{i+Y}^- \phi_{i+1}) - (u_{i+Y}^+ \phi_{i+1} + u_{i+Y}^- \phi_i)}{\Delta x} = \frac{\partial}{\partial x} (u\phi)_i - \left[ \frac{\partial}{\partial x} \frac{\Delta x}{2} \left| u \right| \frac{\partial}{\partial x} \phi \right]_{i+Y} + O\Delta x^2 \tag{B-17}
\]

The upwind discretisation is therefore 1st order accurate, giving rise to a dissipative term, which can be viewed as an additional diffusion term with coefficient $\frac{\Delta x}{2} \left| u \right|$. 

322
B.2 Pressure Correction Schemes

B.2.1 Blended Difference Scheme

The term that governs the accuracy of the pressure correction equation is the mass error term. In the steady state:

\[(\rho u)_i^+ = (\rho u)_i^- - \frac{b_j}{2} \left[ (u_i^+ - u_i^-) (\rho_i^+ - \rho_i^-) \right] \]  \hspace{1cm} B-18

Hence the modified form of the mass error term is:

\[ \frac{\partial}{\partial x_j} \rho u_j - \frac{\partial}{\partial x_j} \frac{\Delta x_j}{2} |u_j| \beta_j \frac{\partial \rho}{\partial x_j} + O(\Delta x_j)^2 \]  \hspace{1cm} B-19

The mass error is therefore second order accurate when \( b_j = 0 \), i.e. when the local directional Mach number is less than \( f_2 \). In regions of very high Mach number flow, where \( b_j = 1 \), then the scheme is first order accurate with an added diffusion term with a coefficient (for the \( x \)-direction) of \( \frac{\Delta x_j}{2} |u_j| \).

B.2.2 Retarded Pressure Scheme

The retarded pressure transformation was stated in section 2.6.4 as:

\[ \bar{P}_{i+1} = P_{i+1} + \mu (\bar{P}_{i+1} - \bar{P}) \]  \hspace{1cm} B-20

This can be expressed as:

\[ \bar{P}_{i+1} = P_{i+1} + \mu \Delta x \left( \frac{\partial \bar{P}}{\partial x} \right)_{i+1} \]  \hspace{1cm} B-21

Successive expansions of the retarded pressure derivative gives:
In this way then the retarded pressure gradient can be seen as the real pressure gradient with additional higher derivatives of pressure. Truncating this to second order terms gives:

\[
\frac{\partial \tilde{p}_{i+\frac{1}{2}}}{\partial x} = \frac{\partial P_{i+\frac{1}{2}}}{\partial x} + \mu \Delta x \left( \frac{\partial^2 P}{\partial x^2} \right)_{i+\frac{1}{2}}
\]

Therefore the modified momentum equation with the retarded pressure scheme becomes:

\[
\frac{\partial}{\partial x} \rho u \cdot u - \mu \frac{\partial^2 u}{\partial x^2} = -\left( \frac{\partial P}{\partial x} + \mu \Delta x \frac{\partial^2 P}{\partial x^2} \right)
\]

From the momentum equation we have:

\[
\frac{\partial P}{\partial x} = -\frac{\partial}{\partial x} \rho u \cdot u
\]

and therefore:

\[
\mu \Delta x \frac{\partial^2 P}{\partial x^2} = -\mu \Delta x \rho u \frac{\partial^2 u}{\partial x^2}
\]

and the modified momentum equation becomes:

\[
\frac{\partial}{\partial x} \rho u \cdot u - \mu \frac{\partial^2 u}{\partial x^2} = -\frac{\partial P}{\partial x} + \mu \Delta x \rho u \frac{\partial^2 u}{\partial x^2}
\]

Thus, the effect of the retarded pressure function is the addition of a dissipation term to the momentum equations.
The definition of $\mu$ has important implications for the stability of the scheme. It was shown by Page [140] that the condition $\mu < 0.5$ must be satisfied in order that the influence of upstream pressure decays with distance. The expansion of the retarded pressure gives:

$$P_i = P_i + \mu \Delta x \left( \frac{\partial P}{\partial x} \right)_{i-\frac{1}{2}}$$

$$= P_i + \mu (P_i - P_{i-1})$$

$$= \frac{P_i - \mu P_{i-1}}{1 - \mu}$$

$$= \frac{P_i}{1 - \mu} - \frac{\mu}{1 - \mu} \frac{P_{i-1} - \mu P_{i-2}}{1 - \mu}$$

$$= \frac{P_i}{1 - \mu} - \frac{\mu}{1 - \mu} \frac{P_{i-1}}{1 - \mu} + \frac{\mu^2}{(1 - \mu)^2} \frac{P_{i-2}}{1 - \mu} + \cdots + (-1)^{n+1} \frac{\mu^n P_{i-n}}{(1 - \mu)^{n+1}}$$

For $\mu < 0.5$ the nearest neighbours have larger influence than upstream nodes. This is essential for numerical stability.
References


References


References


References


References


342


