A quasi-dimensional model for performance and emissions predictions in a dual fuel engine

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A Quasi-Dimensional Model for Performance and Emissions Predictions in a Dual Fuel Engine

by

Stephen Johnson

A Doctoral Thesis
submitted in partial fulfilment of the requirements
for the award of Doctor of Philosophy
of
Loughborough University
2012

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A new quasi-dimensional, multi-zone model has been developed to describe the combustion processes occurring inside a dual fuel engine. A dual fuel engine is a compression ignition engine in which a homogeneous lean premixed charge of gaseous fuel and air is ignited by a pilot fuel spray. The atomisation and preparation of the pilot leads to the formation of multiple ignition centres from which turbulent flame fronts develop. The energy release in a dual fuel engine is therefore a combination of that from the combustion of the pilot fuel spray and lean premixed charge. Hence, the dual fuel combustion process is complex, combining elements of both conventional spark and compression ignition engines. The dual fuel engine is beneficial as it can achieve significant reductions in emissions of carbon dioxide (CO$_2$), as well as reducing emissions of oxides of nitrogen (NO$_x$) and particulate matter (PM).

A review of the dual fuel engine modelling literature highlighted the current lack of understanding regarding the coupling between the combustion of the pilot and the premixed combustion of the gaseous charge. Thus, the objective of this research was to provide a new modelling approach to describe the energy release rate in a dual fuel engine.

The model simulates the combustion processes occurring inside the cylinder during the closed part of the engine cycle. The pilot fuel spray is described using a packet model approach, which includes sub-models for spray development and mixing, swirl, spray wall impingement, ignition and combustion. Flame development is described using an original approach in which flame growth is coupled to the burning zones in the cylinder and is simulated using a turbulent entrainment model. Emissions of NO$_x$ and soot are also evaluated.

Predicted in-cylinder pressures are in good agreement with experimental data obtained from a naturally aspirated, in-line, four-cylinder, direct injection diesel engine operating with methane (CH$_4$) as the gaseous fuel. Furthermore, predicted energy release rates show excellent agreement with experimental data. Breakdowns of the energy release rate provide an excellent insight into the progression of combustion in a dual fuel engine. Trends for emissions of NO$_x$ and soot with gaseous substitution ratio are also presented. A sensitivity analysis provides an improved understanding of the underlying physical mechanisms influencing the performance and emissions of a dual fuel engine.
I would like to thank my supervisor, Dr Andy Clarke, for his help, guidance and encouragement during this work. I would also like to thank the research sponsors, the Hardstaff Group, and Mr Trevor Fletcher (Managing Director) for funding the research. Thanks are also extended to Mr Darryl Hylands of the Hardstaff Group for useful feedback regarding the capabilities of the model.

Further thanks are extended to Prof G Hargrave for useful discussions and suggestions regarding the work. I am also grateful to Dr Jill Stewart for allowing me to use her experimental data. Thanks are also extended to Asish Sarangi for proofreading the work.

I would also like to thank friends and colleagues that I have met throughout my time at Loughborough. Finally, I would like to thank my family for their continuous support.
Conference Papers

Journal Papers
# CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Pages</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABSTRACT</td>
<td>iii</td>
</tr>
<tr>
<td>ACKNOWLEDGEMENTS</td>
<td>iv</td>
</tr>
<tr>
<td>LIST OF PUBLICATIONS</td>
<td>v</td>
</tr>
<tr>
<td>NOMENCLATURE</td>
<td>x</td>
</tr>
</tbody>
</table>

## 1 INTRODUCTION

1.1 BACKGROUND | 1
1.2 EMISSIONS LEGISLATION | 2
1.3 COMBUSTION MODELLING | 5
1.4 RESEARCH AIMS AND OBJECTIVES | 6
1.5 THESIS OUTLINE | 6

## 2 THE DUAL FUEL ENGINE

2.1 COMBUSTION PROCESSES IN DUAL FUEL ENGINES | 8
2.1.1 Combustion in Spark Ignition Engines | 8
2.1.2 Combustion in Diesel Engines | 9
2.1.3 Combustion in Dual Fuel Engines | 13
  2.1.3.1 Energy Release in Dual Fuel Engines | 14
  2.1.3.2 Thermal Efficiency | 15
  2.1.3.3 Brake Specific Energy Consumption (BSEC) | 16
  2.1.3.4 Ignition Delay Period | 17
  2.1.3.5 Dual Fuel Emissions | 18
  2.1.3.6 Combustion at Low Load Operating Conditions | 23
  2.1.3.7 Combustion at High Load Operating Conditions | 25
2.2 CONCLUDING SUMMARY | 26

## 3 COMBUSTION MODELLING

3.1 COMBUSTION MODELLING IN DUAL FUEL ENGINES | 28
  3.1.1 Zero-dimensional Models | 29
  3.1.2 Quasi-dimensional Models | 36
  3.1.3 Multi-dimensional Models | 39
  3.1.4 Summary | 42
3.2 ATOMISATION AND SPRAY MODELLING | 44
  3.2.1 Atomisation | 44
### Contents

3.2.1.1 *Primary Atomisation* 48  
3.2.1.2 *Secondary Atomisation* 49  
3.2.2 Spray Characteristics 51  
3.2.2.1 *Spray Tip Penetration* 53  
3.2.2.2 *Spray Cone Angle* 58  
3.2.2.3 *Liquid Breakup Length* 60  
3.2.2.4 *Representative Diameter* 61  
3.2.2.5 *Swirl* 64  
3.2.3 Spray Modelling 65  
3.2.3.1 *Cummins Model* 65  
3.2.3.2 *Packet Models* 69  
3.3 *Ignition Delay Modelling in Dual Fuel Engines* 71  
3.3.1 Ignition Delay Correlations 71  
3.3.2 The Shell Model 74  
3.4 *Concluding Summary* 76  

### 4 Quasi-Dimensional Dual Fuel Model 78  
4.1 *Introduction* 78  
4.2 *Overview of Dual Fuel Model* 79  
4.3 *Pilot Injection Model* 80  
4.3.1 General Description 80  
4.3.2 Injection 83  
4.3.3 Pilot Fuel Spray Development 84  
4.3.3.1 Description of Pilot Fuel Spray 84  
4.3.3.2 Swirl 86  
4.3.3.3 Spray Wall Impingement 89  
4.3.4 Pilot Mixture Preparation 90  
4.3.4.1 Sauter Mean Diameter (SMD) 90  
4.3.4.2 Entrainment 91  
4.3.4.3 Evaporation 92  
4.3.5 Pilot Heat Release 97  
4.4 *Turbulent Flame Propagation Model* 100  
4.4.1 General Description 100  
4.4.2 Premixed Heat Release 101  
4.4.3 Laminar Burning Velocity 105  
4.5 *Heat Transfer* 106
4.5.1 Convection 107
4.5.2 Radiation 108
4.5.3 Zonal Heat Transfer 109

4.6 EQUILIBRIUM THERMODYNAMICS 110
4.6.1 Methodology of Damköhler and Edse 111
4.6.2 Consideration of Atomic Nitrogen 115
4.6.3 Method of Solution 116

4.7 EMISSIONS FORMATION 118
4.7.1 Nitric Oxide (NO) 118
4.7.2 Particulate Matter (PM) 120

4.8 NUMERICAL SOLUTION 122
4.8.1 General Description 122
4.8.2 Conservation and State Equations 126

4.9 CONCLUDING SUMMARY 128

5 MODEL CALIBRATION AND VALIDATION 129
5.1 INTRODUCTION 129

5.2 OVERVIEW OF ENGINE FACILITY 130
5.2.1 Test Engine 130
5.2.2 Test Bed Facility 131
5.2.3 Emissions Measurement 132
5.2.3.1 Oxides of Nitrogen (NOx) 132
5.2.3.2 Particulate Matter (PM) 133

5.3 EXPERIMENTAL ANALYSIS 133
5.3.1 Energy Release Analysis 133
5.3.2 Start of Combustion (SOC) 135

5.4 MODEL CALIBRATION AND VALIDATION 136
5.4.1 Model Calibration 138
5.4.1.1 Calibration of Pilot Injection Model 138
5.4.1.2 Calibration of Turbulent Entrainment Model 143
5.4.2 Model Validation 146
5.4.2.1 Pressure and Energy Release Diagrams 148
5.4.2.2 Emissions of Nitric Oxide and Soot 162

5.5 CONCLUDING SUMMARY 167
6 SENSITIVITY ANALYSIS

6.1 INTRODUCTION

6.2 SENSITIVITY ANALYSIS

6.2.1 Effect of Input Parameters

6.2.1.1 Effect of Number of Spray Zones

6.2.1.2 Effect of Swirl Ratio

6.2.1.3 Effect of In-cylinder Temperature at Inlet Valve Closure

6.2.2 Effect of Parameters Controlling the Rate of Entrainment into the Pilot Fuel Spray

6.2.3 Effect of Parameters Controlling the Rate of Entrainment and Burning in the Premixed Burning Zone

6.2.3.1 Effect of Integral Length Scale

6.2.3.2 Effect of Turbulence Intensity

6.2.3.3 Effect of Characteristic Burning Time

6.3 DISCUSSION

6.4 CONCLUDING SUMMARY

7 CONCLUSIONS AND FURTHER WORK

7.1 CONCLUSIONS

7.2 RECOMMENDATIONS FOR FURTHER WORK

REFERENCES

APPENDIX A: LIQUID AND GASEOUS PROPERTIES

APPENDIX B: THERMODYNAMIC PROPERTIES

APPENDIX C: EQUILIBRIUM CONSTANTS

APPENDIX D: OVERVIEW OF GRAPHICAL USER INTERFACE
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>Nozzle orifice area (m²)</td>
</tr>
<tr>
<td>$a$</td>
<td>Number of moles of stoichiometric air (kmols)</td>
</tr>
<tr>
<td>$B$</td>
<td>Branching agent</td>
</tr>
<tr>
<td>$b$</td>
<td>Radius (m)</td>
</tr>
<tr>
<td>$c_a$</td>
<td>Orifice area contraction coefficient</td>
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<tr>
<td>$C_d$</td>
<td>Discharge coefficient</td>
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<tr>
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<td>Isobaric specific heat (kJ.kg⁻¹K⁻¹)</td>
</tr>
<tr>
<td>$C_s$</td>
<td>Soot concentration (mg.m⁻³)</td>
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<tr>
<td>$C_v$</td>
<td>Isochoric specific heat (kJ.kg⁻¹K⁻¹)</td>
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<td>Orifice velocity coefficient</td>
</tr>
<tr>
<td>$D$</td>
<td>Diameter (m)</td>
</tr>
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<tr>
<td>$D_{ef}$</td>
<td>Effective hydraulic diameter (m)</td>
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<td>$D_i$</td>
<td>Median diameter of size range (m)</td>
</tr>
<tr>
<td>$D_o$</td>
<td>Sac hole diameter (m)</td>
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<td>$E$</td>
<td>Activation energy (kJ.kmol⁻¹)</td>
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<td>$f_p$</td>
<td>Gaseous fuel concentration (%)</td>
</tr>
<tr>
<td>$h$</td>
<td>Combustion chamber height (m)</td>
</tr>
<tr>
<td>$h_f$</td>
<td>Specific enthalpy (kJ.kg⁻¹)</td>
</tr>
<tr>
<td>$h_f$</td>
<td>Latent heat of evaporation (kJ.kg⁻¹)</td>
</tr>
<tr>
<td>$h_c$</td>
<td>Convective heat transfer coefficient (kW.m⁻²K⁻¹)</td>
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<tr>
<td>$h_c^*$</td>
<td>Corrected convective heat transfer coefficient (kW.m⁻²K⁻¹)</td>
</tr>
<tr>
<td>$h_d$</td>
<td>Mass transfer coefficient (m.s⁻¹)</td>
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<td>Corrected mass transfer coefficient (m.s⁻¹)</td>
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<td>Enthalpy (kJ.kmol⁻¹)</td>
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<td>Equilibrium constant of formation of species</td>
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<td>Definition</td>
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<tr>
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<td>Rate coefficient (\text{mol}^{1-n}\text{cm}^{3n-3}\text{s}^{-1}), for (n)th order reaction</td>
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<td>Rate coefficient (\text{g-C.cm}^2\text{s}^{-1}\text{atm}^{-1}), (\text{g-C.cm}^2\text{s}^{-1}\text{atm}^{-1})</td>
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<td>Absorption coefficient (\text{m}^{-1})</td>
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</tr>
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<td>Integral length scale (m)</td>
</tr>
<tr>
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</tr>
<tr>
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<td>Nozzle length (m)</td>
</tr>
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<td>(LHV)</td>
<td>Lower heating value (\text{kJ.kg}^{-1})</td>
</tr>
<tr>
<td>(L_b)</td>
<td>Jet breakup length (m)</td>
</tr>
<tr>
<td>(L_c)</td>
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<td>(N_d)</td>
<td>Number of droplets</td>
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<td>(N_i)</td>
<td>Number of drops in size range</td>
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<td>(n)</td>
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</tr>
<tr>
<td>(Pr)</td>
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<td>(p)</td>
<td>Partial pressure (kPa)</td>
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<td>(Q)</td>
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</tr>
<tr>
<td></td>
<td>Heat transfer (kJ)</td>
</tr>
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<td></td>
<td>Momentum (\text{kg.m.s}^{-1})</td>
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<td>Volume flow rate (\text{m}^3\text{stroke}^{-1})</td>
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<td>RH</td>
<td>Fuel</td>
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<tr>
<td>(R)</td>
<td>Gas constant (\text{kJ.kg}^{-1}\text{K}^{-1})</td>
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<td>Reaction rate variable (\text{s}^{-1})</td>
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**NOMENCLATURE**

- Reaction rate variable (g-C.cm\(^{-2}\)s\(^{-1}\))
- \(Re\) Reynolds number
- \(R_s\) Swirl ratio
- \(R_{tot}\) Total oxidation rate (g-C.cm\(^{-2}\)s\(^{-1}\))
- \(R_u\) Universal gas constant (8.314 kJ.kmol\(^{-1}\)K\(^{-1}\))
- \(r\) Crankshaft throw (m)
- Nozzle entrance radius (m)
- Radial coordinate (m)
- \(r_c\) Compression ratio
- \(S\) Spray penetration (m)
- \(Sc\) Schmidt number
- \(Sh\) Sherwood number
- \(S_L\) Laminar burning velocity (m.s\(^{-1}\))
- \(S_p\) Mean piston speed (m.s\(^{-1}\))
- \(S_t\) Tangential displacement (m)
- \(S_{uo}\) Reference laminar burning velocity (cm.s\(^{-1}\))
- \(s\) Instantaneous stroke (m)
- \(T\) Temperature (K)
- \(t\) Time (s)
- \(t_b\) Breakup time (s)
- \(U\) Internal energy (kJ)
- \(U'\) Turbulence intensity (m.s\(^{-1}\))
- \(V\) Velocity (m.s\(^{-1}\))
- Volume (m\(^3\))
- \(W\) Work (kJ)
- \(We\) Weber number
- \(w\) Weight factor
- \(x\) Axial coordinate (m)
- Mass fraction
- Stoichiometric coefficient
- \(y\) Mole fraction
- \# Number

**Greek Symbols**

- \(\alpha\) Stoichiometric coefficient
- \(\beta\) Angle from nozzle hole axis to cylinder head (degrees)
### NOMENCLATURE

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<td>$\eta$</td>
<td>Stoichiometric coefficient</td>
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<td>Apparent grey emissivity</td>
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<td>Surface tension (N.m⁻¹)</td>
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### Subscripts

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<tr>
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<td>Unburned zone</td>
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NOMENCLATURE

\[\begin{align*}
  v & \quad \text{Vapour} \\
  w & \quad \text{Wall} \\
  x & \quad \text{Number of carbon atoms} \\
  y & \quad \text{Number of atomic hydrogen atoms} \\
  z & \quad \text{Spray zone} \\
  0 & \quad \text{Initial/Reference condition}
\end{align*}\]

\textit{Superscripts}
\begin{itemize}
  \item \(^+\) \quad \text{Forward}
  \item \(-\) \quad \text{Reverse}
  \item \(\rightarrow\) \quad \text{Vector}
\end{itemize}

\textit{Abbreviations}
\begin{itemize}
  \item AFR \quad \text{Air fuel ratio}
  \item ALPING-LTC \quad \text{Advanced low pilot-ignited natural gas low-temperature combustion}
  \item ATDC \quad \text{After top dead centre}
  \item BDC \quad \text{Bottom dead centre}
  \item BMEP \quad \text{Brake mean effective pressure (kPa)}
  \item BSEC \quad \text{Brake specific energy consumption (kJ.kW}^{-1}.h^{-1})
  \item CA \quad \text{Crank angle}
  \item CI \quad \text{Compression ignition}
  \item CN \quad \text{Cetane number}
  \item EGR \quad \text{Exhaust gas recirculation}
  \item ELR \quad \text{European load response}
  \item ERR \quad \text{Energy release rate (J.CA}^{-1})
  \item ESC \quad \text{European stationary cycle}
  \item ETC \quad \text{European transient cycle}
  \item EVO \quad \text{Exhaust valve opening}
  \item FSN \quad \text{Filter smoke number}
  \item GUI \quad \text{Graphical user interface}
  \item HCCI \quad \text{Homogeneous charge compression ignition}
  \item IDI \quad \text{Indirect injection}
  \item IVC \quad \text{Inlet valve closure}
  \item LPG \quad \text{Liquid petroleum gas}
  \item NEDC \quad \text{New European driving cycle}
  \item NMHC \quad \text{Non-methane hydrocarbons}
\end{itemize}
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO&lt;sub&gt;x&lt;/sub&gt;</td>
<td>Oxides of nitrogen</td>
</tr>
<tr>
<td>PCCI</td>
<td>Premixed charge compression ignition</td>
</tr>
<tr>
<td>PM</td>
<td>Particulate matter</td>
</tr>
<tr>
<td>PN</td>
<td>Particle number</td>
</tr>
<tr>
<td>RON</td>
<td>Research octane number</td>
</tr>
<tr>
<td>SCR</td>
<td>Selective catalytic reduction</td>
</tr>
<tr>
<td>SI</td>
<td>Spark ignition</td>
</tr>
<tr>
<td>SMD</td>
<td>Sauter mean diameter ( \left( D_{32} \right) ) (( \mu )m)</td>
</tr>
<tr>
<td>SOC</td>
<td>Start of combustion</td>
</tr>
<tr>
<td>SOI</td>
<td>Start of injection</td>
</tr>
<tr>
<td>SPICE</td>
<td>Simulation program for internal combustion engines</td>
</tr>
<tr>
<td>TDC</td>
<td>Top dead centre</td>
</tr>
<tr>
<td>uHC</td>
<td>Unburned hydrocarbons</td>
</tr>
<tr>
<td>VCO</td>
<td>Valve covered orifice</td>
</tr>
<tr>
<td>WHSC</td>
<td>World heavy duty steady state cycle</td>
</tr>
<tr>
<td>WHTC</td>
<td>World heavy duty transient cycle</td>
</tr>
</tbody>
</table>

**Chemical Symbols**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>Carbon</td>
</tr>
<tr>
<td>CH&lt;sub&gt;4&lt;/sub&gt;</td>
<td>Methane</td>
</tr>
<tr>
<td>C&lt;sub&gt;12&lt;/sub&gt;H&lt;sub&gt;26&lt;/sub&gt;</td>
<td>n-dodecane</td>
</tr>
<tr>
<td>C&lt;sub&gt;13&lt;/sub&gt;H&lt;sub&gt;28&lt;/sub&gt;</td>
<td>n-tridecane</td>
</tr>
<tr>
<td>CO</td>
<td>Carbon monoxide</td>
</tr>
<tr>
<td>CO&lt;sub&gt;2&lt;/sub&gt;</td>
<td>Carbon dioxide</td>
</tr>
<tr>
<td>H</td>
<td>Atomic hydrogen</td>
</tr>
<tr>
<td>H&lt;sub&gt;2&lt;/sub&gt;</td>
<td>Hydrogen</td>
</tr>
<tr>
<td>H&lt;sub&gt;2&lt;/sub&gt;O</td>
<td>Water</td>
</tr>
<tr>
<td>N</td>
<td>Atomic nitrogen</td>
</tr>
<tr>
<td>N&lt;sub&gt;2&lt;/sub&gt;</td>
<td>Nitrogen</td>
</tr>
<tr>
<td>NH&lt;sub&gt;3&lt;/sub&gt;</td>
<td>Ammonia</td>
</tr>
<tr>
<td>NO</td>
<td>Nitric oxide</td>
</tr>
<tr>
<td>NO&lt;sub&gt;2&lt;/sub&gt;</td>
<td>Nitrogen dioxide</td>
</tr>
<tr>
<td>N&lt;sub&gt;2&lt;/sub&gt;O</td>
<td>Nitrous oxide</td>
</tr>
<tr>
<td>O</td>
<td>Atomic oxygen</td>
</tr>
<tr>
<td>O&lt;sub&gt;2&lt;/sub&gt;</td>
<td>Oxygen</td>
</tr>
<tr>
<td>O&lt;sub&gt;3&lt;/sub&gt;</td>
<td>Ozone</td>
</tr>
<tr>
<td>OH</td>
<td>Hydroxyl</td>
</tr>
</tbody>
</table>
CHAPTER 1
INTRODUCTION

1.1 BACKGROUND

The diesel fuelled compression ignition engine has found widespread use in the transport sector due to its high fuel economy and low exhaust emission characteristics relative to conventional spark ignition engines. Currently, exhaust emissions in Europe are legislated by the Euro V standards. The most challenging of these emissions limits are for oxides of nitrogen (NO\textsubscript{x}) and particulate matter (PM). In recent years, carbon dioxide (CO\textsubscript{2}) emissions have grown in importance due to their link with climate change. There is therefore a need to investigate technologies that have the potential to reduce CO\textsubscript{2} emissions, whilst adhering to current and future emissions standards.

The dual fuel concept has been employed intermittently at times when oil supplies have become scarce or as a method of reducing operational fuelling costs. In recent years, research interest has grown due to ever stringent emissions legislation. A dual fuel engine is a compression ignition engine in which a homogeneous lean premixed charge of gaseous fuel and air is formed inside the cylinder. Typically, the introduction of the gaseous fuel is achieved either through a mixer or by port fuel injection. In recent years, direct injection of the gaseous fuel has also been employed. The lean premixed charge is ignited by a small quantity of diesel, the pilot fuel spray, which is injected towards the end of the compression stroke. The pilot fuel spray atomises into small droplets that penetrate across the cylinder, evaporating and mixing with the high temperature in-cylinder charge. Following the ignition delay period, the pilot fuel spray ignites and flame propagation proceeds from multiple ignition sites. The energy release in a dual fuel engine is therefore a combination of that from the diesel and gaseous fuel. The gaseous fuel employed in dual fuel engines is typically natural gas. The main reasons for this are its availability and inherently cleaner combustion (Kowalewicz and Wojtyniak, 2005). On an energy basis, the stoichiometric combustion of methane (CH\textsubscript{4}), which is the main constituent of natural gas, produces less CO\textsubscript{2} than the stoichiometric combustion of diesel, since methane has a lower carbon-to-hydrogen ratio. The high self-ignition temperature of natural gas also makes it suitable for the high compression ratios used in dual fuel engines.
The dual fuel engine has been employed in a number of applications including: heavy-duty trucks, buses, railway locomotives, marine vessels, and construction and agricultural equipment. Stationary applications include electric power generators, pumps and cogeneration sets. In recent years, there has been increased interest in the haulage sector owing to the reduced costs associated with fuel prices. At this time, the application of dual fuelling in the transport sector is currently by aftermarket products. Because of this trend, gas admission by direct injection is not considered in this work due to its added cost and complexity relative to conventional mixing methods.

The dual fuel engine has a number of advantages relative to diesel engines. Engine-out emissions, specifically CO$_2$, NO$_x$ and PM are improved. Moreover, it retains the thermal efficiency of the diesel engine at full load. Relative to conventional spark ignition engines, the use of a pilot injection provides more reliable ignition and faster combustion of the gaseous charge. This allows much leaner mixtures to be used, thus improving thermal efficiency. Cyclic variability is also reduced (Karim et al., 1988). The main obstacles associated with dual fuel engines are poor low load performance, knock limited power output and increased emissions of carbon monoxide (CO) and unburned hydrocarbons (uHC). Emissions of CO and uHC are particularly high at low load conditions, since the lean gaseous mixture employed under these conditions is unable to support flame propagation. Hence, diesel operation is typically retained at low load and idling conditions.

1.2 EMISSIONS LEGISLATION

In Europe, emissions from vehicles are regulated by European Union Regulations (formerly Directives), which give acceptable limits for engine-out emissions. Emissions from road vehicles are divided between light-duty vehicles (passenger cars and light commercial vehicles) and heavy-duty vehicles (trucks and buses). Table 1.1 shows the progression of the emissions standards for both spark ignition (SI) and compression ignition (CI) engines in light commercial vehicle applications since the year 2000 (Euro III & IV: Directive 98/69/EC, Euro V & VI: EC No 692/2008). The table illustrates the increasingly stringent emissions limits applied to NO$_x$ and PM. For Euro V and VI, a particle number (PN) limit has also been introduced to the CI standards, which must be met in addition to the PM limits. This has been added to control the number of fine particles in the exhaust. Engines are tested against these standards.
<table>
<thead>
<tr>
<th>Standard</th>
<th>Date</th>
<th>Class (Mass Limit / (kg))</th>
<th>CO</th>
<th>uHC</th>
<th>NMHC</th>
<th>NOx</th>
<th>uHC+NOx</th>
<th>PM</th>
<th>PN</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>SI (g·km⁻¹)</td>
<td>CI (g·km⁻¹)</td>
<td>SI (g·km⁻¹)</td>
<td>CI (g·km⁻¹)</td>
<td>SI (g·km⁻¹)</td>
<td>CI (g·km⁻¹)</td>
<td>SI (g·km⁻¹)</td>
</tr>
<tr>
<td>Euro III</td>
<td>2000 I</td>
<td>(≤ 1305)</td>
<td>2.30</td>
<td>0.64</td>
<td>0.20</td>
<td>-</td>
<td>-</td>
<td>0.15</td>
<td>0.50</td>
</tr>
<tr>
<td></td>
<td>2001 II</td>
<td>(1306 - 1760)</td>
<td>4.17</td>
<td>0.80</td>
<td>0.25</td>
<td>-</td>
<td>-</td>
<td>0.18</td>
<td>0.65</td>
</tr>
<tr>
<td></td>
<td>2001 III</td>
<td>(&gt; 1760)</td>
<td>5.22</td>
<td>0.95</td>
<td>0.29</td>
<td>-</td>
<td>-</td>
<td>0.21</td>
<td>0.78</td>
</tr>
<tr>
<td>Euro IV</td>
<td>2005 I</td>
<td>(≤ 1305)</td>
<td>1.00</td>
<td>0.50</td>
<td>0.10</td>
<td>-</td>
<td>-</td>
<td>0.08</td>
<td>0.25</td>
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<tr>
<td></td>
<td>2006 II</td>
<td>(1306 - 1760)</td>
<td>1.81</td>
<td>0.63</td>
<td>0.13</td>
<td>-</td>
<td>-</td>
<td>0.10</td>
<td>0.33</td>
</tr>
<tr>
<td></td>
<td>2006 III</td>
<td>(&gt; 1760)</td>
<td>2.27</td>
<td>0.74</td>
<td>0.16</td>
<td>-</td>
<td>-</td>
<td>0.11</td>
<td>0.39</td>
</tr>
<tr>
<td>Euro V</td>
<td>2009 I</td>
<td>(≤ 1305)</td>
<td>1.00</td>
<td>0.50</td>
<td>0.10</td>
<td>-</td>
<td>-</td>
<td>0.068</td>
<td>0.180</td>
</tr>
<tr>
<td></td>
<td>2010 II</td>
<td>(1306 - 1760)</td>
<td>1.81</td>
<td>0.63</td>
<td>0.13</td>
<td>-</td>
<td>-</td>
<td>0.090</td>
<td>0.235</td>
</tr>
<tr>
<td></td>
<td>2010 III</td>
<td>(&gt; 1760)</td>
<td>2.27</td>
<td>0.74</td>
<td>0.16</td>
<td>-</td>
<td>-</td>
<td>0.108</td>
<td>0.280</td>
</tr>
<tr>
<td>Euro VI</td>
<td>2014 I</td>
<td>(≤ 1305)</td>
<td>1.00</td>
<td>0.50</td>
<td>0.10</td>
<td>-</td>
<td>-</td>
<td>0.068</td>
<td>0.080</td>
</tr>
<tr>
<td></td>
<td>2015 II</td>
<td>(1306 - 1760)</td>
<td>1.81</td>
<td>0.63</td>
<td>0.13</td>
<td>-</td>
<td>-</td>
<td>0.090</td>
<td>0.105</td>
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<tr>
<td></td>
<td>2015 III</td>
<td>(&gt; 1760)</td>
<td>2.27</td>
<td>0.74</td>
<td>0.16</td>
<td>-</td>
<td>-</td>
<td>0.108</td>
<td>0.125</td>
</tr>
</tbody>
</table>

(1) Applicable to vehicles with direct injection
using the New European Driving Cycle (NEDC). This is completed on a chassis dynamometer and includes four test stages: an urban drive cycle, extra urban drive cycle, warm idle tailpipe CO test and crankcase emission test.

Tables 1.2, 1.3 and 1.4 show the progression of the emissions standards for heavy-duty vehicles since the year 2000 (Euro III, IV & V: Directive 2005/55/EC, Euro VI: EU No 582/2011). As stated previously, the most challenging of these emissions limits are for NO\textsubscript{x} and PM. For Euro VI, an ammonia (NH\textsubscript{3}) limit has also been introduced. The purpose of this limit is to control the emission of NH\textsubscript{3} when employing Selective Catalytic Reduction (SCR) systems to reduce NO\textsubscript{x}. Emissions at Euro III, IV and V are tested over three standard test cycles: the European Stationary Cycle (ESC), the European Load Response (ELR) and the European Transient Cycle (ETC). The ESC is completed on an engine dynamometer over a sequence of 13 steady-state modes. The ELR is also completed on an engine dynamometer and is used for the purpose of measuring smoke emissions. The ETC exists as both a chassis and engine dynamometer test. It consists of three sequential test stages: urban driving, rural driving and motorway driving. For Euro VI, emissions will be tested using the World Heavy Duty Steady State Cycle (WHSC) and the World Heavy Duty Transient Cycle (WHTC).

The small pilot fuel quantity and lean gaseous mixture employed in the dual fuel engine are beneficial to the reduction of NO\textsubscript{x} and PM emissions. The combustion of the lean gaseous mixture contributes little NO\textsubscript{x} due to the reduced combustion temperatures, with the main source of NO\textsubscript{x} being due to the relatively small pilot. Particulate emissions are also reduced due to the relative size of the pilot, with the soot that is produced largely oxidised during the expansion stroke.

**Table 1.2 – Emissions standards for diesel heavy-duty vehicles (ESC and ELR)**

<table>
<thead>
<tr>
<th>Standard</th>
<th>Date</th>
<th>CO (g.kW\textsuperscript{-1}h\textsuperscript{-1})</th>
<th>uHC (m\textsuperscript{-1})</th>
<th>NO\textsubscript{x} (g.kW\textsuperscript{-1}h\textsuperscript{-1})</th>
<th>PM (g.kW\textsuperscript{-1}h\textsuperscript{-1})</th>
<th>Smoke (m\textsuperscript{3})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Euro III</td>
<td>2000</td>
<td>2.1</td>
<td>0.66</td>
<td>5.0</td>
<td>0.10</td>
<td>0.13\textsuperscript{(1)}</td>
</tr>
<tr>
<td>Euro IV</td>
<td>2005</td>
<td>1.5</td>
<td>0.46</td>
<td>3.5</td>
<td>0.02</td>
<td>0.5</td>
</tr>
<tr>
<td>Euro V</td>
<td>2008</td>
<td>1.5</td>
<td>0.46</td>
<td>2.0</td>
<td>0.02</td>
<td>0.5</td>
</tr>
</tbody>
</table>

\textsuperscript{(1)} For engines having a swept volume of less than 0.75 dm\textsuperscript{3} per cylinder and a rated power speed of more than 3000 rpm.
### Table 1.3 – Emissions standards for diesel and gas heavy-duty vehicles (ETC)

<table>
<thead>
<tr>
<th>Standard</th>
<th>Date</th>
<th>CO</th>
<th>NMHC</th>
<th>CH₄ (¹)</th>
<th>NOₓ</th>
<th>PM (²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Euro III</td>
<td>2000</td>
<td>5.45</td>
<td>0.78</td>
<td>1.6</td>
<td>5.0</td>
<td>0.16</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.21 (³)</td>
</tr>
<tr>
<td>Euro IV</td>
<td>2005</td>
<td>4.00</td>
<td>0.55</td>
<td>1.1</td>
<td>3.5</td>
<td>0.03</td>
</tr>
<tr>
<td>Euro V</td>
<td>2008</td>
<td>4.00</td>
<td>0.55</td>
<td>1.1</td>
<td>2.0</td>
<td>0.03</td>
</tr>
</tbody>
</table>

(¹) For natural gas engines only
(²) Not applicable for gas fuelled engines
(³) For engines having a swept volume of less than 0.75 dm³ per cylinder and a rated power speed of more than 3000 rpm

### Table 1.4 – Euro VI (2013) emissions standards for diesel and gas heavy-duty vehicles (WHSC and WHTC)

<table>
<thead>
<tr>
<th></th>
<th>CO</th>
<th>uHC</th>
<th>NMHC</th>
<th>CH₄</th>
<th>NOₓ</th>
<th>PM</th>
<th>NH₃</th>
<th>PN</th>
</tr>
</thead>
<tbody>
<tr>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>WHSC (CI)</td>
<td>1.5</td>
<td>0.13</td>
<td>-</td>
<td>-</td>
<td>0.40</td>
<td>0.01</td>
<td>10</td>
<td>8·10¹¹</td>
</tr>
<tr>
<td>WHTC (CI)</td>
<td>4.0</td>
<td>0.16</td>
<td>-</td>
<td>-</td>
<td>0.46</td>
<td>0.01</td>
<td>10</td>
<td>6·10¹¹</td>
</tr>
<tr>
<td>WHTC (SI)</td>
<td>4.0</td>
<td></td>
<td>0.16</td>
<td>0.5</td>
<td>0.46</td>
<td>0.01</td>
<td>10</td>
<td></td>
</tr>
</tbody>
</table>

(¹) Limit to be defined

### 1.3 COMBUSTION MODELLING

Mathematical models are an important part of modern engineering practice. In the study of internal combustion engines, combustion models enable the development of a more complete understanding of the combustion processes, the identification of key parameters affecting the combustion processes and the prediction of performance and emissions trends over different operating ranges. A suitable combustion model allows the determination of quantities that are difficult to measure experimentally and can provide a rational basis for engine development. This can help reduce prohibitive development time and cost. Combustion models are typically classified as zero-dimensional, quasi-dimensional or multi-dimensional. These models vary in complexity, but are interested in the description of the combustion processes on the basis of physical and chemical phenomena.

The dual fuel combustion process is complex, combining elements of both conventional spark ignition and diesel combustion. To date, several numerical studies have been completed to investigate the performance and emissions of dual fuel
engines. In general, these models are qualitative in nature. A review of these models identified that there is currently limited understanding regarding the interaction between the ignition and combustion of the pilot and the premixed combustion of the gaseous charge. Therefore, there is scope to improve the understanding of the progression of these two processes.

1.4 RESEARCH AIMS AND OBJECTIVES

The dual fuel concept offers a number of benefits in terms of engine performance and emissions, but at present the complex combustion processes occurring inside the cylinder are not well understood. Therefore, there is a need to develop tools to advance the current understanding of the dual fuel combustion processes. The aim of the research is to develop a predictive engine model to simulate the in-cylinder pressures and rates of energy release in a dual fuel engine and determine quantitative/qualitative trends for engine-out emissions.

The main objectives of the research are as follows:

- To develop a validated engine model based on phenomenological sub-models that describe the physical and chemical processes occurring inside the cylinder.
- To implement an engine model that can simulate the combustion processes in both a diesel and dual fuel engine.
- To develop a model that can accurately predict the energy release rate in a dual fuel engine.
- To provide a fundamental understanding of the development of premixed gaseous combustion during and after the ignition of the pilot.
- To provide quantitative trends of engine-out emissions for a range of engine operating conditions.

1.5 THESIS OUTLINE

The research contained herein is organised into seven separate chapters. The following gives a brief overview of each chapter.
Chapter 2 contains a review of the dual fuel engine literature. The chapter describes the combustion processes associated with the dual fuel engine with specific focus on the energy release rate, thermal efficiency, brake specific energy consumption (BSEC), ignition delay period and engine-out emissions. The main obstacles associated with dual fuel combustion under low and high load operating conditions are also discussed.

Chapter 3 presents a critical review of the current state of dual fuel combustion modelling. The chapter also discusses atomisation and spray modelling, and ignition delay modelling in dual fuel engines. The chapter concludes with a summary of the limitations of the present models available in the literature and the approach and reasoning for the current work.

Chapter 4 describes the development of a new quasi-dimensional, multi-zone model to describe the combustion processes occurring inside a dual fuel engine. The main focus of the chapter is the description of the spray model concept and the coupling of the combustion of the pilot and premixed combustion of the gaseous charge. Finally, the modelling of the pollutants formation is described and an overview of the numerical solution is presented.

Chapter 5 discusses the calibration and validation of the dual fuel combustion model. The calibration and validation of the model were completed using a naturally aspirated, in-line, four-cylinder, direct injection diesel engine operating with methane as the gaseous fuel. The model was first calibrated against baseline diesel and dual fuel cases. The predictive capability of the model was then assessed by comparing model predictions across a range of gaseous substitution ratios at 1500 rpm under 100 and 50 percent load conditions.

Chapter 6 highlights the underlying physical mechanisms that influence the performance and emissions of a dual fuel engine, through the employment of a sensitivity analysis. Here, the effect of the model inputs/ constants on the prediction of the magnitude and timing of peak in-cylinder pressure, the ignition delay period and emissions of nitric oxide (NO) and soot are assessed.

Chapter 7 concludes the research; the contributions to knowledge are highlighted and recommendations for future work are made.
2.1 COMBUSTION PROCESSES IN DUAL FUEL ENGINES

Combustion processes have an important influence on the performance and emissions of internal combustion engines. Combustion in dual fuel engines includes aspects of both conventional spark ignition and diesel combustion with elements that are unique to dual fuel operation (Turner and Weaver, 1994). In a dual fuel engine, gaseous fuel and air are ingested into the cylinder to form a homogeneous mixture, as in a conventional spark ignition engine. Towards the end of the compression stroke, a small amount of diesel, the pilot fuel spray, is injected into the cylinder. Ignition of the pilot occurs due to the preparation of a combustible mixture and increased temperatures in the cylinder, as in a diesel engine. Flame propagation then proceeds from multiple ignition sites through the premixed charge. This section describes the combustion processes associated with dual fuel engines.

2.1.1 Combustion in Spark Ignition Engines

In a conventional spark ignition engine, a premixed charge is ingested into the cylinder and compressed. As the piston approaches top dead centre (TDC), the charge is ignited by a spark produced by the electrical breakdown of the mixture between the electrodes of the spark plug. A flame kernel forms and the development of a turbulent flame front is established. Termination of the flame front occurs at the cylinder walls, where heat transfer and reduced turbulence levels cause the flame speed to decrease. In this type of engine, the load is controlled by adjusting the mass of mixture ingested into the cylinder via a throttle. At low loads, this is detrimental to the mechanical efficiency of the engine, as the pumping work is increased.

The spark ignition engine can be described using the ideal air standard Otto cycle, for which the thermal efficiency ($\eta_{th,otto}$) is given by

$$\eta_{th,otto} = 1 - \frac{1}{r_c^{k-1}}$$  \hspace{1cm} (2.1)

where $r_c$ is the compression ratio and $k$ is the specific heat ratio. Thus, the thermal efficiency of a spark ignition engine can be improved by increasing the compression ratio.
ratio. In practice, the compression ratio is limited by knock, whereby uncontrolled combustion of the end gases can cause severe damage to the engine. An increased specific heat ratio, which in fuel-air mixtures can be achieved by employing excess air, can also enhance the thermal efficiency.

Higher compression ratios can be achieved by employing lean burn concepts. These promote increased levels of turbulence in the cylinder, allowing leaner mixtures to be burnt, thus reducing the combustion temperature and occurrence of knock. The disadvantage of these types of systems is the high hydrocarbon emissions due to large squish areas and poor surface-to-volume ratios (Stone, 1999).

In conventional spark ignition engines, the emissions of interest are NO\textsubscript{x}, uHC and CO. NO\textsubscript{x} is formed at high temperatures in the burned gases behind the flame front. The formation of NO\textsubscript{x} is also a strong function of oxygen availability and peaks for mixtures just lean of stoichiometric combustion. Furthermore, NO\textsubscript{x} formation is a function of time, with NO\textsubscript{x} emissions increasing for reduced flame speeds (Stone, 1999). Emissions of uHC are a minimum in the presence of excess oxygen since the fuel can readily burn to completion. For increasingly leaner mixtures, emissions of uHC increase due to incomplete combustion caused by partial burning or misfire. Similarly, for increasingly richer mixtures emissions of uHC increase because there is insufficient oxygen available for complete combustion. Other sources of uHC include the flame quench layer, crevice volumes and the oil film. Emissions of CO are primarily caused by the combustion of rich mixtures in which the total oxidation of carbon to carbon dioxide cannot be achieved. Emissions of CO are also present in lean mixtures due to the effects of dissociation caused by high combustion temperatures.

### 2.1.2 Combustion in Diesel Engines

In diesel engines, air is ingested into the cylinder and compressed to high pressures and temperatures. The diesel fuel is injected towards the end of the compression stroke. This atomises into small droplets that penetrate across the cylinder, evaporating and mixing with the high temperature in-cylinder air. Diesel engine combustion can be divided into four phases, as shown in Figure 2.1.
These can be described as follows:

- **Ignition delay.** The period between the start of injection (SOI) and the start of combustion (SOC). During this period both physical and chemical processes take place. The physical processes include the atomisation of the fuel spray, the evaporation of the fuel droplets and the mixing of the fuel vapour and air. The chemical processes include the pre-ignition reactions of the fuel vapour-air mixture which lead to autoignition.

- **Premixed combustion phase.** In this phase, the fuel vapour-air mixture prepared to within combustible limits during the ignition delay period burns rapidly, causing a rapid increase in in-cylinder pressure.

- **Mixing-controlled combustion phase.** Once the initial fuel vapour-air mixture has been consumed, diffusion combustion occurs at the rate at which the fuel-air mixture is prepared.

- **Late combustion phase.** Energy release continues during the expansion stroke due to the combustion of any remaining fuel. A small fraction of energy release may also occur due to the oxidation of soot (Heywood, 1988).

In this type of engine, the load is controlled by varying the amount of fuel injected. Thus, the engine can be operated unthrottled, improving the mechanical efficiency relative to conventional spark ignition engines at low load. Also, since the fuel is
injected close to TDC, the compression ratio is not limited by knock; hence higher compression ratios can be used. The thermal efficiency of a diesel engine ($\eta_{th,diesel}$) can be described using the ideal air standard diesel cycle

$$\eta_{th,diesel} = 1 - \frac{1}{r_c^{k-1}} \left[ \beta^k - 1 \right] \left[ k(\beta - 1) \right]$$

(2.2)

where $\beta$ is the cut-off ratio. This is defined as the inverse of the ratio of the cylinder volumes before and after the combustion process. The thermal efficiency of the diesel cycle differs from the thermal efficiency of the Otto cycle (equation 2.1) by the term in square brackets, which is always greater than unity. Thus, for the same compression ratio, the efficiency of an Otto cycle engine is greater than the efficiency of a diesel cycle engine. However, ultimately, diesel engines can achieve higher efficiencies since higher compression ratios can be employed. The thermal efficiency of a diesel engine can be further improved by turbocharging. This technique has a positive effect on performance and emissions and can be enhanced by employing a charge cooler. Turbocharging spark ignition engines is possible, but is generally more difficult than turbocharging diesel engines due to the increased probability of knock.

An important aspect of diesel engine combustion is the fuel-air mixing rate, which ensures high torque output by means of rapid combustion. This can be enhanced using a number of methods including swirl, improved atomisation and turbulence. Swirl is defined as the organised angular rotation of the charge about the cylinder axis (Heywood, 1988) and promotes the supply of air to the fuel. Swirl is characterised by the swirl ratio ($R_S$). This is defined as the ratio of the angular velocity of a solid-body rotating flow ($\omega_s$) (which has equal angular momentum to the actual flow) to the crankshaft angular rotational speed

$$R_S = \frac{\omega_s}{2\pi N}$$

(2.3)

where $N$ is the engine speed. Atomisation of the fuel into small droplets with high momentum promotes evaporation and air utilisation in the cylinder. This is controlled by the injector and is primarily a function of the injection pressure and nozzle orifice diameter. Turbulence, generated by the gas flow into the cylinder and the piston motion, promotes mixing by the motion of turbulent eddies. Inherent in these methods
is the impact on diesel engine performance and emissions due to variations in combustion duration and local equivalence ratio.

The main emissions of interest in diesel engines are NO\textsubscript{x}, uHC and PM. The lean nature of diesel engine combustion means emissions of CO are minimal. As mentioned previously, NO\textsubscript{x} is a function of temperature, oxygen concentration and time. In diesel engines, NO\textsubscript{x} is formed in the burned gases on the lean side of the flame front, where the oxygen availability is higher. The main source of uHC emissions is by over-leaning of the fuel-air mixture during the ignition delay period. Emissions of uHC are also caused by fuel retained in the injector exiting late in the expansion stroke and bulk quenching. PM or soot is formed on the fuel rich side of the diffusion flame by the pyrolysis of fuel hydrocarbons. The total amount of soot emitted is the net result of soot formation and soot oxidation. Oxidation of the soot occurs during the expansion stroke and is a function of the burnt gas temperature and oxygen concentration. The total soot formation can be reduced by increasing swirl (Figure 2.2) and improving fuel spray atomisation, hence shortening the diffusion combustion phase and giving less time for soot formation and more time for soot oxidation. Increased swirl has the negative effect of increasing the over-leaning process at the periphery of the fuel spray, hence increasing the presence of uHC in the engine-out emissions.

![Figure 2.2 – NO\textsubscript{x} and soot emissions trade-off [Adapted from Herzog (1998)]](image)

Emissions from turbocharged engines are generally lower than those from naturally aspirated engines (Stone, 1999). The higher pressures and temperatures in turbocharged engines result in a reduction in the ignition delay which reduces uHC and
CHAPTER 2  THE DUAL FUEL ENGINE

the increased temperatures during expansion promote soot oxidation. Conversely, emissions of NO\textsubscript{x} increase due to the increase in in-cylinder temperature. However, if a charge cooler is fitted, the NO\textsubscript{x} emissions are again reduced due to the decrease in combustion temperature.

The ignition delay has an important influence on the performance and emissions of the diesel engine. For fuel injected early in the compression stroke, the ignition delay is increased due to the decreased charge temperature at the time of injection. The increased delay promotes mixing and more fuel is burned during the premixed combustion phase. This increases the maximum pressure and temperature in the cylinder around TDC, thus increasing NO\textsubscript{x} and reducing soot emissions. In contrast, fuel injected later in the compression stroke causes lower pressures and temperatures, reducing NO\textsubscript{x} and increasing soot emissions. This is the common emissions trade-off in diesel engines, as shown in Figure 2.2, caused by the opposing trends of NO\textsubscript{x} and soot formation with temperature.

2.1.3 Combustion in Dual Fuel Engines

In dual fuel engines, the premixed charge ingested into the cylinder is compressed to high pressures and temperatures; pre-ignition reactions within the gaseous charge also contribute to the in-cylinder conditions. The mixture does not ignite due to its high self-ignition temperature. As the piston approaches TDC the pilot fuel spray is injected into the cylinder. Following the ignition delay period the diesel fuel ignites. Flame propagation then proceeds from multiple ignition sites through the premixed charge. Radicals and intermediates formed within the gaseous charge during compression have an important influence on the ignition behaviour of the diesel fuel and the subsequent combustion processes. Dual fuel engines are typically unthrottled and the load is controlled by adjusting the total energy admitted to the cylinder. Furthermore, the energy content of the diesel fuel is typically the minimum required for stable combustion of the gaseous charge.

The dual fuel engine retains the mechanical and thermal efficiencies associated with the unthrottled operation and high compression ratios employed in diesel engines. Moreover, the multiple high energy ignition sites provide more reliable ignition and faster combustion of the gaseous charge relative to conventional spark ignition engines. This allows much leaner mixtures to be used (Turner and Weaver, 1994), thus improving the thermal efficiency. The more reliable ignition also reduces the cyclic variability compared to conventional spark ignition engines (Karim et al., 1988).
2.1.3.1 *Energy Release in Dual Fuel Engines*

Karim (2003) described the dual fuel combustion process as consisting of three overlapping stages, as shown in Figure 2.3.

![Figure 2.3](image)

*Figure 2.3 – Schematic representation of the different stages of energy release rate in a dual fuel engine (high load condition) [Adapted from Karim (2003)]*

These can be described as follows:

- **Stage I.** The initial stage of energy release is due the combustion of the pilot fuel vapour and entrained gaseous fuel-air mixture prepared to within combustible limits during the ignition delay period.
- **Stage II.** The second stage of energy release is due to diffusive combustion of the rest of the pilot fuel and the rapid burning of the gaseous fuel in the immediate surroundings.
- **Stage III.** The final stage of energy release is due to turbulent flame propagation through the remaining gaseous charge.

The occurrence of turbulent flame propagation during stage III is dependent on the flammability limit of the gaseous charge (Karim, 1983). Hence, for lean mixtures the bulk of the energy release is from the pilot and entrained gaseous fuel. In this case, the energy release peak during stage III is less prominent, as there is little contribution to the energy release from the gaseous charge away from the pilot fuel zone. As the concentration of gaseous fuel is increased, flame propagation can proceed and the energy release during stage III is larger, as for the high load case illustrated in
Figure 2.3. Increasing the gas substitution results in the eventual amalgamation of stages II and III, where the bulk of the energy release directly follows the ignition of the pilot.

The pilot fuel quantity affects the combustion characteristics of the dual fuel engine, particularly at low loads. Decreasing the pilot fuel quantity reduces the amount of pilot and entrained gaseous fuel prepared for combustion. Hence, the energy release during stage I is reduced. Subsequently, the energy release during stage II is reduced due to the weaker source of ignition, and at low loads flame propagation is unlikely to proceed. Increasing the pilot fuel quantity increases the number of ignition sites and results in a larger volume of charge affected by the combustion of the pilot, thus increasing the proportion of gaseous fuel burnt. Consequently, the energy release during stages I, II and III increases. At high loads, an increase in the pilot fuel quantity leads to a higher brake mean effective pressure (BMEP). This is due to the increased combustion rate of the gaseous fuel as a result of the shorter propagation paths from each ignition site. However, as the power increases, the pilot fuel quantity has to be reduced to control rapid combustion and the occurrence of knock (Poonia et al., 1998).

Poonia et al. (1998) showed that at high load the intake temperature has a dominant effect on the energy release during stages II and III. At high temperatures, the energy release during stage II is significant due to the rapid combustion of the entrained gaseous fuel. Increased temperatures also promote flame propagation during stage III. At lower temperatures, the energy release during stages II and III is less significant. At high loads, the intake temperature does not have a significant influence on the energy release during the first stage of combustion. However, at low load, the effect of increasing the intake temperature is only significant on the first stage of energy release. Here, the increased temperatures cause an increase in the amount of entrained gaseous fuel burned.

2.1.3.2 Thermal Efficiency

A dual fuel engine operating on natural gas can yield a thermal efficiency comparable to and in some cases better than diesel operation at high load. However, at low load, the thermal efficiency is degraded by the lean premixed charge, which is hard to ignite and slow to burn (Daisho et al., 1995).

For constant output conditions at low load, the thermal efficiency of a dual fuel engine can be improved by employing larger pilots. These provide a stronger ignition source
and hence more complete and rapid combustion of the gaseous fuel (Poonia et al., 1999). For small pilots, the thermal efficiency is poor because of extended ignition delay periods, a weak ignition source and slow combustion (Poonia et al., 1999). Increasing the intake air temperature also improves the thermal efficiency. This improvement is due to decreased ignition delay periods and improved combustion of the gaseous fuel. Increased intake air temperatures also lower the volumetric efficiency of the engine, thus increasing the overall richness of the gaseous air mixture and improving combustion.

The thermal efficiency of a dual fuel engine can also be improved by throttling (Daisho et al., 1995, Poonia et al., 1999), although this method is limited by the corresponding decrease in mechanical efficiency as a result of pumping losses. Throttling has the positive effect of allowing the richness of the ingested mixture to be increased, thus improving combustion. At high gas concentrations, Daisho et al. (1995) achieved higher thermal efficiencies compared to normal diesel operation. At low gas concentrations, poor combustion of the diesel fuel (as a result of the throttling process) led to lower thermal efficiencies. Another method for improving the thermal efficiency of a dual fuel engine is hot exhaust gas recirculation (EGR) (Daisho et al., 1995, Poonia et al., 1999). This increases the intake charge temperature and recirculates active radicals which enhance the pre-ignition reactions during the compression stroke, thus improving combustion. Daisho et al. (1995) also showed that for high gas substitutions, a small improvement in thermal efficiency can be achieved by advancing the injection timing.

2.1.3.3 Brake Specific Energy Consumption (BSEC)

For a dual fuel engine, the BSEC is a useful measure of how efficiently an engine is using the supplied fuel energy to produce work. At low load, the BSEC of the dual fuel engine is high compared with diesel operation (Papagiannakis et al., 2008). This is due to the poor utilisation of the gaseous air mixture as a result of the small pilot fuel quantity, air fuel ratio (AFR) and low combustion temperature. At high load, the BSEC converges towards diesel operation as the gaseous fuel utilisation improves.

An increase in the intake temperature causes the BSEC to decrease. Krishnan et al. (2002) attributed this to the higher mass burning rates associated with higher temperatures. Moreover, Gebert et al. (1997) found that advancing the injection timing reduced the BSEC. This can also be attributed to higher in-cylinder temperatures. Furthermore, Gebert et al. (1997) found that the addition of hot EGR
increases the charge temperature and decreases the global AFR leading to a reduction in BSEC.

2.1.3.4 Ignition Delay Period

The ignition delay period of the dual fuel engine varies significantly from the diesel engine, as shown in Figure 2.4. The ignition delay increases with total equivalence ratio to a maximum, before decreasing to a minimum before the total stoichiometric ratio. The total equivalence ratio is based on the combined quantities of gaseous and liquid fuel and the available air (Karim, 2003). The effect of adding a gaseous fuel to the in-cylinder charge is to increase the ignition delay relative to diesel operation.

![Figure 2.4 – Ignition delay versus total equivalence ratio in a dual fuel engine [Adapted from Liu and Karim (1998)]](image)

A number of factors contribute to this behaviour including the charge temperature, oxygen concentration, pilot fuel ignition region and pre-ignition reactions of the gaseous charge (Karim et al., 1989). These factors influence both the physical and chemical ignition processes (Liu and Karim, 1998).

In diesel engines, the most important parameter influencing the ignition delay is the charge temperature. This is affected by changes in the initial intake temperature and changes due to heat transfer and residual gas effects. In dual fuel engines, the charge temperature is further affected by a reduction in temperature as a result of the increase in the overall specific heat of the mixture. In addition, pre-ignition reactions within the gaseous charge during the compression stroke increase the charge temperature.
Residual gases have an important influence on the combustion processes of the subsequent cycle (Liu and Karim, 1995). Here, thermal and chemical kinetic effects reduce the ignition delay by increasing the charge temperature and promoting pre-ignition reactions.

Another effect contributing to the change in ignition delay is the reduction in oxygen concentration with gas substitution. This effect is of minor significance in extending the ignition delay since it decreases with further gas substitution. This is supported by the study of Nielsen et al. (1987) which showed that the addition of nitrogen to the charge only affects the ignition delay slightly. Hence, it was concluded that a decrease in the partial pressure of oxygen had little effect on the ignition delay.

The addition of gaseous fuel to the charge significantly increases the reactive area around the pilot fuel spray. The thickness of the reactive zone also increases, increasing the level of energy release. This partially explains the decrease in ignition delay with gaseous fuel admission and also emphasises the role of chemical effects.

Karim et al. (1989) noted that none of the factors discussed account for the increase in ignition delay for small amounts of gaseous fuel substitution. This is due to the pre-ignition reaction activity of the gaseous charge, whose partial oxidation products can participate in the pre-ignition reactions of the pilot fuel. The oxidation of methane, which is analogous to natural gas, proceeds sequentially via the formation of formaldehyde to CO, and finally to CO$_2$ and water (H$_2$O). Karim et al. (1991) showed that the addition of a small amount of formaldehyde to the charge increases the ignition delay since it competes for the same radicals as the diesel vapour, thus impeding the rate of pre-ignition reactions of the pilot. As the gas substitution is increased, the pre-ignition reactions of the gaseous fuel produce significant amounts of radical species that promote the pre-ignition reactions of the pilot fuel and so the ignition delay decreases (Karim, 1991), as shown in Figure 2.4.

2.1.3.5 Dual Fuel Emissions

The emissions from dual fuel engines are a combination of those produced by both conventional spark ignition and diesel engines, with the main constituents being NO$_x$, uHC, CO and PM. The following describes the parameters that affect dual fuel emissions.
**Oxides of Nitrogen (NO\textsubscript{x})**

Emissions of NO\textsubscript{x} from dual fuel engines are less than those from diesel engines (Papagiannakis and Hountalas, 2004). The lean nature of the gaseous charge in dual fuel engines contributes little NO\textsubscript{x} due to reduced combustion temperatures. The NO\textsubscript{x} is primarily formed in the pilot fuel spray, where high temperatures and long reaction times exist. The pilot fuel quantity and gas concentration have an important influence on the formation of NO\textsubscript{x}, as shown in Figure 2.5. Increasing the size of the pilot increases NO\textsubscript{x} due to the increased combustion volume and energy release. Increasing the gas concentration promotes flame propagation, which increases in-cylinder temperatures, thus increasing NO\textsubscript{x} emissions.

![Figure 2.5](image)

\textit{Figure 2.5} – Concentration of NO\textsubscript{x} with total equivalence ratio for different pilot fuel quantities

[Adapted from Karim et al. (1993)]

Krishnan et al. (2004) showed that emissions of NO\textsubscript{x} can be reduced by employing either advanced (-60 degrees after top dead centre (ATDC)) or retarded injection timings. Retarding the injection timing reduces the ignition delay period resulting in lower combustion temperatures, thus reducing NO\textsubscript{x} emissions. For advanced injection timings, the ignition delay is extended and a lean fuel vapour-air mixture forms which reduces local combustion temperatures.

**Unburned Hydrocarbons (uHC)**

Emissions of uHC in dual fuel engines are high compared to diesel engines (Papagiannakis and Hountalas, 2004). The increase in uHC emissions is inherent in the design of the diesel engine on which dual fuel engines are based. Diesel engines
have large crevice volumes, which in dual fuel operation retain unburned gaseous fuel that is released during the expansion stroke. When the gaseous charge is introduced through a mixer, the large valve overlap period employed in diesel engines to enhance scavenging can also increase uHC emissions. This is because fresh charge is used to clear the burned gases.

A serious source of uHC emissions occurs under low load operating conditions. Under these conditions the gaseous fuel mixture is too lean to support flame propagation and unburned fuel survives to the exhaust (Figure 2.6). At low load, a small amount of entrained gaseous fuel is burned by the pilot. As the gaseous concentration is increased, the reactive area around the pilot increases and so more gaseous fuel is burned. With further gaseous substitution flame propagation can proceed, first through short distances and finally throughout the whole mixture.

![Figure 2.6](image-url)

**Figure 2.6** – Methane conversion with total equivalence ratio for different pilot fuel quantities

[Adapted from Karim et al. (1993)]

At low load, the amount of uHC is dependent on the pilot fuel quantity (Figure 2.6). For larger pilot fuel quantities, more ignition centres exist and hence the volume of gaseous fuel combustion is larger. At high load, the effect of the pilot fuel quantity is insignificant as the flame engulfs the whole mixture. Hence, the minimum pilot quantity for stable combustion can be employed. Emissions of uHC decrease with increasing intake temperature. At high load, uHC decrease due to improved combustion rates, as discussed in section 2.1.3.1. At low load, uHC improve due to increased pre-ignition reaction activity and an increase in the amount of entrained...
gaseous fuel burned. Poonia et al. (1999) showed that for small pilot quantities at high load, emissions of uHC are high for all intake temperatures when employing liquid petroleum gas (LPG) as the gaseous fuel. This is due to over-leaning of the pilot fuel spray, as a result of the extension of the ignition delay, which weakens the ignition source. Karim et al. (1993) showed that different injection characteristics can also have an important influence on uHC emissions.

**Carbon Monoxide (CO)**

Emissions of CO from dual fuel engines are significantly higher than those from diesel engines (Figure 2.7). The formation of CO is primarily a function of oxygen availability. Hence, CO emissions are mainly produced by gaseous fuel within and adjacent to the burning pilot (Karim et al., 1993). Thus, the concentration of CO in the exhaust depends on the size of these regions, with higher CO concentrations observed for larger pilots (Figure 2.7). Under low load operating conditions, CO emissions are also present due to the pre-ignition reaction activity of the gaseous charge. Hence, partially oxidised fuel survives to the exhaust (Liu and Karim, 1997).

![Figure 2.7 - Variation of carbon monoxide with total equivalence ratio for different pilot fuel quantities](image)

For low total equivalence ratios, small amounts of CO are produced mainly by combustion of the pilot. With increasing gaseous fuel concentration, CO formation increases to a maximum due to the increase in the reactive area around the pilot fuel spray and the increase in pre-ignition reaction activity. Beyond the maximum, oxidation of the CO increases due to combustion of the gaseous air mixture.
Figure 2.7 shows that CO formation is independent of the pilot fuel quantity once flame propagation is established. Figure 2.8 shows that higher intake temperatures are found to enhance the oxidation and hence reduction of CO emissions, particularly at high load operating conditions.

![Figure 2.8 – Variation of carbon monoxide with total equivalence ratio for different intake temperatures [Adapted from Karim et al. (1993)]](image)

It has also been shown that different injection characteristics can have an important influence on CO emissions (Karim et al., 1993).

**Particulate Matter (PM)**

Emissions of PM or soot in dual fuel engines are greatly reduced relative to diesel operation (Papagiannakis and Hountalas, 2004). This is because the only soot present is due to the relatively small pilot. Furthermore, the soot produced by the combustion of the pilot is largely oxidised during the remainder of the combustion process. This is particularly true at high loads, where the combustion of the premixed charge increases in-cylinder temperatures. It should be noted that a small amount of particulate matter in the exhaust can be attributed to the lubricating oil (Turner and Weaver, 1994).

**Exhaust Gas Recirculation (EGR)**

Exhaust gas recirculation, whereby exhaust gases are re-circulated back into the intake charge, is a method employed in both spark ignition and diesel engines to improve NOx emissions. The exhaust gases can either be fed directly back into the
intake charge – hot EGR, or cooled beforehand – cooled EGR. EGR reduces NO\textsubscript{x} emissions in three ways. Firstly, by reducing the oxygen content in the intake charge, thus reducing the oxygen available for NO\textsubscript{x} formation. Secondly, the flame temperature is reduced by the dissociation of carbon dioxide and water vapour. Thirdly, the flame temperature is reduced by absorption of combustion heat by the exhaust gases. It is well known that reduced flame temperatures lead to reduced NO\textsubscript{x} emissions (Heywood, 1988). The mechanisms described above are commonly referred to as the dilution, chemical and thermal effects respectively (Ladommatos et al., 1997).

A number of studies have been completed to investigate the use of EGR in dual fuel engines operating on natural gas (Daisho et al., 1995, Gebert et al., 1997, Pirouzpanah and Sarai, 2003). As expected, for increasing EGR fractions NO\textsubscript{x} emissions decrease. Daisho et al. (1995) compared both hot and cooled EGR, showing that cooled EGR gives a greater reduction in NO\textsubscript{x} than hot EGR. This is due to the reduced combustion temperatures associated with cooled EGR. Daisho et al. (1995) also observed a significant reduction in NO\textsubscript{x} with hot EGR. This is due to a reduction in the ignition delay period which reduces subsequent combustion temperatures. Higher intake temperatures also contribute to a reduction in uHC by reducing the lean flammability limit of the gaseous charge. The use of EGR also reduces uHC due to the recirculation and burning of previously unburned fuel. Pirouzpanah and Sarai (2003) completed an experimental study with cooled EGR and observed an increase in CO and uHC emissions with increasing EGR fractions due to the reduction in oxygen availability. Soot emissions were also found to increase with increasing EGR due to decreased in-cylinder temperatures and reduced oxygen concentrations.

2.1.3.6 Combustion at Low Load Operating Conditions

A significant problem associated with the dual fuel engine is the poor low load performance caused by the method of load control. As the load decreases, the gaseous mixture ingested into the cylinder becomes increasingly leaner and the flames originating from the pilot ignition regions cannot propagate throughout the charge. This results in an increase in BSEC, cyclic variations and uHC and CO emissions. Thus, when converting diesel engines to dual fuel operation, diesel operation is typically retained at low load and idling conditions.
The low load performance of the dual fuel engine can be improved by lowering the lean flammability limit of the charge, thus promoting flame propagation (Karim, 1991). A number of methods have been proposed for improving the low load performance of dual fuel engines. These are summarised as follows:

- **Larger pilot quantities.** Increasing the pilot fuel quantity increases the number of ignition sites and results in a larger volume of combustion activity. It also increases the flammability limits of the gaseous charge due to the increased amount of energy release (Karim, 1991). Advancing the injection timing also increases the flammability limits of the gaseous charge due to increased in-cylinder temperatures as a result of the extension of the ignition delay period.

- **Throttling.** Throttling of the gaseous air mixture can provide a richer mixture which will ignite more readily. This method degrades both the mechanical and volumetric efficiency. The same effect could also be achieved by employing variable valve timing, although this technique is not typically used in conventional engines. In turbocharged engines, throttling could be achieved by bypassing excessive boost air at specific engine speed/load points (Gebert et al., 1997).

  Gebert et al. (1997) implemented a skip-fire technique, whereby the number of cylinders in use was reduced to achieve an optimum AFR in the firing cylinders. The number of cylinders to be fired was calculated from the required AFR and the firing order was calculated to give the best uniformity of rotational speed. This technique enabled dual fuel running at idle conditions. The technique also permits the implementation of a rolling skip-fire to achieve a balanced temperature distribution across the engine. Experimental results showed that with three out of six cylinders firing, a significant reduction in uHC and CO emissions could be achieved. A drawback of this method was the significant increase in NOx emissions. Some visible shaking of the engine was also reported. Kusaka et al. (2003) observed similar emissions trends for a four cylinder engine. In an earlier study, Karim (1991) suggested a combination of cylinders running on diesel and dual fuel, although studies of this type have yet to be completed.

- **Preheating the intake gas charge.** Preheating of the gaseous charge, either through preheating or increasing water jacket temperatures, increases the temperature at the end of compression, thus increasing the flammability limits
of the charge, resulting in more gaseous fuel being burned (Karim, 2003). Consequently, the amount of uHC in the exhaust is reduced.

- **Auxiliary fuels.** The addition of small amounts of auxiliary fuel, such as hydrogen or gasoline vapour, enhances the combustion characteristics of the charge (Karim, 1991). The drawback of this method is the increased complexity of the fuelling system.

- **Stratification.** Stratification of the gaseous fuel in air provides a richer mixture in and around the region of the pilot fuel, promoting ignition and combustion of the gaseous fuel. Optimum stratification is likely to reduce exhaust emissions significantly (Karim, 2003).

- **EGR.** The addition of hot EGR to the charge increases the charge temperature, hence promoting combustion. Reactive species present in the EGR also enhance the pre-ignition reaction activity of the gaseous charge. It should be noted, that above an optimum value, the addition of EGR has a negative effect on flame propagation (Poonia et al., 1999).

- **Split injection.** Micklow and Gong (2002) completed a parametric study using a multi-dimensional model (validated for a single injection case) to show that emissions of NO\textsubscript{x}, uHC and CO can be reduced by employing a split injection scheme. The injection quantities and timings of both pulses were shown to have an important effect on engine-out emissions. The first injection pulse creates a pool of radicals which increases the lower flammability limit of the gaseous mixture, thus promoting flame propagation. Consequently, emissions of uHC decrease and the increased in-cylinder temperatures promote CO oxidation. A decrease in NO\textsubscript{x} was predicted due to over-leaning of the first injection pulse as a result of the extended ignition delay due to decreased in-cylinder temperatures at the time of injection.

In an experimental study, Aroonsrisopon et al. (2009) also showed the importance of split injection quantities and timings on the performance and emissions of a dual fuel engine. In contrast to the modelling work of Micklow and Gong (2002), emissions of NO\textsubscript{x}, CH\textsubscript{4} and CO showed little improvement relative to an optimised single injection case. However, split injection was observed to improve combustion stability.

### 2.1.3.7 Combustion at High Load Operating Conditions

A second problem associated with the dual fuel engine is the onset of knock, which limits the maximum power that can be achieved. Knock in dual fuel engines is usually
associated with the autoignition of the charge in the vicinity of the ignition regions, which leads to higher energy release rates and rapid burning of the gaseous mixture (Karim, 2003). Smaller pilot fuel quantities can lead to uncontrolled combustion of the end gases, as in conventional spark ignition engines. Nwafor (2002) also suggested that a third type of knock, referred to as erratic knock, occurs in dual fuel engines as a result of rapid combustion of the premixed charge.

The knock limited power output of the dual fuel engine decreases with intake charge temperature (Karim, 2003). Therefore, the onset of knock can be delayed by lowering the intake temperature or water jacket temperatures and retarding the pilot injection timing. Diluents such as carbon dioxide can also be used to reduce the combustion temperature. A reduced compression ratio can also be used to reduce the occurrence of knock, but this would undermine diesel operation. Knock in the end gases can be avoided by stratification of the gaseous charge, resulting in a less reactive region away from the ignition sites. However, care must be taken with this method not to promote autoignition in the vicinity of the ignition regions.

Karim (2003) describes a simple approach for predicting the onset of knock in dual fuel engines, which assumes that the autoignition of the gaseous fuel is associated with the mean temperature and pressure at the end of combustion of the pilot. Combustion of the pilot is assumed to occur at constant volume and the pre-ignition reactions of the charge are taken into account. Developments of this method consider progressive burning of the pilot, residual gas effects and heat transfer.

### 2.2 CONCLUDING SUMMARY

The dual fuel engine is a compression ignition engine in which a gaseous fuel and air are ingested into the cylinder to form a homogeneous lean premixed charge. This is ignited by a pilot fuel spray, which establishes multiple flame fronts from which flame propagation develops. The energy release in a dual fuel engine is therefore a combination of the combustion of the diesel and gaseous fuel. The current conceptual understanding of dual fuel combustion comprises three stages: combustion of the pilot fuel vapour and entrained gaseous fuel-air mixture prepared to within combustible limits during the ignition delay period; the diffusive combustion of the remainder of the pilot and rapid burning of the surrounding gaseous fuel; and turbulent flame propagation through the remaining premixed charge. The use of a pilot injection ensures reliable ignition and fast combustion of the gaseous charge. Dual fuel
engines are typically unthrottled and the load is controlled by varying the total energy admitted to the cylinder. This is divided between the gaseous and diesel fuel. The introduction of a gaseous fuel increases the specific heat of the charge, thus lowering compression pressures and temperatures. Radicals and intermediates formed within the gaseous charge during compression have a significant influence on the ignition behaviour of the pilot fuel spray, extending the ignition delay relative to diesel operation. The gaseous fuel employed in dual fuel engines is typically natural gas due to its availability and inherently cleaner combustion. Moreover, the high self-ignition temperature of natural gas allows the high compression ratios employed in diesel engines to be maintained. Together with the lean premixed charge, thermal efficiencies comparable to diesel operation can be achieved at high load.

Dual fuel engines can achieve reduced emissions of CO$_2$, NO$_x$ and PM relative to diesel engines. The reduction in CO$_2$ is due to the substitution of diesel with a subsidiary fuel that has a lower carbon-to-hydrogen ratio. The combustion of the lean gaseous mixture contributes little NO$_x$ due to reduced combustion temperatures, with the main source of NO$_x$ being due to the relatively small pilot. Particulate emissions are also reduced due to the relative size of the pilot, with the soot that is produced largely oxidised during the expansion stroke.

The main obstacles associated with dual fuel engines are poor low load performance, knock limited power output and increased emissions of CO and uHC. Emissions of CO and uHC are particularly high at low load conditions, since the lean gaseous mixture employed under these conditions is unable to support flame propagation. Similarly, the BSEC is high at low load, but converges towards diesel operation as gaseous substitution levels are increased and fuel utilisation improves.
CHAPTER 3
COMBUSTION MODELLING

3.1 COMBUSTION MODELLING IN DUAL FUEL ENGINES

Combustion modelling provides an effective means of investigating the combustion phenomena taking place inside the cylinder. A suitable combustion model allows the determination of quantities that are difficult to measure experimentally and can provide a rational basis for engine development, thus reducing prohibitive development time and cost. Combustion models are typically classified as zero-dimensional, quasi-dimensional or multi-dimensional.

Zero-dimensional models are also referred to as thermodynamic or phenomenological models. These terms are related to the formulation of this type of model: zero-dimensional since engine geometry is not considered; thermodynamic since the model is based on the first law of thermodynamics; and phenomenological since individual sub-models are used to describe the different phenomena occurring inside the cylinder. Zero-dimensional models can be further classified into single or multi-zone models. Single-zone models treat the contents of the cylinder as being homogeneously mixed at all times and can either be used to determine the energy release rate from experimental pressure diagrams, or as a predictive tool if either the energy release rate or fuel mass burning rate are specified. The energy release rate can be specified by means of a Wiebe function, which can be used to account for both the premixed and diffusive stages of combustion. Multi-zone models account for temporal and volumetric variations in composition and temperature by dividing the cylinder into zones. Since emissions are a strong function of both composition and temperature, models of this type offer a more realistic representation of the in-cylinder conditions. Quasi-dimensional models are an extension of the zero-dimensional approach and include geometric features such as the diesel fuel spray and flame front shape. Zero-dimensional and quasi-dimensional models both yield a system of ordinary differential equations, which allow for time-efficient solution of combustion problems. The primary objective of these models is to predict the energy release rate on the basis of the physical and chemical processes occurring inside the cylinder.

Multi-dimensional models are fluid dynamic in nature. In this type of model, local equations for mass, momentum, energy and species conservation are solved, yielding
a system of partial differential equations with respect to time and space. Detailed sub-
models for spray and combustion phenomena are also included. Due to their
complexity, these types of model are characterised as being computationally
expensive.

The objective of this section is to review the dual fuel engine models currently
available in the literature, with emphasis placed on the models major assumptions and
predictive capabilities.

3.1.1 Zero-dimensional Models
Mansour et al. (2001) developed a single-zone model to investigate the performance
and emissions characteristics of a naturally aspirated, V8, direct injection engine
operating on natural gas. Detailed chemical kinetics of natural gas and NO_x were
used to predict the main combustion characteristics. The reaction scheme for natural
gas included 493 reaction steps and 81 chemical species. The NO_x scheme included
79 reactions. A quasi-global model of the pilot fuel kinetics was included to predict the
contribution of the pilot to the charge composition. The energy release rate of the pilot
was predicted using a Wiebe function. The ignition delay of the pilot was first
estimated using an empirical correlation for diesel, dependent on the engine speed,
inlet air temperature, and mean pressure and temperature during compression. The
final ignition delay was defined as the time at which the product of the concentration of
oxygen (O_2) and carbon monoxide (CO) was a maximum for the diesel fuel-natural gas
mixture. Wall heat transfer was calculated using the correlation of Woschni (1967).
Experimental data was collected at full load conditions for a range of engine speeds.
The predicted pressure diagrams were shown to be qualitatively consistent with
experimental data for two different engine speeds. However, a comparison of the
experimental and predicted energy release rates was not presented. In general,
trends for CO_2 and CO emissions were poorly predicted. Emissions of uHC exhibited
the correct trend, but were under-predicted by approximately 15 percent at low engine
speeds. Emissions of NO, the main species of NO_x, were predicted using both the
extended Zeldovich mechanism and the NO_x scheme outlined above. The extended
Zeldovich mechanism was observed to over-predict emissions of NO, whereas the
NO_x scheme successfully predicted the correct trend for NO with engine speed.

Karim and Liu (1992) developed a quasi-two zone model to investigate the onset of
autoignition and knock in dual fuel engines operating on methane or propane near full
load. In this model, the gaseous charge, comprising air, gaseous fuel and residuals from the previous cycle, was treated as a single homogeneous zone. Detailed chemical kinetics, comprising 105 reaction steps and 31 species, were used to predict changes in the properties and concentration of the mixture, as well as the energy release rate during compression, combustion and expansion. The pilot fuel was treated as an overlapping subsidiary zone. Following ignition, its contribution to the in-cylinder pressure, temperature and charge composition was considered. It was assumed that the only interaction between the two zones was thermal, thus neglecting the presence of chemical reactions between the gaseous and pilot fuel. The ignition delay period and energy release rate of the pilot were provided either experimentally or empirically. Wall heat transfer was accounted for using the correlation of Woschni (1967). Predicted trends for ignition delay and peak in-cylinder pressure with total equivalence ratio were in good agreement with presented experimental data for propane. Experimental data for methane was not presented.

The quasi-two zone model of Abd Alla et al. (2000, 2001) was used to investigate the combustion characteristics of the dual fuel engine. The effects of total equivalence ratio, pilot fuel quantity and pilot fuel injection timing were considered. In this model, the gaseous charge, comprising air and gaseous fuel, was treated as a single homogeneous zone. The energy release rate of the charge was modelled using detailed chemical kinetics comprising 178 reaction steps and 41 species. The energy release rate of the pilot was predicted using two superposed Wiebe functions to account for the premixed and diffusive stages of combustion. The only interaction between the fuels was considered to be thermal. The prediction of the ignition delay was based on the correlation of Hiroyasu (1985). Here, the correlation was considered to be dependent on the in-cylinder pressure and temperature and the total equivalence ratio of the fuel vapour-gas mixture. Wall heat transfer was determined using the correlation of Woschni (1967). This included an additional radiative term, contrary to the fact that this effect is implicitly included in this correlation. Predicted emissions trends for methane showed good agreement with previous experimental results taken from an indirect injection (IDI) engine.

Pirouzpanah et al. (2007) developed a quasi-two zone model to investigate the effects of EGR on dual fuel combustion at part load. In this model, a detailed chemical kinetic scheme for natural gas was used. This included 112 reaction steps and 34 chemical species. The energy release rate of the pilot was predicted using two superposed
Wiebe functions and the ignition delay was predicted following the work of Abd Alla et al. (2000, 2001). Wall heat transfer was included using the correlation of Annand (1963). The active radicals introduced to the cylinder through EGR were considered to have no effect on the chemical kinetics, but were considered to combine with the free radicals from gaseous fuel ignition. The model was used to predict in-cylinder pressure and temperature, energy release rate and species concentrations. The predicted pressure diagram was in reasonable agreement with experimental data for a naturally aspirated, six-cylinder, direct injection engine operating at 25 percent load with 80 percent gaseous energy substitution. However, pressure data was only plotted at 15 degree crank angle intervals, so it is difficult to comment conclusively. A comparison between the experimental and predicted energy release rates was also not given. Predictions of CO were in poor agreement, although this is expected due to the single-zone nature of the model.

Raine (1990) modified a multi-zone model originally developed at the University of Bath (Simulation Program for Internal Combustion Engines – SPICE) for the prediction of diesel engine combustion to model dual fuel combustion characteristics. Predictions of brake power, brake thermal efficiency and ignition delay were compared against experimental results taken from a naturally aspirated, single-cylinder, direct injection engine operating on methane (Karim and Burn, 1980). The energy release rate of the pilot was predicted using the empirical model of Meguerdichian and Watson (1978) and the ignition delay period was considered to be a function of the mean in-cylinder pressure and temperature during the delay period. The energy release rate of the gaseous charge was predicted using a sine law expression, which included a characteristic burning duration determined from the laminar burning velocity and a semi-empirical constant that accounted for turbulence. The laminar burning velocity was determined using an empirical expression defined by Raine (1990). The wall heat transfer was modelled using the correlation of Annand (1963). The trend for brake power with increasing gaseous substitution was in qualitative agreement with experimental results, but the brake thermal efficiency and ignition delay were in poor agreement.

Liu and Karim (1995b, 1997) developed a multi-zone model to predict low load performance and the onset of knock in a dual fuel engine. In this model, the gaseous charge, comprising air and gaseous fuel, was treated as a homogeneous mixture in which detailed chemical kinetics were used to describe the oxidation of the gaseous
fuel during compression, combustion and expansion. The initial model employed 138 reaction steps and 32 chemical species, while the latter model employed 157 reaction steps and 38 chemical species. Following pilot fuel injection, gaseous charge was entrained into the fuel spray forming three zones: a rich diesel fuel zone, a flammable zone and a lean gaseous fuel zone (Figure 3.1).

![Figure 3.1 – Schematic of the zone division adopted by Liu and Karim (1997) during fuel injection [Adapted from Liu and Karim (1997)]](image)

The pilot fuel spray was described using steady state gas jet theory supplemented by experimental correlations for spray cone angle (Hiroyasu et al., 1980) and spray breakup and penetration (Hiroyasu et al., 1983). Entrainment of the gaseous mixture into each zone was defined by equivalence ratio boundaries. Corrections for increasing entrainment with swirl and spray wall impingement were also included.

Following ignition (Hiroyasu, 1985), combustion of the pilot, entrained gaseous fuel and premixed charge were assumed to proceed simultaneously. At this stage, the cylinder contents were viewed as being split into an unburned pilot fuel zone, unburned gaseous fuel zone, diffusion burned zone and propagation burned zone (Figure 3.2).
Under high load conditions, a flame front was considered to develop and the energy of the unburned gaseous mixture was assumed to be released as it crossed the flame front. However, at low load conditions, combustion was assumed to be confined to the diffusion burned zone and a reacting zone was added to account for partial oxidation of the premixed charge. The combustion of the pilot and entrained gaseous fuel were described using two superposed Wiebe functions under the assumption that the gaseous fuel was directly influenced by the burning of the pilot. Heat transfer was determined using the correlation of Annand (1963).

Experimental data was taken from a naturally aspirated, single-cylinder, direct injection engine operating on methane (Khan, 1969). Predicted values for in-cylinder pressure showed good agreement with experimental data, although the pressure was slightly over-predicted during the final stage of combustion. The corresponding energy release rates were not presented. Emissions trends with total equivalence ratio were also in good agreement. Emissions of CO and uHC were in qualitative agreement with experiment results, although they were both under-predicted.

Hountalas and Papagiannakis (2000, 2001, 2002) and Papagiannakis et al. (2005) developed a two-zone model to investigate the combustion characteristics of the dual fuel engine. Here, the latest model (Papagiannakis et al., 2005) is described. In this model, the gaseous charge, comprising air and gaseous fuel, was treated as a
homogenous zone into which a second conical zone penetrated during injection of the pilot. The conical zone formed as a result of the atomisation of the pilot and subsequent entrainment of the gaseous charge. The spray cone was described by correlations for spray cone angle (Hiroyasu et al., 1980) and spray penetration (Hiroyasu et al., 1983). Wall impingement was also included. The quantity of gaseous fuel entrained into the burning zone was determined from its volume change. The two zones were referred to as the unburned and burning zones respectively (Figure 3.3).

Figure 3.3 – Definition of burning zone adopted by Papagiannakis et al. (2005) before initiation of combustion [Adapted from Papagiannakis et al. (2005)]

Following ignition, the outer boundary of the burning zone was defined by a flame front, which propagated into the unburned zone in a direction perpendicular to the burning zones surface (Figure 3.4). The subsequent energy release was controlled by the rate of flame propagation. This was given by a laminar burning velocity correlation (Al-Himyary and Karim, 1987) corrected for the effects of turbulence.
In this model, the ignition delay (Kadota et al., 1976) was considered to be a function of the burning zone pressure, temperature and equivalence ratio. The rate of energy release of the pilot and entrained gaseous fuel were described using the preparation model of Whitehouse-Way (1971) and an Arrhenius type function respectively. Dissociation of the combustion products was included using the method of Vickland et al. (1962). The formation of NO was predicted using the extended Zeldovich mechanism. Emissions of CO were determined using two kinetically controlled reactions (Ramos, 1989). Here, the oxidation of CO was mainly attributed to the reaction between carbon monoxide (CO) and hydroxyl (OH). An empirical function for the total soot formation (Hiroyasu et al., 1983) was also included.

The predictions of Papagiannakis et al. (2005) were compared against experimental data taken from a naturally aspirated, direct injection engine operating on natural gas for a range of engine loads. In these experiments, the pilot fuel quantity was held constant. The pressure and energy release diagrams were in good agreement with the experimental work, although the model over-predicted the energy release rate during flame propagation. Predictions of engine efficiency against load were well predicted and emissions trends for CO and NO were found to be in good agreement, although the trend for NO emissions was slightly under-predicted. Soot emissions were under-predicted at low load conditions, but converged towards experimental values at high loads. It was found that the agreement between the predicted and experimental ignition delay period decreased with decreasing load. The model was
further used to investigate the effects of advanced injection timings on combustion characteristics. In a later study (Papagiannakis et al., 2007), the model was used to study the effects of pilot fuel quantity and injection timing on the performance and emissions of the dual fuel engine.

The studies of Patterson et al. (2006) and Stewart et al. (2007) described a three-zone energy release analysis model to investigate the performance and emissions of three different fuels in a stationary dual fuel engine. The experimental work was completed using a naturally aspirated, four-cylinder, direct injection engine. In this model, the cylinder was split into three zones: a diesel fuel zone, an unburned zone and a burned zone. The unburned zone was treated as a homogeneous mixture containing air, gaseous fuel and exhaust gas residuals. The pilot fuel zone appeared following injection and was assumed to contain only vaporised fuel. The burned zone appeared following the SOC. This was determined from the minimum in the first derivative of the pressure crank angle diagram following the SOI (Stone, 1999). Combustion in the pilot was assumed to occur due to the entrainment of the pilot and gaseous fuel in stoichiometric proportions to air. Turbulent flame propagation was implicitly included in the energy release analysis, by including the burning of the remainder of the gaseous fuel once the pilot had been consumed.

3.1.2 Quasi-dimensional Models
Pirouzpanah and Kashani (1999) developed a quasi-dimensional, multi-zone model to predict emissions in dual fuel engines at full load. In this model, the gaseous charge, comprising air and gaseous fuel, was treated as a homogeneous mixture and the pilot was modelled as a gaseous jet (Shahed et al., 1975). Combustion of the premixed charge was described using a Wiebe function, which included the characteristic combustion duration defined by Raine (1990). Combustion of both fuels was considered to begin following the ignition delay period. During the ignition delay, there was assumed to be no chemical interaction between the gaseous fuel and pilot. Wall heat transfer was predicted using the correlation of Annand (1963). The model included the ability to predict emissions of NO, uHC, CO and PM. Emissions of NO, uHC and CO were considered to originate from all burning zones, whereas PM was attributed solely to the pilot fuel zones. Emissions of NO were predicted using the extended Zeldovich mechanism and CO emissions were determined using the two-step approach of Bazari (1992), which considers the net effect of CO formation and oxidation. Soot was predicted using an empirical function. Calculations of chemical
equilibrium were based on the methods of Olikara and Borman (1975) and Benson (1975). The predicted pressure diagram was compared against experimental data taken from a heavy-duty, naturally aspirated, six-cylinder, direct injection engine at full load. The predicted values were in good general agreement with the experimental data, although the value for peak pressure was under-predicted. The energy release rate, which is a useful tool for understanding engine-out emissions, was not given. The predicted trend for NO emissions with engine speed was in good agreement with experimental data, although values of NO were under-predicted by approximately 50 percent. Predicted values of CO and PM at full load were in good agreement with experimental results, but predictions of uHC were poor.

Pirouzpanah and Saray (2006) described a quasi-dimensional, multi-zone model used to investigate the combustion characteristics of a dual fuel engine operating on natural gas. The model was used to predict the pressure, temperature and energy release rate for changes in equivalence ratio, injection timing, pilot fuel quantity and air throttling. The gaseous charge, comprising air and natural gas, was treated as a homogeneous mixture in which detailed chemical kinetics were used to predict the properties of the mixture and the energy release during compression, combustion and expansion. The chemical reaction scheme included 184 reaction steps and 50 species. The pilot fuel was modelled as a gaseous jet (Shahed et al., 1975). Following the ignition delay period, the contribution of the pilot to the energy release, heating of the gaseous charge and cylinder composition was included. During the ignition delay, there was assumed to be no chemical interaction between the gaseous fuel and pilot. Pirouzpanah and Saray (2006) claimed that there was good agreement between the predicted and experimental pressure diagrams for a heavy-duty, naturally aspirated, six-cylinder, direct injection engine at full load. However, at first sight the agreement is poor. At part load, the predicted and experimental pressure diagrams are in better agreement. However, during the combustion phase it is difficult to comment on the predictive capabilities of the model, as the pressure data is only plotted at 15 degree crank angle increments. Moreover, the predicted energy release rate was not compared against the experimental diagram. Predicted emissions results were compared at 25 percent load. Emissions of NOx were in good agreement, but predictions of CO and uHC emissions were poor.

Krishnan et al. (2007) developed a quasi-dimensional, multi-zone model to describe Advanced Low Pilot-Ignited Natural Gas Low-Temperature Combustion (ALPING-
LTC), whereby the pilot fuel in a dual fuel engine is injected approximately -60 degrees ATDC. In this model, the cylinder was divided into pilot fuel zones, an unburned zone, a flame zone and a burned zone. The number of pilot fuel zones, or packets, was specified as an input to the model and each one was of equal mass. The spray was considered to be axisymmetric and spray penetration was determined using the correlation of Dent (1971). Entrainment of the gaseous charge into the spray was calculated using the correlation of Bell and Caton (1988). This correlation accounts for lower entrainment rates in zones that are close to the spray centreline, lower entrainment rates in zones injected later and decreasing rates of entrainment following the SOI. In this model, the pilot fuel spray breaks up at the nozzle exit, forming droplets that subsequently evaporate to form zones of combustible fuel vapour-gas mixture. For simplicity, an initial droplet diameter of 30 μm was assumed.

Due to difficulties predicting the ignition delay period with empirical correlations at the advanced injection timings employed, the Shell autoignition model (Halstead et al., 1977) was used. This is a phenomenological model that uses a simplified reaction mechanism to predict the autoignition of hydrocarbon fuels. A modified version of the Shell autoignition model (Kong and Reitz, 1993), used to predict the ignition of diesel fuel, was employed to predict the ignition delay period of the pilot. Hence, any chemical interaction between the gaseous fuel and pilot was neglected. Following ignition, the pilot and entrained gaseous fuel were each assumed to burn according to a single-step global reaction mechanism (Westbrook and Dryer, 1981). A premixed turbulent flame was also assumed to propagate. This was modelled using a turbulent entrainment and laminar burn-up model (Tabaczynski et al., 1977). The flame area was assumed to be proportional to the sum of the instantaneous enflamed areas, calculated on a dimensional basis as $\frac{V^2}{3}$. The burned zone was created at the SOC and comprised burned products from the flame zone. Burned packets were also added to the burned zone if the temperature of the packet was lower than a critical temperature, more than 90 percent of the fuel had been burned or the reaction rates were negligible. The wall heat transfer was determined using the correlation proposed by Woschni (1967). Experimental data was obtained from a single-cylinder, direct injection engine which could replicate turbocharged cylinder conditions. The gaseous fuel employed was natural gas. The model was able to formulate predictions for pressure and energy release rate in qualitative agreement with experimental results. The initial energy release rate and combustion duration were well predicted, but towards the end of combustion the energy release rate and consequently pressure were over-predicted.
3.1.3 Multi-dimensional Models

The rapid development of computing power means multi-dimensional models are becoming ever more practical as an investigative tool. This type of model predicts the turbulent flow field inside the engine. In this way, the associated heat transfer and combustion processes that depend on the turbulent flow field can be predicted. The computational demands of these models are typically high. This is inherent in the finite volume approach, which produces a large amount of data. In general, the solution time and storage constraints restrict the detail of this type of model. A number of multi-dimensional studies have been completed to investigate the combustion characteristics of dual fuel engines. These are all based on the KIVA 3V code, with modifications to enable dual fuel combustion modelling.

The model of Zhang et al. (2003) used the KIVA 3V code to study the combustion characteristics of the dual fuel engine. Experimental data was taken from a naturally aspirated, six-cylinder, direct injection engine operating on natural gas. In this model, methane was treated as being representative of natural gas and the ignition delay was predicted using the Shell autoignition model (Kong and Reitz, 1993). Combustion of the pilot and gaseous fuel was modelled on a diffusion basis. The predicted pressure and energy release diagrams were in qualitative agreement with the experimental data for the two load conditions presented. In both cases, the pressure and energy release rate were over-predicted during the final stage of combustion. The model was further used to perform a parametric study to investigate the effects of diesel fuel quantity, injection rate shape and injection timings on dual fuel combustion.

Singh et al. (2004) modified the model of Zhang et al. (2003) and used it to investigate the performance and emissions of dual fuel engines. Experimental data was taken from a single-cylinder, direct injection engine operating on natural gas. Turbocharged conditions were simulated by controlling the intake and exhaust pressures. As in the model of Zhang et al. (2003), methane was treated as being representative of natural gas and the ignition delay was predicted using the Shell autoignition model (Kong and Reitz, 1993). The predicted pressure and energy release diagrams were in poor agreement for different levels of natural gas substitution. In general, the pressure and energy release rate were under-predicted during the initial stage of combustion and over-predicted during the final stage of combustion. The ignition delay period was also over-predicted. The emissions trends of interest were for NOx and uHC. The NOx
emissions were predicted using the extended Zeldovich mechanism. Emissions trends were in qualitative agreement with experimental data, but the uHC emissions were increasingly under-predicted as the percentage of natural gas substitution was increased. Predictions for the effect of changes in the inlet charge temperature were also completed. Emissions of NO_x were in qualitative agreement, but were under-predicted by approximately 25 percent. The disagreement between predicted and experimental pressure and energy release rate diagrams was attributed to the combustion model, which was developed primarily for prediction of diffusion combustion. Hence, Singh et al. (2006) proposed the implementation of a flame propagation model into the KIVA 3V code. The model was compared with experimental data for different engine loads, injection timings and inlet temperatures. The predicted pressure and energy release diagrams were in good agreement, although the prediction of the final stage of combustion was slightly over-predicted for all cases. Emissions of NO_x and uHC were in qualitative agreement, but uHC emissions were consistently under-predicted.

Cordiner et al. (2007) used the KIVA 3V code to model the working cycle of the dual fuel engine. In this model, the contribution of the pilot fuel (which provided 10 percent of the total energy) to combustion was neglected and treated as a source of ignition. The ignition delay was calculated using the Shell autoignition model (Kong and Reitz, 1993). The combustion of natural gas was predicted based on the hypothesis of a flamelet combustion model. Experimental data was taken from a turbocharged, six-cylinder, direct injection engine operating on natural gas at 50 percent load. The comparison between predicted and experimental data was in good agreement. The pressure was slightly under-predicted during the initial stage of combustion as the contribution of the pilot fuel was neglected. A comparison between the experimental and predicted energy release rates was not given. The model was used to analyse the effect of the turbulent flow field on the spray, its breakup and evaporation, and subsequent autoignition. A later work by the same author (Cordiner et al., 2008) compared the suitability of the diffusion and flamelet type model. It was concluded that each model had its own merits depending on the local conditions in the cylinder.

Tamagna et al. (2008, 2007) used the KIVA 3V code to predict the combustion characteristics of a gasoline-diesel dual fuel engine. The studies were based on a naturally aspirated, single-cylinder, direct injection engine. The KIVA 3V code was coupled with detailed chemical kinetics in which heptane and iso-octane were
assumed to be representative of diesel and gasoline respectively. The chemical scheme included 55 reaction steps and 32 species. The model was first validated for homogeneous charge compression ignition (HCCI) and premixed charge compression ignition (PCCI) combustion. A parametric study was then completed for a number of dual fuel cases. In the initial study, a comparison of the diffusion type combustion model and detailed chemical kinetics was completed. Predictions of NO\textsubscript{x} and soot emissions were also included. The ignition delay was predicted using the Shell autoignition model (Kong and Reitz, 1993). In the latter study, the suitability of four different combustion models were analysed to describe the flame front. The model was used to study the effects of injection timing and mixture composition for two different injectors.

A number of multi-dimensional studies have been completed to investigate emissions reduction at low load conditions. Kusaka et al. (2000, 2002) investigated the effects of EGR and intake heating on the performance and emissions of a dual fuel engine at low load. Experimental data was taken from a naturally aspirated, four-cylinder, direct injection engine operating on natural gas at 20 percent load. In the initial study, the KIVA 3V code was used to describe NO\textsubscript{x} and uHC emissions at the tested load condition. Emissions of NO\textsubscript{x} were predicted using the extended Zeldovich mechanism. Predicted pressure and energy release diagrams were in good agreement, as were the emissions of NO\textsubscript{x}. In the latter study, the KIVA 3V code was coupled with detailed chemical kinetics in which heptane and methane were assumed to be representative of diesel and natural gas respectively. The chemical scheme included 173 reaction steps and 43 chemical species. In this study, predicted and experimental data for pressure and energy release rate were in qualitative agreement, but the baseline dual fuel case was under-predicted.

Micklow and Gong (2002) investigated the effects of multiple injections on the performance and emissions of a dual fuel engine at low load. In this study, the gaseous fuel was treated as methane. The predicted in-cylinder pressure was in good agreement with experimental data at 50 percent load and 85 percent natural gas energy substitution. A comparison between the experimental and predicted energy release rates was not given. Predicted emissions of uHC and CO were also in good agreement. Emissions of NO\textsubscript{x}, predicted using the extended Zeldovich mechanism, were under-predicted by 40 percent. The model was used to predict the optimum
injection timing and pilot fuel quantity for each injection pulse to give the best reduction in uHC and CO emissions at low load.

Kusaka et al. (2003) used the KIVA 3V code coupled with detailed chemical kinetics to study the performance and emissions characteristics of a dual fuel engine operating on a reduced number of cylinders. The chemical scheme included 290 reaction steps and 57 species. Experimental data was taken from a naturally aspirated, four-cylinder, direct injection engine operating on natural gas. In this model, heptane and methane were treated as being representative of diesel and natural gas respectively. The predicted pressure and energy release rate diagrams for the four cylinder baseline case were in good agreement with experimental results. For two cylinder operation, the pressure and energy release rate were under-predicted during the final stage of combustion. The model was used to analyse the pilot fuel concentrations and temperature distributions in the cylinder, as well as the CO and NO formation processes.

3.1.4 Summary
As described in Chapter 2, the combustion processes occurring inside the dual fuel engine are a complex combination of those present in both conventional spark ignition and diesel engines. In recent years, a number of models have been developed to describe the combustion phenomena present in dual fuel engines. As mentioned previously, the primary objective of these models is to predict the energy release rate on the basis of the physical and chemical processes occurring inside the cylinder. The following is a brief summary of the current state of dual fuel modelling.

The zero-dimensional model has been widely employed to simulate dual fuel combustion. In recent years, detailed chemical kinetic modelling has been extensively used to study pre-ignition reaction activity, low load performance and emissions, and knock. However, in this type of model, the energy release of the pilot is generally described using a specified mass burning rate, thus neglecting the important spray mixing process. Liu and Karim (1995b, 1997) and Papagiannakis et al. (2005) modelled simple spray geometries using experimental correlations. Papagiannakis et al. (2005) coupled the spray model to a flame propagation model in which flame growth was described from the surface of a conical spray. This model also included the ability to model spray wall impingement. In general, the zero-dimensional models studied were unable to predict engine-out emissions. This is because temporal and
spatial variations in composition and temperature are not adequately described by this type of model. Moreover, the effects of turbulence, swirl and spray wall impingement were either neglected or described using model constants rather than on the basis of appropriate physical phenomena.

At present, the development of quasi-dimensional models has been limited. Pirouzpanah and Kashani (1999) used a quasi-dimensional description of the pilot fuel spray, but employed a specified mass burning rate to describe the energy release of the premixed charge. In a later model, Pirouzpanah and Saray (2006) used detailed chemical kinetics to describe the energy release of the gaseous fuel, but in general, the predictive capability of the model was poor. Krishnan et al. (2007) developed a multi-zone spray model coupled to a turbulent entrainment model. This accounted for the effects of varying turbulence intensity and length scales on the flame propagation process. However, this model made a number of simplifying assumptions when considering spray development, such as employing a constant droplet diameter at spray breakup and neglecting swirl and spray wall impingement. Thus far, the quasi-dimensional model has not been used to perform an extensive study of emissions trends. Pirouzpanah and Saray (2006) and Pirouzpanah and Kashani (1999) both predicted emissions, but for only one load condition. An emissions trend for NO\textsubscript{x} with engine speed was presented by Pirouzpanah and Kashani (1999), but this was under-predicted.

In general, the combustion models studied were only validated by comparison of the predicted and experimental pressure diagrams. Few studies also compared the predicted and experimental energy release rates. The energy release rate can provide important information about the progression of combustion and aid the explanation of emissions formation. In general, studies that presented the energy release rate were in qualitative agreement with experimental data. However, the energy release rate during flame propagation was generally over-predicted. At this time, the prediction of energy release rates from multi-dimensional models is no better than the zero- or quasi-dimensional approach. Coupled with the high computational demands of this type of model, a zero- or quasi-dimensional approach is viewed as being more suitable for the investigation of the fundamental aspects of dual fuel combustion.

At present, the coupling between the combustion of the pilot and the premixed combustion of the gaseous charge is not well understood. Current modelling
methodologies for dual fuel combustion lead to an over-prediction of the energy release during the premixed combustion of the gaseous charge. Therefore, a new approach is needed to couple these two processes. Spray development and mixing has an important effect on the ignition process and subsequent flame growth, as well as the combustion of the entrained gaseous fuel. Hence, the next section will describe atomisation and spray modelling, with a view to describing spray phenomena using experimental correlations, rather than subjective model constants.

3.2 ATOMISATION AND SPRAY MODELLING

In diesel engines, liquid fuel is injected into the cylinder at high pressure through small diameter orifices. This results in spray breakup in the atomisation regime. This is characterised by jet breakup at the nozzle exit and the formation of droplets with diameters much less than the nozzle diameter. Breakup in the atomisation regime is advantageous, as it has an important influence on air utilisation and the fuel-air mixing rate.

The structure of a typical diesel fuel spray can be described by a number of characteristics. These include the spray tip penetration, spray cone angle, breakup length and representative diameter. Characterisation of the spray is useful in engine modelling, as it allows prediction of the spray development and subsequent combustion processes. In general, spray characteristics are described using correlations determined from experimental work. These are mainly dependent on the liquid properties, injection pressure, in-cylinder conditions, and nozzle design and geometry.

This section describes the main breakup regimes of a liquid jet and the mechanisms of breakup specific to the atomisation regime. The main correlations used to describe a typical diesel fuel spray are compared and the main spray models in the literature are reviewed.

3.2.1 Atomisation

The high injection pressures employed in modern diesel engines result in spray breakup in the atomisation regime. There are four different breakup regimes in total: the rayleigh regime, first-wind induced regime, second wind-induced regime and
atomisation regime (Reitz and Bracco, 1986). These breakup regimes can be classified using the liquid Weber number, Reynolds number and Ohnesorge number.

The liquid Weber number ($We_l$) is a dimensionless group which compares the external pressure forces acting to breakup a jet with the surface tension forces trying to reform the jet

$$We_l = \frac{\rho_l V^2 D}{\sigma_l} \quad (3.1)$$

where $\rho_l$ is the liquid fuel density, $V$ is the velocity of the jet, $D$ is the nozzle orifice diameter and $\sigma_l$ is the liquid fuel surface tension.

The Reynolds number ($Re$) is a dimensionless group which is defined as the ratio of the inertial forces to viscous forces of the jet

$$Re = \frac{\rho_l V D}{\mu_l} \quad (3.2)$$

where $\mu_l$ is the liquid fuel dynamic viscosity.

The Ohnesorge number ($Oh$) eliminates the velocity from both the Weber and Reynolds number and is an indication of jet stability.

$$Oh = \frac{\sqrt{We_l}}{Re} = \frac{\mu_l}{\sqrt{\sigma_l \rho_l D}} \quad (3.3)$$

Figure 3.5, commonly referred to as an Ohnesorge diagram, classifies the four breakup regimes by plotting the Ohnesorge number against the Reynolds number on a logarithmic scale.
Here, with the liquid properties and nozzle diameter held constant, each subsequent breakup regime is encountered with an increase in jet velocity. Figure 3.6 shows the relationship between the jet velocity and jet breakup length. Ramos (1989) defines the jet breakup length ($L_b$) as the distance from the nozzle exit to the point where droplets are formed on the liquid surface.

**Figure 3.5** – Classification of the different jet breakup regimes [Adapted from Lefebvre (1989)]

**Figure 3.6** – Breakup length of a liquid jet as a function of velocity: (A-C) B-C drip flow; C-D Rayleigh regime; E-F first wind-induced regime; F-G (F-H) second wind-induced regime; beyond G (H) atomisation regime [Adapted from Reitz and Bracco (1986)]
The drip flow regime occurs at low injection velocities. In the Rayleigh regime, the jet breakup length increases with jet velocity. Upon reaching a maximum, the jet breakup length decreases throughout the first and second-wind-induced regimes. However, in some cases, the breakup length in the second wind-induced regime has been found to increase, as described by Reitz and Bracco (1986). At the high injection velocities encountered in the atomisation regime, the breakup length drops to zero.

Figure 3.5 can be extended to include the additional effects of gas density (Figure 3.7), whereby jet breakup is enhanced by increasing the gas density. The effect of methane in air, as for the premixed charge in a dual fuel engine, is to reduce the gas density, thus hindering the atomisation process.

1. **Rayleigh breakup.** This occurs at low Reynolds numbers and is caused by axisymmetric oscillation of the jet surface, caused by surface tension. The droplet diameters are larger than the jet diameter.

2. **First wind-induced breakup.** In this regime, the oscillations caused by the surface tension are amplified by the relative velocity of the jet and surrounding
gas. Breakup occurs many jet diameters away from the nozzle. The droplet diameters are approximately the same size as the jet diameter.

3. **Second wind-induced breakup.** Breakup is caused by the growth of short-length surface waves caused by the relative velocity of the jet and surrounding gas. This wave growth is opposed by the surface tension. Breakup occurs several nozzle diameters downstream of the nozzle. The average droplet diameters are much less than the jet diameter.

4. **Atomisation.** Breakup occurs at high Reynolds numbers and at the nozzle exit. Average droplet diameters are much less than the jet diameter.

There are two stages of atomisation in a diesel fuel spray: primary atomisation and secondary atomisation. These are described in the following sections.

### 3.2.1.1 Primary Atomisation

Primary atomisation is the breakup of the liquid jet into droplets and ligaments. Several mechanisms of primary atomisation have been proposed. These include turbulence, hydrodynamic cavitation, aerodynamic forces and relaxation of the velocity profile. Reitz and Bracco (1982) found that none of these breakup mechanisms alone can explain the onset of atomisation. It is generally agreed that atomisation is a combination of these breakup mechanisms. The breakup mechanisms are described below.

Turbulence-induced breakup is caused by radial turbulent velocity fluctuations inside the jet. Here, the kinetic energy of the radial fluctuations overcomes the surface tension force of the jet, forming primary droplets (Wu and Faeth, 1995).

Hydrodynamic cavitation is the formation of bubbles and cavities in the nozzle due to localised decreases in static pressure below the vapour pressure of the fuel caused by the nozzle geometry. During injection, a vena contracta forms at the nozzle hole entrance and the resultant decrease in static pressure inside the recirculation zone causes the fuel to evaporate and vapour bubbles to be produced (Chaves et al., 1995). The vapour bubbles start as micro-bubbles, which are either present in the fuel or at the nozzle wall due to surface imperfections (Baumgarten, 2006). Upon entering the cylinder, the decay of the vapour bubbles leads to an increase in the turbulence level and hence spray disintegration (Blessing et al., 2003). Cavitation can also result in an
asymmetrical flow inside the nozzle, which can have a significant effect on the spray geometry (Blessing et al., 2003).

Aerodynamic-induced breakup is caused by the high velocity of the jet relative to the surrounding gas. During injection, small surface waves are setup on the surface of the jet as a result of turbulence inside the nozzle. Aerodynamic forces amplify the surface waves (Chen and Veshagh, 1993), which become unstable and breakup to form primary droplets. Since aerodynamic forces are time-dependant, this breakup mechanism does not explain the breakup of the spray at the nozzle exit. Therefore, it is considered to be of secondary importance.

Relaxation of the velocity profile occurs for fully turbulent pipe flow in which there is no cavitation (Baumgarten, 2006). Here, the viscous forces inside the jet cause the outer region of the jet to accelerate upon exiting the nozzle. This acceleration causes internal instabilities that result in jet breakup (Lefebvre, 1989). This method of breakup is also considered to be of secondary importance because in modern day injection systems, where cavitation is present, relaxation of the velocity profile is unlikely to occur.

3.2.1.2 Secondary Atomisation

Secondary atomisation is the subsequent breakup of droplets by aerodynamic forces. The aerodynamic forces cause the growth of surface waves, which can lead to disintegration of the droplet. The aerodynamic forces are opposed by surface tension forces, which try to retain the droplets shape. The ratio of aerodynamic forces to surface tension forces is described by the gas phase Weber number ($We_g$)

$$We_g = \frac{\rho_g V_{rel}^2 D}{\sigma_l}$$

(3.4)

where $\rho_g$ is the gas density and $V_{rel}$ is the relative velocity between the droplet and surrounding gas. Above a critical Weber number, given by Baumgarten (2006) as twelve, the droplet disintegrates into a number of smaller droplets. These droplets are then subjected to the same process. The smaller the droplets the larger the surface tension forces and the bigger the relative velocity required to breakup the droplet. Different mechanisms of disintegration exist for different size Weber numbers.
Arcoumanis et al. (1997) describe six breakup modes. With reference to Figure 3.8, these are described as follows:

1. **Vibrational breakup** ($We_g \approx 12$). The droplet flattens out and the centre narrows causing two droplets of almost identical diameter to form. A droplet of smaller diameter often forms at the point where the droplet narrows (Wierzba, 1990).

2. **Bag breakup** ($12 < We_g < 18$). The droplet flattens out into a thin film surrounded by a liquid rim. The film develops into a bag-like structure and disintegrates into a number of smaller droplets. The rim then disintegrates into a number of larger drops, resulting in a bimodal size distribution.

3. **Bag and streamer breakup** ($18 < We_g < 45$). This breakup mode is similar to bag breakup, but with the development of a streamer. The streamer breaks up shortly after the bag-like structure, disintegrating into droplets of similar size.

4. **Chaotic breakup** ($45 < We_g < 100$). This is a transitional stage of breakup where both bag breakup and stripping of small droplets from the boundary layer occur. At a critical deformation, the droplet breaks up into a number of larger droplets, causing a bimodal size distribution.

5. **Stripping breakup** ($100 < We_g < 1000$). Small droplets are stripped from the boundary layer of the droplet by shear forces. As with chaotic breakup, once the droplet reaches a critical deformation it breaks up into larger droplets, causing a bimodal size distribution.

6. **Catastrophic breakup** ($We_g > 1000$). The droplet abruptly breaks up into a number of smaller droplets.

All of the breakup mechanisms described above are present in diesel engines. Generally, secondary atomisation occurs close to the nozzle exit where the gas phase Weber numbers are high. Downstream of the nozzle, the Weber numbers are typically smaller due to smaller droplet sizes caused by breakup, evaporation and reduction of the relative velocity by drag forces.
Secondary breakup can also be caused by droplet collision. Droplet collision can result in a number of scenarios, including shattering collision, bouncing collision, grazing collision and permanent coalescence (Arcoumanis et al., 1997). These collisions can result in changes in droplet size and velocity, hence affecting the development of the spray.

### 3.2.2 Spray Characteristics

Figure 3.9 shows the structure of a typical diesel fuel spray. Immediately after the SOI, the spray breaks up into droplets and ligaments, forming a dense liquid core. The leading droplets and ligaments are decelerated by aerodynamic forces. This reduces the resistance encountered by the following droplets, which can then penetrate further. The faster moving droplets entering the spray push the slower moving droplets to the spray periphery, causing the spray to diverge. This divergence is characterised by the spray cone angle ($\theta$). The interaction of the spray with the surrounding gas leads to the exchange of momentum and the entrainment of the high temperature in-cylinder charge.
The spray breakup leads to the formation of droplets of different sizes. These are characterised by a representative diameter, the Sauter Mean Diameter (SMD), which will be discussed in section 3.2.2.4. The proceeding evaporation of the fuel leads to the formation of a fuel vapour-air mixture. In the early stages of injection, this forms alongside the liquid core (Dec, 1997). Sometime after the SOI, the liquid core reaches its maximum penetration length, referred to as the liquid breakup length \((L_c)\). Following maximum penetration of the liquid core, the fuel vapour-air mixture continues to penetrate, but at a decreasing rate, ultimately forming a head vortex. The penetration distance of the spray is referred to as the spray tip penetration \((S)\).

The spray characteristics described above have an important influence on air utilisation and the fuel-air mixing rate. The spray penetration and corresponding spray cone angle are important for ensuring adequate air utilisation. Over penetration of the fuel spray can degrade emissions as a result of spray wall impingement, whilst under penetration can lead to inadequate mixing. Small droplet size is also important to ensure rapid evaporation and mixing. The spray characteristics highlighted in Figure 3.9 commonly appear as correlations in engine modelling. These correlations are discussed in the following sections.
3.2.2.1 Spray Tip Penetration

Many correlations for spray tip penetration ($S$) have been proposed. A review of the early literature, completed by Hay and Jones (1972), recommended the correlations of Wakuri et al. (1960) and Dent (1971). Dent’s correlation, based on gas jet mixing theory, is frequently cited in the literature and is given by

$$S = 3.07 \left[ \frac{(\Delta P)}{\rho_g} \right]^{0.5} tD \left( \frac{294}{T_g} \right)^{0.25}$$

(3.5)

where $\Delta P$ is the pressure differential between the injection pressure and mean in-cylinder pressure (in Pa), $t$ is time and $T_g$ is the gas temperature. The correlation satisfied data from many sources and was recommended by Hay and Jones (1972) for in-cylinder pressures up to 100 bar.

Another notable spray tip correlation, widely cited in the literature, was proposed by Arai et al. (1984). They proposed a correlation for the spray tip penetration before and after the breakup time. Figure 3.10 shows a schematic, based on their experimental work, of spray tip penetration against time. During the early stages of injection, the injection rate is proportional to time. After a short period, characterised by the breakup time ($t_b$), the spray penetration is assumed to be proportional to the square root of time, as given by gas jet mixing theory.

![Spray Tip Penetration](image)

**Figure 3.10** – Schematic of spray tip penetration [Adapted from Arai et al. (1984)]
On this basis, Arai et al. (1984) proposed the following correlation for spray tip penetration before and after breakup.

Before breakup, $0 < t < t_b$

$$S = 0.39 \left( \frac{2\Delta P}{\rho_l} \right)^{0.5} t \quad \text{(3.6)}$$

After breakup, $t > t_b$

$$S = 2.95 \left( \frac{\Delta P}{\rho_g} \right)^{0.25} (tD)^{0.5} \quad \text{(3.7)}$$

where $t_b$ is the breakup time

$$t_b = 28.65 \left( \frac{\rho_lD}{\rho_g \Delta P} \right)^{0.5} \quad \text{(3.8)}$$

This correlation contains a discharge coefficient of 0.39, which is embedded within the constant. Jung and Assanis (2001) stated that modern injector nozzles have discharge coefficients in the range between 0.6 and 0.8. They noted that after breakup ($t > t_b$), the correlation of Arai et al. (1984) shows good agreement with experimental data for a range of discharge coefficients. However, before breakup ($t < t_b$), the correlation was updated for application to injectors with different discharge coefficients ($C_d$).

Before breakup, $0 < t < t_b$

$$S = C_d \left( \frac{2\Delta P}{\rho_l} \right)^{0.5} t \quad \text{(3.9)}$$

where the breakup time, $t_b$, equals
\[ t_b = 4.351 \left( \frac{\rho_l D}{C_d^2 (\rho_g \Delta P)^{0.5}} \right) \] (3.10)

The correlation employed by Jung and Assanis (2001) was validated against the experimental data of Dan et al. (1997) for injection pressures ranging from 550 to 1200 bar. The ambient gas used was nitrogen (N\(_2\)) and the fuel injected was n-tridecane (C\(_{13}\)H\(_{28}\)). This extended the validity of the pressure range of the original correlation and makes it applicable to modern common rail systems using single-hole mini-sac nozzles. It was observed that the modified spray correlation over-predicts penetration in the early stages of fuel injection. Kennaird et al. (2002) compared both single mini-sac, multi-hole mini-sac and valve covered orifice (VCO) nozzles and proposed a new constant for the correlation of Arai et al. (1984) after breakup. This was given as 6.5. Interestingly, the single-hole VCO nozzle required an additional time offset to account for an initial hesitation period at the SOI. This phenomenon was also observed by Morgan et al. (2001) and Abdelghaffar et al. (2007).

Table 3.1 outlines the key parameters and weights of the current spray tip penetration correlations available in the literature. All of the correlations agree that the key parameters affecting spray tip penetration are time, nozzle orifice diameter, pressure differential across the injector and in-cylinder gas density. The weights of these parameters are in good agreement. It is generally agreed that following breakup the spray penetration is proportional to the square root of time. For increasing pressure differentials the spray penetrates further as a result of increasing momentum, whilst for increasing gas density spray penetration decreases due to increased drag forces. An increase in the orifice diameter increases the momentum of the spray and hence the spray penetration increases. The correlations of Wakuri et al. (1960), Schihl et al. (1996), Naber and Siebers (1996) and Arrège et al. (1999) also include the spray cone angle, \( \theta \), as a key parameter. This parameter and the spray penetration are intrinsically linked; the spray cone angle reducing (increasing) for an increase (decrease) in spray penetration. Varde and Popa (1983) and Renner and Maly (1994) include a characteristic nozzle parameter, the ratio of nozzle length to nozzle orifice diameter (\( L/D \)), to account for the effects of nozzle geometry on spray tip penetration. The effect of the \( L/D \) ratio is discussed in more detail in relation to the spray cone angle in the next section.
Dent (1971) is the only author to account for the effects of evaporation by including a temperature term which predicts a reduction in the spray tip penetration. This is caused by cooling of the hot entrained gases, which increases the local gas density, thus decreasing the spray penetration. Morgan et al. (2001) commented that this term does not adequately compensate for this effect, since the correlation only predicts a 5 percent change in penetration, whilst the observed results are 13 to 18 percent. Naber and Siebers (1996) noted that the effects of evaporation decrease with increasing gas density.

In the correlation of Renner and Maly (1994), the weight of the nozzle diameter parameter is primarily attributed to the effective hydraulic diameter ($D_{\text{eff}}$). This accounts for separation of the flow from the nozzle wall, which results in a smaller effective nozzle diameter. Renner and Maly (1994) also included a viscosity ratio ($\mu_l/\mu_g$) to account for the effect of spray breakup on spray penetration.

The effect of methane in air is to decrease the in-cylinder pressure, thus increasing the pressure differential across the injector, and to decrease the gas density. This results in an increase in spray penetration. Since the spray penetration and spray cone angle are intrinsically linked, the effect of methane in air is to decrease the spray cone angle. This is because as the gas density decreases a smaller mass of fuel is pushed to the spray periphery. The main parameters affecting the spray cone angle are discussed in the next section.
Table 3.1 – Comparison of spray tip penetration correlations

<table>
<thead>
<tr>
<th>Reference</th>
<th>$t$</th>
<th>$D$</th>
<th>$\Delta P$</th>
<th>$\rho_g$</th>
<th>$\rho_l$</th>
<th>$\Delta\rho$</th>
<th>$\theta$</th>
<th>$\tan\left(\frac{\theta}{2}\right)$</th>
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<th>$T_g$</th>
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(1) Injection pressure, $P_{inj}$
3.2.2.2 Spray Cone Angle

Lefebvre (1989) defines the spray cone angle (θ) as the angle formed by two straight lines drawn from the discharge orifice to cut the spray contours at a specific distance from the atomizer (nozzle) face. Arai et al. (1984) defined this distance as sixty orifice diameters downstream of the nozzle (Figure 3.11).

![Figure 3.11 – Definition of spray cone angle [Adapted from Arai et al. (1984)]](image)

The spray cone angle is usually measured using photographic techniques. Several correlations for the spray cone angle have been proposed. The two main correlations cited in the literature are by Reitz and Bracco (1979) and Hiroyasu et al. (1980). According to Reitz and Bracco (1979), the spray cone angle can be determined by combining the radial velocity of the fastest growing unstable surface wave with the axial injection velocity. This gives the following expression for the spray cone angle

\[
\tan \left( \frac{\theta}{2} \right) = \frac{4\pi}{A} \left( \frac{\rho_g}{\rho_t} \right)^{0.5} \cdot f^\pi \left( \frac{\rho_t}{\rho_g} \frac{Re}{We_t} \right)^2
\]  

(3.11)

where

\[
A = 3.0 + 0.28 \left( \frac{L}{D} \right)
\]

(3.12)

for sharp edge inlet nozzles. The function \( f^\pi \) is shown in Figure 3.12 and tends to \( \sqrt{3}/6 \) when the argument of the operating conditions is greater than unity, which is typically the case for sprays in the atomisation regime (Chehroudi et al., 1985).
The correlation of Hiroyasu et al. (1980) is given by

$$\theta = 0.05 \left( \frac{\rho_g \Delta P D^2}{\mu_g^2} \right)^{0.25}$$

(3.13)

where $\mu_g$ is the gas dynamic viscosity. Hiroyasu and Arai (1990) later proposed the following correlation, applicable to sac hole nozzles

$$\theta = 83.5 \left( \frac{L}{D} \right)^{-0.22} \left( \frac{D}{D_o} \right)^{0.15} \left( \frac{\rho_g}{\rho_l} \right)^{0.26}$$

(3.14)

where $D_o$ is the sac hole diameter. The $L/D$ and $D/D_o$ terms consider the effects of nozzle geometry on cavitation and its subsequent effect on the spray cone angle. Small values of $L/D$ lead to an increase in the spray cone angle due to the decay of cavitation bubbles beyond the nozzle exit. Large values of $D/D_o$ promote cavitation at the nozzle entrance, resulting in an increase in spray cone angle due to increased turbulence (Baumgarten, 2006).

Table 3.2 outlines the parameters and weights of the spray cone angle correlations currently available in the literature. Aside from the early proposal of Hiroyasu et al. (1980), all the other correlations show no dependence on pressure (Arrègle et al. (1999) $\Delta P \to 0$). Hiroyasu and Arai (1990) later showed that for a spray in the atomisation regime, the spray cone angle is independent of pressure.
### Table 3.2 – Comparison of spray cone angle correlations

<table>
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<td>-</td>
</tr>
<tr>
<td>Varde et al. (1984)</td>
<td>-</td>
<td>-</td>
<td>0.33</td>
<td>-0.33</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Hiroyasu and Arai (1990)</td>
<td>0.15</td>
<td>-</td>
<td>0.26</td>
<td>-0.26</td>
<td>-0.22</td>
<td>-0.15</td>
<td></td>
</tr>
<tr>
<td>Arrègle et al. (1999)</td>
<td>0.508</td>
<td>0.00943(^{(1)})</td>
<td>0.335</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

\(^{(1)} \) Injection pressure, \( P_{inj} \)

From Table 3.2, the main parameter affecting the spray cone angle is the gas density, but there is little agreement over the importance of this parameter. As gas density increases the spray penetration decreases, resulting in a larger mass of fuel being pushed to the spray periphery, thus increasing the spray cone angle. Arrègle et al. (1999) showed that for a common rail system, the nozzle orifice diameter also has an important influence on the spray cone angle. An increase in the nozzle orifice diameter reduces the spray cone angle due to the formation of larger initial droplets, which take longer to breakup and entrain surrounding gas. As discussed, nozzle geometry also has an important influence on the spray cone angle due to the inception of cavitation.

### 3.2.2.3 Liquid Breakup Length

The liquid breakup length \( (L_c) \) is measured along the spray centreline and refers to the distance from the nozzle exit to the point of breakup of the dense liquid core. The following correlations for liquid breakup length were obtained using an electrical resistance method in which the working fluid was water. Arai et al. (1984) proposed a correlation for the breakup length given by

\[
L_c = 15.8 \left( \frac{\rho_l}{\rho_g} \right)^{0.5} D
\]  

where the breakup length is considered to be dependent on the density ratio \( \rho_l/\rho_g \) and the nozzle orifice diameter, \( D \). Hiroyasu and Arai (1990) later proposed a more detailed correlation, including terms to account for nozzle shape and in-flow conditions.
where \( r \) is the nozzle entrance radius and \( P_g / \rho_l V^2 \) is the dimensionless cavitation number. The liquid breakup length trends can be summarised as follows. The effect of increasing the gas density is to decrease the liquid breakup length due to increased aerodynamic forces. Increased cavitation, also promoted by decreased inlet rounding, results in a decreased liquid breakup length due to increased levels of turbulence. Moreover, the effect of larger \( L / D \) ratios is to increase the liquid breakup length. An increase in nozzle diameter increases the liquid breakup length due to the formation of larger droplets, which have higher momentum. The influence of methane in air is to increase the liquid gas density ratio \( \rho_l / \rho_g \); this increases the breakup length due to the decrease in aerodynamic forces.

### 3.2.2.4 Representative Diameter

Sprays are characterised by a mean droplet diameter which is representative of the entire spray. There are a number of different mean diameters \( D_{ab} \), as discussed by Lefebvre (1989). These can be expressed in general form by

\[
D_{ab} = \left[ \frac{\sum N_i D_i^a}{\sum N_i D_i^b} \right]^{1/(a-b)}
\]

(3.17)

where \( a \) and \( b \) refer to the effect investigated (Table 3.3), \( i \) is the size range considered, \( N_i \) is the number of drops in the size range and \( D_i \) is the median diameter of the size range.

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length</td>
<td>1</td>
</tr>
<tr>
<td>Area</td>
<td>2</td>
</tr>
<tr>
<td>Volume</td>
<td>3</td>
</tr>
</tbody>
</table>

In combustion modelling, spray droplets are characterised by the Sauter Mean Diameter (SMD). Hiroyasu and Kadota (1974) describe the SMD as the diameter of a
droplet that has the same volume to surface ratio as that of the total spray. This can be expressed by

\[
SMD = D_{32} = \frac{\sum N_i D_i^3}{\sum N_i D_i^2}
\]  

(3.18)

The SMD is used because the surface area and volume have important effects on the evaporation and combustion events in engines. There are a number of different experimental techniques for determining the SMD, as described by Hiroyasu and Kadota (1974). An early study by these authors used a liquid emersion technique to obtain an SMD correlation for a nozzle opening pressure of 99 bar.

Elkobt (1982) obtained the following correlation for the SMD using a liquid emersion technique and a maximum injection pressure of 1180 bar

\[
SMD = 107(Re)^{-0.183}(We)_{l}^{-0.442}(C_d)^{-0.442}\left(\frac{\rho_l}{\rho_g}\right)^{-0.05} D
\]  

(3.19)

Hiroyasu et al. (1989) obtained a correlation for the SMD using the Fraunhofer diffraction technique with injection pressures ranging from 35 to 900 bar.

\[
SMD = 0.38(Re)^{0.25}(We)_{l}^{-0.32}\left(\frac{\mu_l}{\mu_g}\right)^{0.37}\left(\frac{\rho_l}{\rho_g}\right)^{-0.47} D
\]  

(3.20)

The measurements in the above study were taken across a sample volume of the spray and therefore, as a description of the entire spray include a degree of uncertainty. Yamane et al. (1994) used a technique to measure the SMD of the entire spray for injection pressures ranging from 550 to 1330 bar. Their correlation expresses the effects of the nozzle diameter, injection velocity and the gas density on the SMD.

\[
SMD = 47(Re)^{-0.5}\left(\frac{\rho_g}{\rho_l}\right)^{0.26} D
\]  

(3.21)

Table 3.4 outlines the parameters and weights of the current SMD correlations available in the literature. The main parameters affecting the SMD are the liquid and
gas density, and the Reynolds and liquid Weber number. There is little agreement
over the weight of these parameters, which is most probably due to the range of
experimental techniques used to collect the data. In the work of Renner and Maly
(1994), the non-dimensional group for liquid and gas density is in contrast to the other
correlations, which account for coalescence with increasing gas density. In general,
the SMD decreases with increasing velocity due to increases in the turbulence and
aerodynamic forces that promote breakup. In contrast, the SMD increases with liquid
viscosity and surface tension, which oppose breakup. The nozzle diameter also
increases the SMD due to the initial formation of larger droplets.

Table 3.4 – Comparison of SMD correlations

<table>
<thead>
<tr>
<th>Reference</th>
<th>$D$</th>
<th>$\Delta P$</th>
<th>$\rho_g$</th>
<th>$\rho_l$</th>
<th>$\mu_l/\mu_g$</th>
<th>$Re$</th>
<th>$We$</th>
<th>$C_d$</th>
<th>$Q$ (1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hiroyasu and Kadota (1974)</td>
<td>-</td>
<td>-0.135</td>
<td>0.121</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.131</td>
</tr>
<tr>
<td>Elkobt (1982)</td>
<td>1</td>
<td>-</td>
<td>0.05</td>
<td>-0.05</td>
<td>-</td>
<td>-0.183</td>
<td>-0.442(l)</td>
<td>-0.422</td>
<td>-</td>
</tr>
<tr>
<td>Varde et al. (1984)</td>
<td>1</td>
<td>0.26</td>
<td>-</td>
<td>-</td>
<td>0.26</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Hiroyasu et al. (1989)</td>
<td>1</td>
<td>-0.11</td>
<td>0.11</td>
<td>0.37</td>
<td>0.25</td>
<td>0.37</td>
<td>-</td>
<td>-</td>
<td>-0.32(l)</td>
</tr>
<tr>
<td>Renner and Maly (1994)</td>
<td>1</td>
<td>-0.26</td>
<td>-0.26</td>
<td>-</td>
<td>-0.5</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

(1) $Q$ (m$^3$.stroke$^{-1}$)

The effect of methane in air is to decrease the in-cylinder pressure, thus increasing the
jet velocity. This increases the external pressure forces acting on the jet and promotes
the effects of turbulence. However, the addition of methane also reduces the gas
density, which can lead to a reduction in aerodynamic forces. The addition of methane
also reduces the probability of permanent coalescence.
3.2.2.5 Swirl

In diesel engines, many combustion chambers employ in-cylinder swirl to promote fuel-air mixing rates. Figure 3.13 shows the geometry of a fuel spray in the presence of swirl. As the fuel spray is decelerated it becomes increasingly deflected in the tangential direction. Figure 3.13 demonstrates the importance of swirl, illustrating the significant increase in the size of the fuel vapour-air mixture.

![Schematic of a fuel spray in the presence of swirl](image)

Figure 3.13 – Schematic of a fuel spray in the presence of swirl

The effect of swirl on the spray characteristics is to reduce the spray penetration and increase the spray cone angle. Chiu et al. (1976) and Hiroyasu et al. (1983) included correction factors to account for the effect of swirl on the spray penetration in their respective spray models. The spray penetration with swirl ($S_S$), as expressed by Chiu et al. (1976), is given by

$$\frac{S - S_S}{S} = 0.35 \left( \frac{S_S Q_g}{D Q_j} \right)^{0.44}$$  \hspace{1cm} (3.22)

where $Q_g$ and $Q_j$ are the momenta of the gas and fuel jet respectively

$$Q_g = \rho_g S_S^2 \omega_S^2$$ \hspace{1cm} (3.23)

$$Q_j = \rho_l V_0^2$$ \hspace{1cm} (3.24)
and $\omega_S$ is the angular velocity (in rps) of the cylinder charge and $V_0$ is the initial velocity of the fuel spray. Hiroyasu et al. (1983) expressed the reduction in spray penetration as

$$S_S = \left(1 + \frac{\pi R_S N S}{30 V_0}\right)^{-1} S$$  \hspace{1cm} (3.25)

where $N$ is the engine speed (in rpm). Moreover, Hiroyasu et al. (1980) expressed the effect of swirl on the spray cone angle. Accordingly, the spray cone angle with swirl ($\theta_S$) is given by

$$\theta_S = \left(1 + \frac{\pi R_S N S}{30 V_0}\right)^2 \theta$$  \hspace{1cm} (3.26)

### 3.2.3 Spray Modelling

Several models have been developed to describe fuel spray formation in internal combustion engines. One of the most important aspects of these models is the calculation of the entrainment rate, as this has an important influence on the subsequent combustion processes. Many models use correlations, as described in sections 3.2.2.1 through 3.2.2.5, to describe the spray development and hence gas entrainment rate. The simplest method of describing a fuel spray is via a single zone. The drawback of this method is that quantitative predictions of emissions cannot be made due to the heterogeneous nature of fuel sprays. Hence, more complex models divide the fuel spray into multiple zones to account for temporal and spatial variations in composition and temperature. In the following, the most important spray models identified in the literature are described and reviewed.

#### 3.2.3.1 Cummins Model

The Cummins model (Shahed et al., 1975, Chiu et al., 1976) treats the spray as a steady gas jet in which the fuel is considered to be a vapour. In this approach, the spray geometry is described using correlations for spray tip penetration, spray width growth rate and spray trajectory. The fuel distribution within the spray is described by a similarity profile across the spray cross-section and a hyperbolic profile along the spray axis.
The rates of combustion and pollutant formation are determined by superimposing discrete zones onto the spray geometry, with each zone bounded by equivalence ratio limits. Figure 3.14 shows the progression of the boundary zones.

Zone A corresponds to the surrounding gases into which the fuel is injected. The central zone, zone C, corresponds to the dense liquid core and zone B to the prepared mixture. Zone B is further divided and bounded by fuel equivalence ratios between the rich and lean flammability limits, $\phi_R$ and $\phi_L$, of zones C and A respectively.

At each time step, following the definition of the spray geometry, the equivalence ratio boundaries of each zone are calculated. This is achieved by proceeding from the leanest flammability limit towards the richest flammability limit on the basis that the mass of fuel in each zone remains the same. The gases entrained into zone C are then assigned to a new sub-division of zone B. Fuel beyond the lean flammability limit is added to zone A. Once the zone boundaries have been defined, the combustible mixture preparation and entrainment rate for each zone are calculated. The entrainment rate is equal to the change in mass of the sub-zone. In this model, combustion is assumed to have no effect on the fuel-gas mixing rate.

The Cummins model is also able to predict spray behaviour in the presence of swirl. This is achieved by using a correction factor for the spray penetration (equation (3.22)) in conjunction with definitions for the spray trajectory and average cross-section of the spray. The tangential displacement due to swirl ($S_T$) is given by
\[ S_t = D \left( \frac{Q_g}{Q_j} \right) \left( \frac{r}{D} \right)^{2.217} \]  

(3.27)

where \( r \) is the radial coordinate in the combustion chamber. The average cross-section of the spray, with reference to Figure 3.15, is given by

\[ b = \sqrt{\frac{b_3(b_1 + b_2)}{2}} \]  

(3.28)

where the radius change with spray direction (\( x \)) is given as

\[ \frac{db_1}{dx} = 0.12 \left( 1 + \frac{\rho_g}{\rho_j} \right) \]  

(3.29)

and

\[ b_2 = b_1(1 + 0.0016Re^{0.66}) \]  

(3.30)

\[ b_3 = b_1 + 0.11x \left( \frac{\rho_g}{\rho_j} \right) \]  

(3.31)

The Reynolds number in equation (3.30) is given in terms of the angular velocity, \( \omega_s \), in (rps)

\[ Re = \frac{2\pi\rho_g r\omega_s D}{\mu_g} \]  

(3.32)
As described, the Cummins model treats the fuel spray as a steady gas jet, thus neglecting atomisation and the subsequent evaporation process. A major drawback of this assumption is that chemical kinetics cannot be used to predict the ignition delay period, since the local fuel vapour-oxygen concentrations are not modelled. Another consequence of assuming that the spray is a gaseous jet is under-prediction of the fuel spray penetration. A further drawback of the Cummins model is that a detailed description of spray wall impingement is not considered.

Figure 3.15 – Definition of the average cross-section of a spray in the presence of swirl as defined by the Cummins model [Adapted from Chiu et al. (1976)]
3.2.3.2 Packet Models

The packet model (Figure 3.16), originally proposed by Hiroyasu et al. (1983) and later applied and developed by several other authors, for example Bazari (1992), Stiesch and Merker (1999), Jung and Assanis (2001) and Hountalas et al. (2002), is frequently used to describe spray formation in diesel engines. In this approach, the spray is modelled as a number of discrete packets, whose spatial distribution are representative of the overall spray geometry. In general, the spray behaviour is defined by experimental correlations for spray tip penetration and spray cone angle.

![Figure 3.16 – Schematic of the packet model [Merker et al. (2006)]](image)

The discretization of the spray is achieved by dividing it in the axial and radial directions on the basis that there is equal mass of fuel in each packet for a given spray segment. The division of the packets in the radial direction is fixed geometrically. In the axial direction, the divisions occur at equal time increments.

Figure 3.17 shows the progression of the composition of an individual spray packet. Each packet is considered as a thermodynamic control volume, in which atomisation, evaporation, mixing, ignition, combustion and pollutant formation occur. Initially, the spray packets contain only liquid fuel. Following spray breakup, surrounding gases are entrained into the spray packets on the basis of momentum conservation. The sub processes of evaporation, mixing, ignition, combustion and pollutant formation then proceed. At any one time, each packet may contain fuel droplets, fuel vapour, entrained gases and combustion products. The growth of the spray is determined by the entrainment rate and the expansion of each packet as a result of combustion. All the sub processes occur with the assumption that there is no mass or energy transfer between packets. Therefore, each packet has its own temperature and composition history and the total energy release rate and emissions are calculated by summing the individual packets. In general, in this type of model, it is assumed that combustion has no effect on entrainment, although in the original model, Hiroyasu et al. (1983) did account for a reduction in the entrainment rate following the SOC.
The packet model has the potential to predict spray behaviour for the cases of in-cylinder swirl and spray wall impingement. In the case of in-cylinder swirl, a correction factor (equation (3.25)) is often applied to the correlation for spray tip penetration and a tangential deflection is applied to each packet.

A major difference between the Cummins and packet model is the way in which the spray is divided into zones. In the packet model, zone division is completed at spray inception, whereas in the Cummins model zone division is completed later. Hence, the packet model allows pollutant formation to be directly coupled to each zone. With reference to dual fuel modelling, the packet model allows the direct coupling of the ignition and flame propagation processes. By coupling the ignition of individual packets to the development of the flame front area, ignition of the pilot fuel spray has a direct influence on the rate of premixed combustion.

**Figure 3.17** – Schematic of the composition of an individual spray packet [Adapted from Merker et al. (2006)]
3.3 IGNITION DELAY MODELLING IN DUAL FUEL ENGINES

The ignition delay period has a significant influence on the subsequent combustion processes and overall performance and emissions of an engine. Hence, suitable methods for predicting the ignition delay are important for predicting engine performance and emissions. The ignition delay period is defined as the time between the SOI and SOC. In experimental work, the definition of ignition is arbitrary and has been defined in a number of ways, as described by Zhou and Karim (1994). It is usually defined as the point at which an increase in in-cylinder pressure due to exothermic energy release is detected.

3.3.1 Ignition Delay Correlations

In general, dual fuel combustion models employ diesel engine correlations to predict the ignition delay period ($\tau$). These are commonly expressed in the form presented by Liu and Karim (1995a)

$$\tau = AP^a \phi^b \exp \left( \frac{c}{T_g} \right)$$  \hspace{1cm} (3.33)

where $P$ and $T_g$ are the mean in-cylinder pressure (in atm) and mean charge temperature during the ignition delay period, and $\phi$ is the fuel-air equivalence ratio of the charge. The constants $A$, $a$, $b$ and $c$ are determined experimentally. This approach gives limited agreement with experimental data, as shown in the studies of Raine (1990), where $b$ is taken to be equal to zero, and Papagiannakis et al. (2005). This is due to the additional effects that contribute to the ignition delay in dual fuel engines, as discussed in Chapter 2 (section 2.1.3.4). These include changes in the physical properties of the charge; the occurrence of pre-ignition reactions; changes in the heat transfer characteristics; and the effects of exhaust gas residuals.

Liu and Karim (1995a) extended the general expression for ignition delay to include these effects by considering their contribution to the charge temperature and pressure.

$$\tau + \Delta \tau = A(P + \Delta P)^a(\phi + \Delta \phi)^b \exp \left( \frac{c}{T_g + \Delta T} \right)$$  \hspace{1cm} (3.34)
CHAPTER 3 COMBUSTION MODELLING

This correlation was used in conjunction with detailed chemical kinetics to perform a study of the effects of intake concentration on the ignition delay for a range of gaseous fuels. The chemical scheme included 138 reaction steps with 32 species. Due to the strong dependence of the ignition delay on temperature, the pre-ignition reactions, heat transfer and residual gases were considered to have an important influence on the ignition delay. It was observed that the ignition delay in a dual fuel engine is strongly dependent on the type of gaseous fuel employed and its concentration in the cylinder.

Prakash et al. (1999) modified the ignition delay correlation of Hardenberg and Hase (1979) for application to dual fuel engines. The correlation was adapted to consider changes in temperature at the end of compression and oxygen concentration in the charge due to the induction of a gaseous fuel. According to Prakash et al. (1999), the ignition delay for a dual fuel engine is given by

\[ \tau = A C_f O_c^k \exp(E \cdot P + Q^{0.63}) \]  

(3.35)

where

\[ A = 0.36 + 0.22 S_p \]  

(3.36)

\[ E = \frac{618840}{CN + 25} \]  

(3.37)

\[ P = \frac{1}{R_u T_{BDC} r_c^{n_{df} - 1}} - \frac{1}{17190} \]  

(3.38)

and

\[ Q = \frac{21.2}{P_m r_c^{n_{df} - 12.4}} \]  

(3.39)

In the above, \( C_f \) is a modified correction constant, \( S_p \) is the mean piston speed, \( O_c \) is the relative oxygen concentration, \( k \) is a constant, \( R_u \) is the universal gas constant, \( T_{BDC} \) is the temperature at bottom dead centre (BDC), \( n \) is the polytropic index of
compression and $P_m$ is the intake manifold pressure (in bar). Equation (3.37) gives the activation energy, $E$, as a function of the Cetane number (CN) of the diesel fuel.

In equation (3.35), the relative oxygen concentration, $O_c$, accounts for the reduction in oxygen concentration due to the induction of a gaseous fuel. This is defined as the ratio of the concentration of oxygen in the cylinder to the concentration of oxygen in atmospheric air. Though the oxygen concentration decreases with gas concentration, it increases with load. This is due to the increased temperatures of the combustion products, which aid the scavenging of the cylinder, leading to a reduced mass of residuals.

Prakash et al. (1999) showed that the polytropic index of compression, $n$, decreases linearly with gaseous fuel concentration ($f_p$) (Figure 3.18).

![Figure 3.18](image)

**Figure 3.18** – Variation of polytropic index of compression with gaseous fuel concentration at different loads [Adapted from Prakash et al. (1999)]

This variation affects the temperature at the SOI, which has a significant effect on the ignition delay. The relationship between the polytropic index of compression and the gaseous fuel concentration can be expressed as

$$n_{df} = n_d - 0.23 f_p$$  \hspace{1cm} (3.40)

where the subscripts $df$ and $d$ correspond to dual fuel and diesel operation respectively.
The effect of load on the ignition delay was considered by including $T_{BDC}$. This was calculated using the method of Pedersen and Qvale (1974), whereby the exhaust gas residuals and inducted charge are treated as ideal gases which are mixed adiabatically. The temperature at BDC increases with load, but decreases with increasing gas substitution. This results in lower temperatures at the point of injection, which increases the ignition delay.

Prakash et al. (1999) validated the correlation against experimental data taken from a naturally aspirated, single-cylinder, direct injection engine operating on biogas. The predicted ignition delay periods were in good agreement with experimental data, with the majority of the data being within 10 percent degrees crank angle of the predicted ignition delay. It was concluded that further improvements could be made if pre-ignition reactions were also considered.

### 3.3.2 The Shell Model

The Shell model (Halstead et al., 1977) is a phenomenological model that uses a simplified reaction mechanism to predict the autoignition of hydrocarbon fuels, and was originally used to study knock in spark ignition engines. The model was later modified by Kong and Reitz (1993) to predict ignition in diesel engines. The model assumes that degenerative branching controls the two-stage ignition and cool flame phenomena observed during hydrocarbon autoignition.

The Shell model consists of eight reactions and five generic species. The reactions are as follows:

**Initiation:**

$$RH + O_2 \xrightarrow{k_q} 2R^* \quad (3.41)$$

**Propagation:**

$$R^* \xrightarrow{k_p} R^* + P + \text{Heat} \quad (3.42)$$

**Propagation:**

$$R^* \xrightarrow{f_{1k_p}} R^* + B \quad (3.43)$$

**Propagation:**

$$R^* \xrightarrow{f_{4k_p}} R^* + Q \quad (3.44)$$
Propagation:

\[ R^* + Q \xrightarrow{f_2k_p} R^* + B \quad (3.45) \]

Branching:

\[ B \xrightarrow{k_b} 2R^* \quad (3.46) \]

Linear termination:

\[ R^* \xrightarrow{f_3k_p} \text{termination} \quad (3.47) \]

Quadratic termination:

\[ 2R^* \xrightarrow{k_t} \text{termination} \quad (3.48) \]

where RH is the fuel, R* is a generalised radical, B is a branching agent, Q is an intermediate species and P represents the products CO, CO₂ and H₂O. The rate coefficients in equations (3.41) to (3.48) are given by

\[ f_i = A_{fi}\exp\left(-E_{fi}/R_uT\right)[O_2]^{x_i}[RH]^{y_i} \quad (3.49) \]

\[ k_j = A_j\exp\left(-E_j/R_uT\right) \quad (3.50) \]

\[ k_p = \left[ \frac{1}{k_{p1}[O_2]} + \frac{1}{k_{p2}} + \frac{1}{k_{p3}[RH]} \right]^{-1} \quad (3.51) \]

where \( i \) and \( j \) take the terms 1, 2, 3, 4 and, \( p1, p2, p3, q, b \) and \( t \) respectively. In total there are twenty six different parameters, which are adjusted to predict the autoignition of different fuels. Kong et al. (1995) present the parameters for three fuels of different octane ratings in their study. Krishnan et al. (2007) used the original model coefficients for 90 research octane number (RON) fuel, but modified the pre-exponential factor controlling fuel consumption (\( A_{p3} \)) to match the experimentally observed data for dual fuel engines operating at advanced injection timings.

In the original Shell model (Halstead et al., 1977), the ignition point was set using an arbitrary temperature of 1100 K. This temperature was determined using an energy balance which considered the chemical heat release, heat loss rate and work due to piston motion. The ignition temperature for the reviewed dual fuel studies ranged from 1000 K to 1200 K (Cordiner et al. (2008) and Zhang et al. (2003) respectively).
3.4 CONCLUDING SUMMARY

Suitable combustion models can describe details of complicated mixing, combustion and emissions processes in internal combustion engines. At this time, the development of such models for dual fuel engines has been limited. This is mainly due to the complex nature of the combustion phenomena occurring inside the cylinder. The following conclusions can be drawn from the current chapter:

- The majority of dual fuel modelling studies are validated by comparison of experimental and predicted pressure diagrams. Few studies also compare the experimental and predicted energy release rates.

- The understanding of flame development following diesel ignition is lacking. This is reflected in the current models, which over-predict the pressure and energy release rate during the final stage of combustion. In their quasi-dimensional model, Krishnan et al. (2007) identified the strong influence that spray combustion has on the turbulent combustion of the gaseous mixture in an ALPING-LTC engine. This type of study has yet to be applied to a conventional dual fuel engine.

- In recent years, a number of multi-dimensional models have been developed to investigate dual fuel combustion. At present, this type of model is unable to accurately predict the turbulent combustion of the gaseous charge. Hence, for the prediction of pressure and energy release rate diagrams, the multi-dimensional model is currently no better than the zero- or quasi-dimensional approach. Coupled with the high computational demands of this type of model, the zero- or quasi-dimensional approach is viewed as being more suitable for the investigation of the fundamental aspects of dual fuel combustion.

- The current zero-dimensional dual fuel modelling studies only allow qualitative predictions of engine-out emissions. The current quasi-dimensional models are interested in the prediction of dual fuel engine performance and only compare emissions for limited operating conditions. Thus, the quasi-dimensional model, which is able to represent the heterogeneous nature of a diesel fuel spray, has been underused for the prediction of engine-out emissions.
• The main characteristics of the spray, including spray tip penetration, spray cone angle, breakup length and SMD can be described using correlations obtained from experimental work. Currently, there is no general expression for the description of each of the spray characteristics, although the main parameters affecting them are agreed in each case.

• There is currently no accepted method for the prediction of the ignition delay period in dual fuel engines. Currently, the majority of models employ standard or modified versions of correlations used to predict diesel ignition.

A suitable approach needs to be developed that can simulate the complex combustion and emissions processes present in the dual fuel engine. On this basis, a new quasi-dimensional combustion model has been developed (as discussed in the following chapter) that considers the phenomena associated with fuel injection, atomisation, mixing of the diesel and gaseous charge, autoignition, combustion and pollutant formation. The aim of the work is to predict in-cylinder pressures and rates of energy release during combustion and allow quantitative/qualitative trends of engine-out emissions. The main purpose of the model is to couple the diesel and gaseous combustion sub-models, and accurately describe the final phase of dual fuel combustion. This will significantly increase the understanding of the combustion phenomena associated with dual fuel engines, and aid the explanation and prediction of emissions trends.
4.1 INTRODUCTION

As discussed in Chapter 2, the dual fuel concept has many advantages as a future engine technology. However, at present, the combustion processes occurring inside the cylinder are not well understood. Therefore, there is a need to develop tools to advance the current understanding of the dual fuel combustion processes. Suitable combustion models can provide an effective means of investigating the combustion phenomena taking place inside the cylinder and a number of models have been developed for dual fuel engines (as discussed in Chapter 3, section 3.1). These range from relatively simple zero-dimensional models, to increasingly complex quasi-dimensional and multi-dimensional models.

Zero-dimensional models are based on specified or empirical energy release functions, or chemical kinetic schemes and are characterised as being computationally efficient. However, zero-dimensional models are unable to account for the temporal and spatial variations in composition and temperature within the cylinder. In contrast, multi-dimensional models are based on the finite element approach and solve for conservation of mass, momentum, energy and species. Although this type of model provides in-depth information about the temporal and spatial conditions inside the cylinder, the large amounts of data produced mean that this type of model is characterised as being computationally expensive. The quasi-dimensional model is beneficial to combustion analysis, as it provides the temporal and spatial information required for quantitative prediction of performance and emissions, whilst remaining computationally efficient.

The main obstacle to modelling the combustion processes occurring inside a dual fuel engine is understanding the coupling between the combustion of the pilot and the premixed combustion of the gaseous charge. This is demonstrated by the large number of approaches that have been adopted to describe the energy release in dual fuel engines (see Chapter 3, section 3.1). Based on the current conceptual understanding of dual fuel combustion, in which the combustion of the pilot controls the subsequent burning of the premixed charge, the model in this study is based on a quasi-dimensional, multi-zone packet model (Hiroyasu et al., 1983) which has been
coupled to a turbulent entrainment model (Tabaczynski et al., 1980). The model includes sub-models for spray development and mixing, swirl, spray wall impingement, ignition and combustion, and pollutant formation. The main objective of the model is to predict in-cylinder pressures and rates of energy release on the basis of the physical and chemical phenomena occurring inside the cylinder.

This chapter begins with an overview of the dual fuel model, before describing in detail the development of the pilot injection and turbulent entrainment models. The calculations are based on equilibrium thermodynamics and a revised model is described and implemented into the combustion simulation. Pollutant formation is considered following the development of the energy release model.

### 4.2 OVERVIEW OF DUAL FUEL MODEL

A new quasi-dimensional, multi-zone model has been developed to describe the combustion processes occurring inside a dual fuel engine during the closed part of the engine cycle (inlet valve closure (IVC) to exhaust valve opening (EVO)). The model simulates the injection of a pilot fuel spray into a homogenous lean premixed charge of natural gas and air (Figure 4.1). The liquid fuel is assumed to be n-dodecane (C$_{12}$H$_{26}$) and the natural gas is considered to be 100 percent methane (CH$_4$).

![Figure 4.1 – Schematic of the dual fuel model concept](image-url)
The lean premixed charge ingested into the cylinder is treated as a single homogeneous zone. This is referred to as the unburned gaseous zone. At the point of fuel injection, spray segments containing liquid fuel are formed at equal time increments. These are divided into zones of equal mass in both the radial and circumferential direction. Following spray breakup, the lean premixed charge is entrained into the pilot fuel spray. The spray droplets formed during breakup evaporate and ignition occurs following the ignition delay of the pilot. Following ignition, combustion of the prepared fuel vapour and entrained gaseous fuel proceed simultaneously under stoichiometric conditions.

Burning zones within the spray act as flame kernels from which flame fronts develop, as illustrated in Figure 4.1. In an original approach, the burning zones are adiabatically mixed and a single spherical flame front is assumed to propagate at the turbulent burning velocity. The premixed charge crossing this flame front is added to a separate burning zone, thus retaining the integrity of the burning zones in the pilot fuel spray.

The total energy release rate and pollutant formation are calculated by summing the respective values in each burning zone. Dissociation of the combustion products is accounted for by the method of Damköhler and Edse (1943)\(^1\) (as described by Gaydon and Wolfhard (1960)), which has been modified to include eleven product species. Emissions of NO\(_x\) are calculated using the extended Zeldovich mechanism and PM is calculated using a simple two-step approach which accounts for soot formation and soot oxidation. Emissions of PM are attributed solely to the spray burning zones and the instantaneous soot density of each zone is incorporated into a radiative heat transfer model. Convective heat transfer is considered using the model proposed by Annand (1963).

### 4.3 PILOT INJECTION MODEL

#### 4.3.1 General Description

The pilot fuel spray is modelled as a number of discrete zones, whose spatial distribution are representative of the overall spray geometry (Figure 4.2). The discretization of the spray is achieved by dividing it in three dimensions. At each time step, a new spray segment is formed. This segment is further divided in both the

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\(^1\) Due to its scarcity this paper could not be obtained
radial and circumferential directions. The division of the segment in the radial and
circumferential directions is fixed. However, in the axial direction, the number of spray
segments varies depending on the injection duration and the time step used. The
mass of fuel in each segment is divided equally between the zones. It is assumed that
there is no mass or energy transfer between the spray zones and that each zone has
its own temperature and composition history.

The spray behaviour is defined by empirical correlations for spray breakup, spray tip
penetration, spray cone angle and SMD. Initially, the injected fuel is assumed to form
a continuous liquid jet which travels at the fuel injection velocity. After a characteristic
breakup time, the injected fuel atomises and the velocity of the spray decreases.
Following spray breakup, the spray contents are assumed to reside within the spray
cone angle (Figure 4.2). The spray cone angle of each segment is unique and is a
function of the instantaneous in-cylinder conditions at the point of segment breakup.

Figure 4.3 shows the development of an individual spray zone. Following spray
breakup, it is assumed that the pilot fuel spray atomises into a large number of
droplets of equal diameter. These are characterised by the SMD. Similarly to the
spray cone angle, the SMD is unique to each spray segment and is a function of the
instantaneous in-cylinder conditions at the point of segment breakup.

The entrainment of gaseous mixture into the pilot fuel spray also starts at the point of
spray breakup and is based on the principle of conservation of momentum, whereby
the total momentum imparted on the fuel during the injection process is conserved.
CHAPTER 4 QUASI-DIMENSIONAL DUAL FUEL MODEL

Figure 4.3 – Temporal evolution of spray zone composition

throughout spray development. The entrainment rate depends on the position of each zone within the pilot fuel spray, with spray zones at the spray periphery entraining more gas than those close to the centreline. The effects of swirl and spray wall impingement on the entrainment rate are also considered.

Immediately after breakup, evaporation proceeds and a combustible mixture forms in each spray zone. Combustion in each spray zone is assumed to occur following the ignition delay of the pilot. This is measured from the SOI and is based on the in-cylinder pressure, and individual zone temperature and equivalence ratio. Following ignition, combustion of the prepared fuel vapour and entrained gaseous fuel proceed through stoichiometric single-step reactions.

Heat transfer is modelled on a zonal basis and includes both convective and radiative heat transfer. Convective heat transfer is calculated globally and distributed between the model zones, whilst radiative heat transfer is calculated for each spray burning zone as a function of soot formation and soot oxidation. Heat transfer from the spray burning zones to the premixed burning zone and unburned zone is also considered.

The sub-models included in the pilot injection model are described in the following sections. The properties of the liquid fuel (n-dodecane) can be found in Appendix A.
4.3.2 Injection
Following the SOI, the injected liquid fuel is divided into spray zones. During injection, axial spray segments are formed at equal time increments given by the combustion simulation interval. In the present work, the mass of fuel in each spray segment is determined by dividing the total mass injected between each segment on the basis of the fuel line pressure. The mass in each segment is then divided equally between the radial and circumferential spray zones. The total number of axial spray segments is given by the injection duration, which is determined from the recorded needle lift. The numbers of radial and circumferential zones are specified as model constants.

For a quasi-steady, incompressible, one dimensional flow, the instantaneous injection rate \( \frac{dm_t}{dt} \) is given by Heywood (1988) as

\[
\frac{dm_t}{dt} = C_d A \sqrt{2 \rho_l \Delta P}
\]

(4.1)

where \( C_d \) is the discharge coefficient, \( A \) is the nozzle orifice area, \( \rho_l \) is the liquid fuel density and \( \Delta P \) is the instantaneous pressure differential across the injector (in Pa). Thus, knowing the mass apportioned to each spray segment, the instantaneous pressure differential across the injector, \( \Delta P \), can be determined. The instantaneous injection velocity \( V_0 \) can then be calculated from

\[
V_0 = C_d \frac{2 \Delta P}{\sqrt{\rho_l}}
\]

(4.2)

In equations (4.1) and (4.2), a constant discharge coefficient of 0.39 has been found to give satisfactory results by many authors. In the present work, a discharge coefficient of 0.66 has been employed, following the work of Dan et al. (1997), as this is more representative of modern diesel injectors. The mass of liquid fuel apportioned to each spray zone \( m_{t,z} \) in the cycle simulation interval \( \Delta \varphi \) is given by

\[
m_{t,z} = \frac{(dm_t/dt)(\Delta \varphi/6N)}{j_{max} \cdot k_{max}}
\]

(4.3)
where \( N \) is the engine speed (in rpm) and \( j_{\text{max}} \) and \( k_{\text{max}} \) are the maximum number of radial and circumferential zones respectively.

### 4.3.3 Pilot Fuel Spray Development

Spray development, which has an important influence on gas entrainment, has a significant effect on the subsequent combustion processes occurring inside the cylinder. The spray behaviour is described using empirical correlations for spray breakup, spray tip penetration, spray cone angle and SMD. The correlations used in the present work are discussed in the following sections. The effect of swirl and spray wall impingement are also discussed.

#### 4.3.3.1 Description of Pilot Fuel Spray

In the present work, the spray tip penetration is determined based on the empirical correlation of Arai et al. (1984). This correlation has been cited by many authors, for example Bazari (1992), Stiesch and Merker (1999) and Jung and Assanis (2001). Here, the formulation of Jung and Assanis (2001) has been adopted in which different discharge coefficients can be considered.

The injected fuel is initially assumed to form a continuous liquid jet which penetrates across the cylinder in proportion to time. After a short period, characterised by the breakup time \( t_b \), the liquid jet atomises. The breakup time, \( t_b \), is given by Jung and Assanis (2001) as

\[
\begin{align*}
t_b &= 4.351 \left( \frac{\rho_l D}{C_d^2 (\rho_g \Delta P)^{0.5}} \right) \quad (4.4)
\end{align*}
\]

where \( D \) is the nozzle orifice diameter and \( \rho_g \) is taken to be the instantaneous unburned gas density at the time of injection of the spray segment. Following breakup, the spray penetrates in proportion to the square root of time. The spray tip penetration \( S \) is given by

\[
S = 2.95 \left( \frac{\Delta P}{\rho_g} \right)^{0.25} (tD)^{0.5} \quad (4.5)
\]

where \( \rho_g \) is the instantaneous unburned gas density and \( t \) is the time elapsed since the SOI of the spray segment. Equation (4.5) gives the penetration of the spray along
the spray centreline in the absence of swirl and spray wall impingement. These two parameters are accounted for in sections 4.3.3.2 and 4.3.3.3.

To account for reduced penetration at the spray periphery due to aerodynamic forces, spray similarity is considered. According to Abramovich (1963),

\[
\frac{V}{V_{cl}} = f^n \left( \frac{r}{x} \right)
\]  

(4.6)

where \( V \) is the velocity at an arbitrary point in the spray, \( V_{cl} \) is the centreline velocity and \( r \) and \( x \) are radial and axial coordinates respectively. Thus, the velocity at any point in the spray can be determined from the centreline velocity, where the centreline velocity is obtained from the derivative of the spray tip penetration with respect to time.

\[
V_{cl} = \frac{dS}{dt} = 1.475 \left( \frac{\Delta P}{\rho_g} \right)^{0.25} \left( \frac{D}{t} \right)^{0.5}
\]  

(4.7)

The radial velocity profile can be considered to follow a Gaussian profile (Desantes et al., 2006, Pastor et al., 2000). Thus,

\[
V = V_{cl} \exp \left( -\alpha \left( \frac{r}{x} \right)^2 \right)
\]  

(4.8)

where \( \alpha \) is the shape factor for the Gaussian distribution. From this point onwards \( \alpha \) is referred to as the entrainment factor. Expressing \( r/x \) as a function of the spray zone angle, \( \theta_z \) (Figure 4.4), the velocity of any spray zone \( (V_z) \) can be expressed as

\[
V_z = V_{cl} \exp(-\alpha \cdot tan^2 \theta_z)
\]  

(4.9)

In the present work, individual spray zone angles are calculated by dividing the spray cone angle equally between the radial zones (Figure 4.2). The spray cone angle \( \theta \) is determined according to the correlation of Reitz and Bracco (1979)

\[
tan\left( \frac{\theta}{2} \right) = \frac{2\pi}{A} \left( \frac{\rho_g}{\rho_l} \right)^{0.5}
\]  

(4.10)
where the constant $A$ has been defined previously (see Chapter 3, section 3.2.2.2).

4.3.3.2 Swirl

Swirl has an important influence on spray development and gas entrainment. As discussed in Chapter 2 (section 2.1.2), in-cylinder swirl is characterised by the swirl ratio ($R_s$). This can be obtained experimentally and is given as a model input. Assuming a solid-body rotating flow, the definition of the swirl ratio, $R_s$, can be used to calculate the angular velocity of the charge motion ($\omega_s$) at IVC.

$$\omega_{s,IVC} = R_{s,IVC}2\pi N$$  \hspace{1cm} (4.11)

The variation of angular velocity with crank angle is calculated by solving for the conservation of angular momentum of the cylinder contents. In the present work, the method of Dent and Derham (1974) is used. This method accounts for the decrease in angular momentum due to frictional effects between the cylinder contents and the surrounding surfaces.

According to Perini and Mattarelli (2011), the effect of swirl on spray development can be determined by considering the local velocity components associated with a non-swirling spray and the swirling motion of the in-cylinder charge. This approach is adopted in the present work. Assuming a solid-body rotating flow, the swirl velocity ($V_s$) associated with the in-cylinder charge is given by

$$V_s = \omega_s r$$  \hspace{1cm} (4.12)
where \( r \) is the radial coordinate of an arbitrary point relative to the cylinder origin. Since the swirl velocity, \( V_s \), is proportional to the radial cylindrical coordinate, \( r \), the swirl velocity increases towards the cylinder periphery (Figure 4.5).

The coordinate system employed in the present work is illustrated in Figures 4.5 and 4.6. Figure 4.5 shows the cylinder coordinate system. Here, the \( x-y \) plane is considered to be parallel to the cylinder head with the \( z \)-axis perpendicular to this plane. Figure 4.6 shows the spray coordinate system. Here, the initial injection direction is along the \( x_1 \)-axis with the spray direction given by the radial coordinates \( r_1 \) and \( y_1 \). In the present work, the \( x \)-axis is considered to be in line with the initial injection direction.

**Figure 4.5** – Calculation of in-cylinder swirl [Based on a diagram from Petersen and MacGregor (1996)]
The effect of swirl on spray development is determined by resolving the spray coordinate system onto the cylinder coordinate system. The velocity of a spray zone in a non-swirling spray is given by

\[
\vec{V} = \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} = \begin{pmatrix} V_{r_1} \sin(\beta) + V_{x_1} \cos(\beta) \\ -V_{y_1} \\ V_{x_1} \sin(\beta) - V_{r_1} \cos(\beta) \end{pmatrix} \tag{4.13}
\]

where \( \beta \) is the angle between the nozzle hole axis and cylinder head, and the velocity components \( V_{x_1}, V_{r_1} \) and \( V_{y_1} \) are given by

\[
V_{x_1} = V_z \tag{4.14}
\]

\[
V_{r_1} = V_z \tan(\theta_z) \cos(\theta_{r_1,y_1}) \tag{4.15}
\]

\[
V_{y_1} = V_z \tan(\theta_z) \sin(\theta_{r_1,y_1}) \tag{4.16}
\]

where \( \theta_{r_1,y_1} \) is the circumferential spray cone angle (Figure 4.6). As stated previously, the effect of swirl on the spray zone velocity is calculated by considering the local components of velocity associated with a non-swirling spray and the swirling motion of the in-cylinder charge. Hence, with reference to Figure 4.5, the velocity components are given by
where $\theta$ is the angle from the $x$-axis to the spray zone location. Following the calculation of the spray zone velocity, the spray zone coordinates are calculated as follows

$$
\begin{pmatrix}
S_{x,S} \\
S_{y,S} \\
S_{z,S}
\end{pmatrix} = \begin{pmatrix}
V_{x,S} \\
V_{y,S} \\
V_{z,S}
\end{pmatrix} \left( \Delta \varphi / 6N \right) \quad (4.18)
$$

These are used to define the radial coordinate, $r$, in the following time step, and for the determination of spray wall impingement (discussed in the next section). For simplicity, the coordinates of each spray zone are only calculated following spray breakup and spray penetration is assumed to start at the cylinder origin.

### 4.3.3.3 Spray Wall Impingement

In engines with small combustion chamber geometries, spray wall impingement is an inherent part of the mixture formation process due to the high injection pressures employed in modern injection systems. In the present work, spray wall impingement is only considered to occur within the piston bowl, thus neglecting impingement against the piston crown and cylinder liner. At each time step, spray zone locations are checked against the relative position of the piston bowl. If a spray zone exceeds the physical boundaries defined by the bowl geometry, then spray wall impingement is considered to have occurred. The piston bowl geometry considered in the present work is shown in Figure 4.7.

Hiroyasu and Nishida (1989) found that the velocity of the spray after wall impingement decreases in proportion to $t^{-0.75}$. In the present work, the spray velocity after impingement is assumed to decrease in proportion to $t^{-c}$, where $c$ is an adjustable constant greater than 0.5. Hence, after impingement, the spray centreline velocity is given by

$$
V_z = 1.475 \left( \frac{\Delta \rho}{\rho_g} \right)^{0.25} \frac{t_{\text{imp}}^{c-0.5}}{t^c} D^{0.5} \quad (4.19)
$$
where \( t_{imp} \) is the impingement time. Thus, the velocity of the spray decreases following spray wall impingement.

\[
\text{SMD} = 4.12 (Re)^{0.12} (We)^{-0.75} \left( \frac{\mu_l}{\mu_g} \right)^{0.54} \left( \frac{\rho_l}{\rho_g} \right)^{0.18} D \tag{4.20}
\]

**4.3.4 Pilot Mixture Preparation**

The rate of preparation of a combustible mixture inside the pilot fuel spray has an important effect on the energy release in a dual fuel engine. The pilot mixture preparation is controlled by the droplet diameter following breakup, the rate of entrainment of fresh unburned gaseous mixture and the rate of evaporation. These processes are discussed in the following sections.

**4.3.4.1 Sauter Mean Diameter (SMD)**

Following spray breakup, the liquid fuel atomises into small droplets characterised by the SMD \( (D_{32}) \). In the present work, the SMD is determined from the correlations of Hiroyasu et al. (1989), whereby the maximum of two correlations is assumed to represent the SMD.
\[
SMD = 0.38(Re)^{0.25}(We_l)^{-0.32}\left(\frac{\mu_l}{\mu_g}\right)^{0.37}\left(\frac{\rho_l}{\rho_g}\right)^{-0.47} D
\] (4.21)

Equations (4.20) and (4.21) describe the SMD for low and high velocity jets, where \(\mu_l/\mu_g\) and \(\rho_l/\rho_g\) are the viscosity and density ratios of liquid fuel to gaseous mixture. The Reynolds number \((Re)\) and liquid Weber number \((We_l)\) have been defined previously (see Chapter 3, section 3.2.1).

The droplets within each spray segment are assumed to be of equal diameter, thus neglecting droplet size distribution and secondary atomisation. Therefore, the number of droplets in each spray zone for a given segment \(N_{d,z}\) can be expressed as

\[
N_{d,z} = \frac{6m_{l,z}}{\rho_l \pi \cdot SMD^3}
\] (4.22)

### 4.3.4.2 Entrainment

The mass of unburned gaseous mixture entrained into each spray zone \(m_{g,z}\) is determined from the principle of conservation of momentum, whereby the total momentum imparted on the fuel during the injection process is conserved throughout spray development.

\[
m_{l,z,0}V_0 = \text{const} = (m_{l,z,0} + m_{g,z})V_z
\] (4.23)

From equation (4.23), the mass of gaseous mixture entrained into each zone, \(m_{g,z}\), can be expressed as

\[
m_{g,z} = \frac{m_{l,z,0}(V_0 - V_z)}{V_z}
\] (4.24)

Therefore, the entrainment of gaseous mixture into the fuel spray is proportional to the zone velocity. Thus, entrainment is a strong function of the spray zone location. This approach accounts for increased entrainment rates towards the spray periphery and increased entrainment rates as a result of swirl and spray wall impingement. During model calibration, an adjustable constant \((C_b)\) is applied to equation (4.24) to modify the rate of entrainment to match the engine type being studied.
4.3.4.3 Evaporation
Following atomisation, the high temperature gases entrained into the pilot fuel spray heat up the spray droplets and evaporation begins. The evaporation of the droplets is due to heat transfer to the droplet and mass transfer away from the droplet. The rate of evaporation depends on the droplet diameter, in-cylinder pressure, liquid fuel vapour pressure, transport and state properties of the droplet vapour-gas boundary layer, and relative velocity between the droplets and unburned gaseous mixture.

For typical injection temperatures, the initial droplet temperature and hence vapour pressure at the droplet surface are low and little mass transfer occurs. During this time, most of the energy reaching the droplet surface heats up the liquid. At the same time, the fuel vapour pressure increases and so does the evaporation rate. As the evaporation rate increases, heat transfer to the droplet surface is reduced due to the increased amount of energy required to heat the additional vapour in the droplet boundary layer. The following section describes the mathematical formulation of this process, as used in the present study.

Droplet evaporation is calculated using the single droplet model of Borman and Johnson (1962). In this model, droplet evaporation is based on the empirical heat and mass transfer coefficients of Ranz and Marshall (1952), with corrections for high rates of evaporation.

The energy balance for a single droplet is given by

\[
\frac{d(m_l h_l)}{dt} = \frac{dQ_l}{dt} + \frac{dm_l}{dt} \cdot h_{fg}
\]  

where the rate of change of energy of the droplet is equal to the difference between the rate of heat transfer to the droplet and the rate at which enthalpy is carried away from the droplet.

Substituting for isobaric specific heat \((C_p = dh/dT)\) and rearranging in terms of the rate of change of liquid temperature \((dT_l/dt)\), equation (4.25) becomes

\[
\frac{dT_l}{dt} = \frac{1}{m_l C_{p,l}} \left( \frac{dQ_l}{dt} + \frac{dm_l}{dt} \cdot h_{fg} \right)
\]  

(4.26)
where $m_l$ is the mass of the droplet and $C_{p,l}$ and $h_{fg}$ are the isobaric specific heat and latent heat of evaporation of the liquid fuel respectively.

In this model, the rate of heat transfer to the droplet ($dQ_l/dt$) is assumed to be solely by convection. Hence,

$$\frac{dQ_l}{dt} = hA(T_g - T_l) \quad (4.27)$$

where $h$ is the convective heat transfer coefficient, $A$ is the surface area of the droplet and $T_g$ is the temperature of the surrounding gases. The convective heat transfer coefficient is obtained from an appropriate Nusselt number ($Nu$) correlation, where the Nusselt number is a measure of the convection occurring at the droplet surface. Ranz and Marshall (1952) found that for low rates of evaporation

$$Nu = \frac{\bar{h} \cdot \text{SMD}}{\bar{k}_m} = 2 + 0.6Re_m^{0.5}Pr_m^{1/3} \quad (4.28)$$

where $\bar{k}_m$, $Re_m$ and $Pr_m$ are the thermal conductivity and Reynolds and Prandtl numbers for the mean vapour-gas boundary layer. The Reynolds number is defined in terms of the relative velocity of the spray zone ($V_{rel,z}$) and the droplet diameter, SMD.

$$Re_m = \frac{\rho_m V_{rel,z} \cdot \text{SMD}}{\mu_m} \quad (4.29)$$

Following Hiroyasu and Nishida (1989), the relative velocity, $V_{rel,z}$, between the droplet and entrained gaseous mixture is assumed to be 30 percent of the instantaneous zone velocity. The Prandtl number is defined as the ratio of momentum diffusivity to thermal diffusivity and is given by

$$Pr_m = \frac{C_{p,m} \mu_m}{\bar{k}_m} \quad (4.30)$$

For high rates of evaporation, the convective heat transfer coefficient must be corrected to account for the heating of additional fuel vapour in the droplet boundary.
layer. The corrected heat transfer coefficient ($\tilde{h}^*$) is given as (Borman and Ragland, 1998)

$$\tilde{h}^* = \tilde{h}Z \quad (4.31)$$

where

$$Z = \frac{z}{e^z - 1} \quad (4.32)$$

$$z = -\frac{(dm_l/dt)C_{p,v}}{\tilde{h}A} \quad (4.33)$$

and $C_{p,v}$ is the isobaric specific heat of the fuel vapour. Taking $A = \pi \cdot \text{SMD}^2$, substituting the corrected convective heat transfer coefficient (equation (4.31)) into equation (4.27) and expressing the Nusselt number (equation (4.28)) in terms of the convective heat transfer coefficient, the rate of heat transfer to the droplet becomes

$$\frac{dQ_l}{dt} = \pi \cdot \text{SMD} \cdot \tilde{k}_m(T_g - T_l) \cdot \frac{z}{e^z - 1} \left(2 + 0.6Re_m^{0.5}Pr_m^{1/3}\right) \quad (4.34)$$

The only unknown in equation (4.34) is the rate of change of liquid mass (from equation (4.33)). Mass diffusion is considered to occur across a concentration gradient, where the driving force is the difference between the partial pressure of the vapour at the droplet surface ($p_{v,s}$) and the surroundings ($p_{v,g}$). Hence, the rate of change of liquid mass is given by

$$\frac{dm_l}{dt} = -\tilde{h}_D A (p_{v,s} - p_{v,g}) \quad (4.35)$$

where $\tilde{h}_D$ is the mass transfer coefficient and $R_v$ is the vapour gas constant. The mass transfer coefficient is obtained from an appropriate Sherwood number ($Sh$) correlation, where the Sherwood number is a measure of the mass transfer due to convection at the droplet surface. Ranz and Marshall (1952) found that for low rates of evaporation
CHAPTER 4 QUASI-DIMENSIONAL DUAL FUEL MODEL

\[ Sh = \frac{\tilde{h}_D \cdot \text{SMD}}{D_{v,g}} = 2 + 0.6 Re_m^{0.5} Sc_m^{1/3} \]  

(4.36)

where \( D_{v,g} \) is the mass diffusivity and \( Sc_m \) is the Schmidt number of the vapour-gas boundary layer. In the case of dual fuel operation, the diffusivity of the liquid fuel vapour into a homogeneous mixture of methane and air has also been considered (Appendix A). The Schmidt number is defined as the ratio of momentum diffusivity and mass diffusivity and is given by

\[ Sc_m = \frac{\mu_m}{\rho_m D_{v,g}} \]  

(4.37)

For higher rates of evaporation, the corrected mass transfer coefficient (\( \tilde{h}_D^* \)) is given as (Borman and Ragland, 1998)

\[ \frac{\tilde{h}_D^*}{\tilde{h}_D} = \ln \left( \frac{P_{cyt} - P_{v,g}}{P_{cyt} - P_{v,s}} \right) / \left( \frac{P_{v,s} - P_{v,g}}{P_{cyt}} \right) \]  

(4.38)

where \( P_{cyt} \) is the in-cylinder pressure. Taking \( A = \pi \cdot \text{SMD}^2 \), substituting equation (4.38) into equation (4.35) and expressing the Sherwood number (equation (4.36)) in terms of the mass transfer coefficient, the rate of change of liquid mass becomes

\[ \frac{dm_i}{dt} = -\left( \frac{\pi \cdot \text{SMD} \cdot D_{v,g} P_{cyt}}{R_v T_m} \right) \ln \left( \frac{P_{cyt} - P_{v,g}}{P_{cyt} - P_{v,s}} \right) (2 + 0.6 Re_m^{0.5} Sc_m^{1/3}) \]  

(4.39)

The properties of the vapour-gas boundary layer are evaluated at the mean temperature and concentration as follows

\[ T_m = T_i + \frac{T_g - T_i}{2} \]  

(4.40)

\[ y_{v,m} = y_v + \frac{y_g - y_v}{2} \]  

(4.41)

\[ y_{g,m} = 1 - y_{v,m} \]  

(4.42)
where $T$ is the temperature, $y_v$ is the mole fraction of fuel vapour and $y_g$ is the mole fraction of the gaseous mixture. The subscripts $m$ and $l$ refer to the mean vapour-gas boundary layer and liquid fuel properties respectively. It can be shown that equation (4.40) simplifies to

$$T_m = \frac{T_g + T_l}{2} \tag{4.43}$$

and that if the fuel vapour concentration far away from the droplet is assumed to be zero, equation (4.41) simplifies to

$$y_{v,m} = \frac{y_v}{2} \tag{4.44}$$

The average film properties are subsequently given by

$$M_m = y_{g,m} M_g + y_{v,m} M_v \tag{4.45}$$

$$\rho_m = \frac{P_{cycl} M_m}{R_u T_m} \tag{4.46}$$

$$\tilde{k}_m = y_{g,m} \tilde{k}_g + y_{v,m} \tilde{k}_v \tag{4.47}$$

$$\mu_m = y_{g,m} \mu_g + y_{v,m} \mu_v \tag{4.48}$$

$$C_{p,m} = y_{g,m} C_{p,g} + y_{v,m} C_{p,v} \tag{4.49}$$

where $M$ is the molecular weight and $R_u$ is the universal gas constant. The properties $D_{v,g}, \tilde{k}_g, \tilde{k}_v, \mu_g, \mu_v, C_{p,g}$ and $C_{p,v}$ are evaluated at $T_m$, while the properties $h_{fg}, p_{v,s}$ and $C_{p,l}$ are evaluated at $T_l$. The correlations used to evaluate these properties are given in Appendices A and B.

The total rate of heat of vaporisation provided to the droplets in a single spray zone ($dQ_{l,tot,x}/dt$) is given by
Following Rakopoulos et al. (1995), it is assumed that the total heat of vaporisation is provided by both the spray zone and the unburned gaseous zone. This is because, at spray zone inception, the internal energy of the spray zone cannot provide the heat required for rapid rates of evaporation. The contribution of the spray zone and unburned gaseous zone (subscript $u$) to the total heat of vaporisation is determined on the basis of zone mass and temperature:

$$
\frac{dQ_{t,i}}{dt} = \frac{m_i}{m_u T_u + m_z T_z} \cdot \frac{dQ_{t,tot,z}}{dt}
$$

(4.51)

where $i$ denotes the zone under consideration.

### 4.3.5 Pilot Heat Release

The ignition delay period is defined as the time between the SOI and SOC. During this time, both physical and chemical processes take place and a combustible fuel vapour-gas mixture is formed. The physical processes include the atomisation of the fuel spray, the evaporation of the fuel droplets and the mixing of the fuel vapour-gas mixture. The chemical processes include the pre-ignition reactions of the fuel vapour-gas mixture which lead to autoignition.

In general, the ignition delay ($\tau$) of a given fuel is a function of pressure, temperature and equivalence ratio (Heywood, 1988). In the present work, ignition is considered to be due to the pilot and is determined according to the Arrhenius-type expression of Nishida and Hiroyasu (1989):

$$
\tau = 4 \cdot 10^{-3} P_{cy}^{-2.5} \Phi_z^{-1.04} \exp \left( \frac{E}{R_u T_z} \right)
$$

(4.52)

where $P_{cy}$ is the in-cylinder pressure (in MPa) and $\Phi_z$ and $T_z$ are the local equivalence ratio and temperature. Thus, any chemical interactions between the liquid and gaseous fuel are neglected. In the work of Nishida and Hiroyasu (1989), the value of $E/R_u$ in equation (4.52) was assigned a value of 6000 K.
During the ignition delay period, the in-cylinder pressure and local in-cylinder temperature change as a result of piston motion and heat transfer. Moreover, the local equivalence ratio changes as a result of the entrainment and evaporation processes. In order to account for these changes, the ignition delay is determined from the following integral

\[ \int_0^t \frac{1}{t} dt \geq 1 \]  

(4.53)

where \( t \) and 0 refer to the ignition delay period and SOI respectively. This is solved using the trapezoidal rule. Equation (4.53) is evaluated for each spray zone to account for temporal and spatial variations in equivalence ratio and temperature. Combustion is considered to begin when the ignition integral from the previous step is greater than or equal to one.

Following ignition in the respective spray zones combustion begins. In a dual fuel engine, the rate of energy release from the pilot fuel spray is a combination of that from the prepared fuel vapour and entrained gaseous fuel. It is assumed that the combustion of each fuel proceeds via a stoichiometric single-step reaction

\[ \text{Fuel} + \alpha O_2 \rightarrow \beta CO_2 + \gamma H_2O \]  

(4.54)

where \( \alpha, \beta \) and \( \gamma \) are stoichiometric coefficients. In the present work, the gaseous fuel is assumed to burn under the direct influence of the pilot, following the study of Liu and Karim (1997). Thus, following the consumption of the prepared fuel vapour, combustion in that spray zone ceases to exist. The consumption rate of the fuel vapour by the combustion reaction (equation (4.54)) is described using the Arrhenius-type expression of Nishida and Hiroyasu (1989)

\[ \frac{d\rho_v}{dt} = 5 \cdot 10^{10} \rho_{mix}^2 x_v x_{O_2}^5 \exp \left(-\frac{12000}{T_z}\right) \]  

(4.55)

where \( \rho_v \) is the fuel vapour density, \( \rho_{mix} \) is the density of the mixture to be burned, \( x_v \) is the mass fraction of fuel vapour available and \( x_{O_2} \) is the mass fraction of oxygen available. Similarly to the ignition delay, equation (4.55) is evaluated for each spray zone to account for spatial variations in composition and temperature. The exponents

---

98
of the fuel vapour and oxygen mass fractions are such that the maximum rate of burning occurs under stoichiometric conditions, as illustrated in Figure 4.8.

![Figure 4.8](image)

**Figure 4.8** – Change in vapour density due to combustion reaction (Pressure and temperature determined following isentropic compression: \( P_0 = 1 \) bar, \( T_0 = 300 \) K, \( r_c = 18.5 \), \( k = 1.4 \))

In this study, the gaseous fuel and pilot burn in stoichiometric proportions as defined by the stoichiometric air fuel ratio (AFR\(_{st}\))

\[
\text{AFR}_{st} = \frac{\{\alpha \left( x_l + \frac{y_l}{4} \right) + \beta \left( x_g + \frac{y_g}{4} \right)\} \cdot 4.76M_{air}}{\alpha(x_lM_C + y_lM_H) + \beta(x_gM_C + y_gM_H)}
\]  

(4.56)

where

\[
\alpha = \frac{m_l}{m_l + m_g}
\]  

(4.57)

\[
\beta = \frac{m_g}{m_l + m_g}
\]  

(4.58)

and \( x \) and \( y \) represent the number of atoms of carbon (C) and atomic hydrogen (H) in the liquid and gaseous fuel.

The combustion rate of the liquid and gaseous fuel is limited by the total mass of evaporated fuel and the total mass of entrained gaseous fuel. The combustion rate
can also be limited by the availability of entrained air, in which case, the air is divided between the two fuels on a stoichiometric basis. The subsequent chemical energy release rate for each spray zone \( \frac{dQ_{ch,z}}{dt} \) is given by

\[
\frac{dQ_{ch,z}}{dt} = LHV_l \left( \frac{dm_{l,b,z}}{dt} \right) + LHV_g \left( \frac{dm_{g,b,z}}{dt} \right)
\]

(4.59)

where \( m_{l,b} \) and \( m_{g,b} \) are the masses of burned liquid and gaseous fuel and \( LHV_l \) and \( LHV_g \) are their lower heating values respectively. The lower heating values, \( LHV_l \) and \( LHV_g \), are given as 44574 and 50048 kJ.kg\(^{-1}\) respectively (Borman and Ragland, 1998).

### 4.4 TURBULENT FLAME PROPAGATION MODEL

#### 4.4.1 General Description

In a dual fuel engine, flames are initiated at multiple locations by the ignition of the pilot. These flames propagate across the cylinder at the turbulent burning velocity. Accordingly, the rate of energy release from the premixed charge is a function of the velocity of the ‘flame front’. Turbulent flame propagation is currently not well understood. At present, knowledge of the turbulent flow field, laminar burning velocity and flame geometry are generally used as a basis for flame propagation modelling.

In the present work, turbulent flame propagation is considered to begin when ignition first occurs in any spray zone. Conceptually, spray burning zones are considered to act as flame kernels from which flame fronts develop. In an original approach, the burning zones are adiabatically mixed and a single spherical flame front is assumed to propagate from the surface of an equivalent sphere with equal volume to zone volume. The premixed charge crossing this flame front is added to a premixed burning zone. On subsequent steps, all spray burning zones, as well as the premixed burning zone, are lumped together to determine the flame front surface from which propagation develops. Burning occurs via a single-step reaction at the lean condition of the charge. Any mixture not burned is carried over to the next time step.

The turbulent flame propagation model employed in the present work is described in the following section. The model is based upon the entrainment and burn-up of turbulent eddies and is commonly referred to as a turbulent entrainment model.
4.4.2 Premixed Heat Release
In the present work, the turbulent entrainment model of Tabaczynski et al. (1980) is used to determine the rate of burning through the premixed charge. In this method, the small scale turbulence structure is based on the work of Tennekes (1968) (Figure 4.9). This assumes that the vorticity in the turbulent flow field is represented by vortex tubes characterised by the Kolmogorov scale ($\eta$). The spacing of the vortex tubes is given by the Taylor microscale ($\lambda$). Combustion on the Kolmogorov scale, $\eta$, is assumed to be instantaneous and reaction sheets are considered to propagate between the vortex tubes at the laminar burning velocity ($S_L$), as shown in Figure 4.10. According to Tabaczynski et al. (1980), ignition sites propagate along the vortex tubes at a velocity $U' + S_L$, where $U'$ is the turbulence intensity. Thus, the rate at which mass is entrained into the flame front ($\frac{dm_e}{dt}$) is given by

$$\frac{dm_e}{dt} = \rho_g A_e (U' + S_L)$$ (4.60)

where $A_e$ is the area of the entrainment front. In conventional spark ignition engines, the flame surface area changes as a function of the relative position of the flame front and combustion chamber geometry. In a dual fuel engine, the flame front is initiated at multiple locations, hence tracking each flame front relative to the combustion chamber geometry and accounting for agglomeration of individual flame fronts is a complex task. In the present work, the flame geometry is assumed to be spherical (Heywood, 1988). However, this approach leads to an increase in the entrainment area with each time step.

In the present work, the flame is initially assumed to propagate freely across the cylinder. Then, following the entrainment of a characteristic mass ($C_m$), termed the transition time ($tr$), the entrainment area is described by an exponential decay. At higher gaseous equivalence ratios, where the flame is more likely to engulf the entire mixture, this is indicative of a reducing flame area due to the coalescence of individual flame fronts. At lower gaseous equivalence ratios, this is attributed to the effects of bulk quenching. The entrainment area is subsequently defined as a weighted mean of the entrainment area at the transition time, $tr$, and the entrainment area described by the exponential decay.
Figure 4.9 – Small scale turbulence structure as proposed by Tennekes (1968) [Adapted from Tabaczynski et al. (1980)]

Figure 4.10 – Schematic of burning in a small scale turbulent structure [Adapted from Tabaczynski et al. (1980)]
\( A_e = (1 - w)A_{e, tr} + wA_{e, sph} \left[ 1 - \exp \left( \frac{-m_u}{C_e \cdot m_{g, cyl}} \right) \right] \)  

(4.61)

where \( m_u \) is the mass of the unburned zone and \( C_e \) is a constant used to shape the exponential decay. Here, the subscript \( sph \) denotes the spherical flame front. The weight factor, \( w \), increases with time and is a function of the mass available for entrainment and the mass that was available at the transition time.

\[
w = 1 - \frac{m_u}{(m_u)_{tr}}
\]

(4.62)

The rate of burning behind the flame front \( (dm_{g,b,p}/dt) \) is given by

\[
\frac{dm_{g,b,p}}{dt} = \frac{m_e - m_b}{\tau}
\]

(4.63)

where \( \tau \) is the characteristic time for a reaction sheet to propagate across the Taylor microscale, \( \lambda \), at the laminar burning velocity, \( S_L \).

\[
\tau = \frac{C_T \lambda}{S_L}
\]

(4.64)

Here, \( C_T \) is a constant, modified to match the characteristic burning time, \( \tau \), to the engine type being studied. Assuming isotropic turbulence, the Taylor microscale, \( \lambda \), can be expressed as a function of the integral length scale (\( L \)) and the turbulent Reynolds number (\( Re_T = U'L/v \)) (Heywood, 1988)

\[
\frac{\lambda}{L} = 15.0^{0.5} \left( \frac{U'L}{v} \right)^{-0.5}
\]

(4.65)

where \( v \) is the kinematic viscosity and the integral length scale, \( L \), represents the overall size of a turbulent eddy. Following the start of premixed gaseous combustion, the unburned charge is assumed to be compressed at a rate sufficiently fast that rapid distortion theory can be applied. In engines, rapid distortion theory is applicable when the turbulent flow field is distorted more rapidly by the mean flow than by interactions with itself and assumes that the angular momentum of individual eddies is conserved.
CHAPTER 4 QUASI-DIMENSIONAL DUAL FUEL MODEL

(Wong and Hoult, 1979). Conservation of mass and angular momentum of a turbulent eddy leads to the following expressions for the turbulence intensity, $U'$, and integral length scale, $L$,

$$U' = U_i' \left( \frac{\rho_g}{\rho_{g,i}} \right)^{\frac{1}{3}}$$  \hspace{1cm} (4.66)

$$L = L_i \left( \frac{\rho_{g,i}}{\rho_g} \right)^{\frac{1}{3}}$$  \hspace{1cm} (4.67)

where the subscript $i$ denotes the conditions immediately before initiation of the flame front. Equations (4.66) and (4.67) predict an increase in turbulence intensity and decrease in length scale with compression (Heywood, 1988). They also imply that leaner mixtures will burn more slowly, due to less compression ahead of the flame front (Tabaczynski et al., 1977). The turbulence intensity and integral length scale before the initiation of the flame front are considered to be proportional to the mean piston speed ($S_p$) and instantaneous chamber height ($h$) respectively

$$U_i' = C_{U'} S_p$$  \hspace{1cm} (4.68)

$$L_i = C_L h$$  \hspace{1cm} (4.69)

where $C_{U'}$ and $C_L$ are constants modified to match the engine type being studied. The relationship expressed in equation (4.68) is made under the assumption that the turbulence intensity does not change considerably with the start of combustion of the premixed gaseous charge.

Following the depletion of the unburned gaseous mixture, the turbulent flame front ceases to exist. However, a small volume of unburned gaseous fuel may still exist within the premixed burning zone. This is subsequently burned according to the following expression (Keck, 1982)

$$\frac{dm_{g,b,p}}{dt} = \left( \frac{dm_{g,b,p}}{dt} \right)_t e^{ \left( t - t_t \right) / \tau_t}$$  \hspace{1cm} (4.70)
where the subscript \( t \) denotes the time at which flame termination occurred.

The chemical energy release rate from the premixed zone \( (dQ_{ch,p}/dt) \) is given by

\[
\frac{dQ_{ch,p}}{dt} = LHV_g \left( \frac{dm_{g,b,p}}{dt} \right) \tag{4.71}
\]

4.4.3 Laminar Burning Velocity

The laminar burning velocity, \( S_L \), is defined as the velocity at which the unburned gases pass through the flame front in the direction normal to the flame surface (Kuo, 2005). In combustion modelling, correlations for the laminar burning velocity are needed for the range of pressures, temperatures and equivalence ratios observed in internal combustion engines. Several authors have proposed empirical correlations for the laminar burning velocity. At present, there is a large body of literature on the laminar burning velocity of methane-air mixtures. However, there are limited studies that cover the range of pressures and temperatures observed in internal combustion engines. Table 4.1 shows the laminar burning velocity correlations that best cover the range of pressures, temperatures and equivalence ratios observed. It should be noted that the correlation of Elia et al. (2001) also includes the ability to predict the influence of diluents on the laminar burning velocity. This effect is not considered in the present work.

<table>
<thead>
<tr>
<th>Reference</th>
<th>Pressure Range ( / (\text{atm}) )</th>
<th>Temperature Range ( / (\text{K}) )</th>
<th>Equivalence Ratio ( (\Phi) ) Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Iijima and Takeno (1986)</td>
<td>0.5 - 30.0</td>
<td>291 - 500</td>
<td>0.8 - 1.3</td>
</tr>
<tr>
<td>Al-Himyary and Karim (1987)</td>
<td>1.0 - 70.0</td>
<td>323 - 473</td>
<td>0.62 - 1.35</td>
</tr>
<tr>
<td>Göttgens et al. (1992)</td>
<td>1.0 - 40.0</td>
<td>290 - 800</td>
<td>( \Phi_{\text{limit}} - 1.0 )</td>
</tr>
<tr>
<td>Elia et al. (2001)</td>
<td>0.75 - 70.0</td>
<td>298 - 550</td>
<td>0.8 - 1.2</td>
</tr>
</tbody>
</table>

The laminar burning velocity is calculated based on the correlation of Elia et al. (2001). It is noted that this correlation is only valid for equivalence ratios between 0.8 and 1.2. However, in a dual fuel engine, much leaner mixtures have been observed to burn (Stewart, 2006). Hence, in the present work, the relation that relates the laminar
burning velocity at standard temperature and pressure to equivalence ratio is described using an S-shaped curve (Wiebe function) fitted to the numerical data of Gottgens et al. (1992) at 1 bar and 298 K (Figure 4.11). This study presented numerically determined data for the laminar burning velocities of methane-air mixtures down to an equivalence ratio of 0.4. Subsequently, the expression for the laminar burning velocity (in cm.s\(^{-1}\)) is given by

\[
S_L = S_{u0}(1 - \exp[-a\Phi^b]) \left(\frac{T_g}{T_0}\right)^{\alpha} \left(\frac{P_{cyl}}{P_0}\right)^{\beta}
\]  

(4.72)

where the constants \(a\) and \(b\) are assigned values of 4.75 and 4.25 respectively. The laminar burning velocity at the reference conditions, \(S_{u0}(= 37.5\ \text{cm.s}^{-1})\), and the exponents \(\alpha(= 1.857)\) and \(\beta(= -0.435)\) are taken from the correlation of Elia et al. (2001), where the reference temperature and pressure (\(T_0\) and \(P_0\)) are 298 K and 1 atm respectively. It is proposed that this gives a better description of the laminar burning velocity for the gaseous equivalence ratios employed in dual fuel engines.

\[\text{Figure 4.11} \quad \text{– Curve fit (Wiebe function) to the numerical data of Göttgens et al. (1992) (1 bar, 298 K)}\]

\[\text{4.5 HEAT TRANSFER}\]

In internal combustion engines, heat transfer between the cylinder contents and surrounding surfaces is by forced convection and radiation (Annand, 1986). The relative proportion of these two processes varies between conventional spark ignition
and diesel engines. In diesel engines, soot particles formed during diffusion combustion can contribute significantly to the radiative heat transfer, whereas in conventional spark ignition engines, levels of radiative heat transfer are comparatively low. Generally, these processes are modelled on a global basis (Annand, 1963, Woschni, 1967). In the present work, the combustion volume of the liquid fuel and subsequent mass of soot formed will vary considerably from diesel to dual fuel operation. Thus, a zonal approach to modelling radiative heat transfer is adopted, following the approach of Bazari (1992). Convective heat transfer is modelled on a global basis using the method proposed by Annand (1963). In the present work, heat transfer from the spray burning zones to the surrounding gas is also considered. These processes are discussed in the following sections.

4.5.1 Convection

The rate of wall heat transfer due to convection \( \frac{dQ_{wc}}{dt} \) is given by

\[
\frac{dQ_{wc}}{dt} = \tilde{h}A(T_w - T_b)
\]

(4.73)

where \( A \) is the combustion chamber surface area, \( T_b \) is the bulk average cylinder temperature and \( T_w \) is the wall temperature. The wall temperature, \( T_w \), is a model constant and is adjusted to match the engine type being studied. According to Annand (1963), the heat transfer coefficient, \( \tilde{h} \), can be expressed as follows

\[
\tilde{h} = a \frac{k_g}{B} Re^b
\]

(4.74)

where \( k_g \) is the gas thermal conductivity and \( B \) is the bore diameter. The constant \( a \) is related to the charge motion and combustion chamber design, and generally takes a value in the range 0.1 to 0.3; the constant \( b \) is typically assigned a value of 0.8 (Annand, 1986). The Reynolds number, \( Re \), is defined in terms of the mean piston speed, \( S_p \), and bore diameter, \( B \),

\[
Re = \frac{\rho_{cyl}S_pB}{\mu_g}
\]

(4.75)

where the density of the cylinder contents, \( \rho_{cyl} \), is given by
\[ \rho_{\text{cyl}} = \frac{m_{\text{cyl}}}{V_{\text{cyl}}} \]  

here, \( m_{\text{cyl}} \) is the gaseous cylinder mass and \( V_{\text{cyl}} \) is the instantaneous cylinder volume. Following Ferguson and Kirkpatrick (2001), air data is used to calculate the thermal conductivity and viscosity of the cylinder gases.

\[ \bar{k}_{\text{air}} = 3.17 \cdot 10^{-4} T_b^{0.772} \]  

(4.77)

\[ \mu_{\text{air}} = 3.3 \cdot 10^{-7} T_b^{0.7} \]  

(4.78)

Equations (4.77) and (4.78) were taken from Rakopoulos and Giakoumis (1997) and Heywood (1988) respectively. The bulk cylinder temperature, \( T_b \) is calculated on a mass average basis

\[ T_b = \frac{m_u T_u + m_p T_p + \sum z m_z T_z}{m_u + m_p + \sum z m_z} \]  

(4.79)

where \( m \) and \( T \) are the mass and temperature of the unburned zone, spray zones and premixed burning zone denoted by the subscripts \( u, z \) and \( p \) respectively. The heat transferred to the walls due to convection is distributed between the model zones on the basis of zone mass and temperature

\[ \frac{dQ_{wc_i}}{dt} = \frac{m_i T_i}{m_u T_u + m_p T_p + \sum z m_z T_z} \cdot \frac{dQ_{wc}}{dt} \]  

(4.80)

where \( i \) denotes the zone type under consideration.

4.5.2 Radiation

There are two sources of radiative heat transfer within the cylinder: the high temperature burned gases and the soot particles produced by the diffusion flame. The radiative heat transfer from the high temperature burned gases is small in comparison to that from the soot particles (Heywood, 1988), thus only radiation due to soot is considered in the present model.
The contribution of each spray zone to the rate of wall heat transfer due to radiation \( \frac{dQ_{w,z}}{dt} \) is calculated according to

\[
\frac{dQ_{w,z}}{dt} = \varepsilon_a \sigma A (T_w^4 - T_z^4)
\]  

where \( \varepsilon_a \) is the apparent grey emissivity of the soot cloud, \( \sigma \) is the Stefan Boltzmann constant and \( A \) is the droplet surface area. According to Annand (1974), the apparent grey emissivity, \( \varepsilon_a \), for a cloud of soot particles is given by

\[
\varepsilon_a = 1 - \exp(-k_a L)
\]

where \( k_a \) is the absorption coefficient and \( L \) is a length scale. Field et al. (1967) suggested that the absorption coefficient, \( k_a \), is related to the soot cloud density \( \rho_s \) by

\[
k_a = 1200 \rho_s
\]

and that the length scale, \( L \), for a soot cloud of arbitrary shape is given by

\[
L = 3.4 \frac{V_z}{A_z}
\]

where \( V_z \) and \( A_z \) are the instantaneous volume and surface area of the spray zone. In the present work, the surface area is considered to be equal to that of an equivalent sphere with equal volume to zone volume. Equation (4.84) is given under the assumption that the soot cloud fills the spray zone.

### 4.5.3 Zonal Heat Transfer

Zonal heat transfer is typically neglected in quasi-dimensional models. However, Cui et al. (2001) accounted for heat transfer from the spray zones to the surrounding gas, citing a better description of the heat transfer processes occurring inside the cylinder.

In the present work, heat transfer from the spray burning zones to the premixed burning zone and unburned zone is considered. The heat transfer from each spray burning zone is given by
where $\xi$ is a constant and $h$ is the specific enthalpy. The total heat transferred from the spray burning zones is divided between the premixed burning zone and unburned zone on a mass basis.

4.6 EQUILIBRIUM THERMODYNAMICS

For the prediction of performance in internal combustion engines, the combustion products can be considered to be in chemical equilibrium at a given pressure and temperature. Here, the dissociation and recombination paths of each chemical reaction can be considered to be equal. Therefore, there is no net change in the composition of the mixture. In engine modelling, this assumption is used to determine the composition and thermodynamic properties of the burned gases. In the present work, eleven product species (CO$_2$, CO, H$_2$O, O$_2$, H$_2$, OH, H, O, N$_2$, NO and N) are considered and the equilibrium combustion products are solved using a modified version of the method of Damköhler and Edse (1943).

Several computer programmes have been developed for the calculation of chemical equilibrium. The most widely cited are those of Svehla and McBride (1973), Olikara and Borman (1975) and Ferguson and Kirkpatrick (2001). Svehla and McBride (1973) developed a comprehensive chemical equilibrium code, using Lagrange multipliers to compute the chemical equilibrium for a range of thermodynamic inputs. Olikara and Borman (1975) proposed a method based on twelve product species, using equilibrium constants and mole fractions to compute the chemical equilibrium for a given pressure and temperature. Ferguson and Kirkpatrick (2001) adapted this method, but reduced the number of product species to ten, omitting argon and atomic nitrogen. The primary objective of the models of Olikara and Borman (1975) and Ferguson and Kirkpatrick (2001) was to provide a rapid method of calculation for use in combustion modelling.

Gaydon and Wolfard (1960) described the iterative scheme of Damköhler and Edse (1943) for calculation of the equilibrium combustion products. This method is based on the solution of equilibrium constants and considers ten product species. The implementation of this model is described in the following sections.
4.6.1 Methodology of Damköhler and Edse

This section describes the method of Damköhler and Edse (1943) for the solution of the equilibrium combustion product composition. The use of equilibrium constants requires the equilibrium reactions and hence combustion products to be specified. Damköhler and Edse (1943) specified ten product species – CO$_2$, CO, H$_2$O, O$_2$, H$_2$, OH, H, O, N$_2$ and NO. The general combustion reaction for these species can be written as

$$C_xH_y + \frac{\alpha}{\Phi}(O_2 + 3.76N_2) \rightarrow n_1CO_2 + n_2CO + n_3H_2O + n_4O_2$$

$$+n_5H_2 + n_6OH + n_7H + n_8O + n_9N_2 + n_{10}NO$$ (4.86)

where $\alpha$ is the number of moles of air for stoichiometric combustion and $n_i$ is the number of moles of the $i$th component.

For the species considered, the equilibrium reactions for the solution of the combustion product composition are given as follows

$$CO_2 \leftrightarrow CO + \frac{1}{2}O_2$$ (4.87)

$$H_2O \leftrightarrow H_2 + \frac{1}{2}O_2$$ (4.88)

$$H_2O \leftrightarrow \frac{1}{2}H_2 + OH$$ (4.89)

$$\frac{1}{2}H_2 \leftrightarrow H$$ (4.90)

$$\frac{1}{2}O_2 \leftrightarrow O$$ (4.91)

$$\frac{1}{2}N_2 + \frac{1}{2}O_2 \leftrightarrow NO$$ (4.92)

For the generalised form of the above equations
\[ x_A A + x_B B \leftrightarrow x_C C + x_D D \] (4.93)

in which \( x_i \) represents the stoichiometric coefficients of the reactants and products, the equilibrium constant \( (K_P) \) for chemical equilibrium can be defined as

\[ K_P = \frac{p_C^{x_C} p_D^{x_D}}{p_A^{x_A} p_B^{x_B}} \] (4.94)

where \( p_i \) are the partial pressures in bar. For the dissociation equilibria considered, equations (4.87) to (4.92), the equilibrium constants are given by

\[ K_{P1} = \frac{p_{\text{CO}} \sqrt{p_{\text{O}_2}}}{p_{\text{CO}_2}} \] (4.95)
\[ K_{P2} = \frac{p_{\text{H}_2} \sqrt{p_{\text{O}_2}}}{p_{\text{H}_2\text{O}}} \] (4.96)
\[ K_{P3} = \frac{p_{\text{OH}} \sqrt{p_{\text{H}_2}}}{p_{\text{H}_2\text{O}}} \] (4.97)
\[ K_{P4} = \frac{p_{\text{H}}}{\sqrt{p_{\text{H}_2}}} \] (4.98)
\[ K_{P5} = \frac{p_{\text{O}}}{\sqrt{p_{\text{O}_2}}} \] (4.99)
\[ K_{P6} = \frac{p_{\text{NO}}}{\sqrt{p_{\text{N}_2} p_{\text{O}_2}}} \] (4.100)

The equilibrium constants for equations (4.95) to (4.100) were determined using the relation

\[ \log_{10}(K_P)_{\text{reaction}} = \sum x_i \log_{10}(K_f)_i \] (4.101)

where \( (K_f)_i \) are the equilibrium constants of formation of species from the elements in their standard state. These were obtained from the JANAF tables (1998). Curve fits for the temperature range 600 K to 4000 K were determined using the expression of Olikara and Borman (1975)

\[ \log_{10}K_P = A \ln(T) + \frac{B}{T} + C + DT + ET^2 \] (4.102)

where \( T \) is in kK. The curve fit coefficients are given in Appendix C.
Equations (4.95) to (4.100) give six of the ten equations needed for the solution of the ten unknown partial pressures. From the reactants, equations for the mole ratios of carbon, oxygen and nitrogen to hydrogen can be determined.

\[
\frac{n_C}{n_H} = \frac{p_{CO_2} + p_{CO}}{N} \quad (4.103)
\]

\[
\frac{n_O}{n_H} = \frac{2p_{H_2O} + 2p_{H_2} + p_H + p_{OH}}{N} \quad (4.104)
\]

\[
\frac{n_N}{n_H} = \frac{2p_{N_2} + p_{NO}}{N} \quad (4.105)
\]

Furthermore, addition of the number of moles of each element in the products and substituting for \( n_i = \frac{N}{p} p_i \) from the definition of the ideal gas relation gives

\[
\left( \frac{p}{N} \right) n_C = p_{CO_2} + p_{CO} \quad (4.106)
\]

\[
\left( \frac{p}{N} \right) n_H = 2p_{H_2O} + 2p_{H_2} + p_H + p_{OH} \quad (4.107)
\]

\[
\left( \frac{p}{N} \right) n_O = 2p_{CO_2} + p_{CO} + p_{H_2O} + 2p_{O_2} + p_{OH} + p_O + p_{NO} \quad (4.108)
\]

\[
\left( \frac{p}{N} \right) n_N = 2p_{N_2} + p_{NO} \quad (4.109)
\]

For the products being considered, the total pressure \( (P) \) is given by Dalton’s law as the sum of the partial pressures.

\[
P = p_{CO_2} + p_{CO} + p_{H_2O} + p_{O_2} + p_{H_2} + p_{OH} + p_O + p_{N_2} + p_{NO} \quad (4.110)
\]

Equations (4.95) to (4.100), (4.103) to (4.105) and (4.110) yield the ten equations needed for the solution of the ten unknown partial pressures. Figure 4.12 shows the method of substitution used to calculate the ten partial pressures, starting with initial estimations of \( p_{CO_2}/p_{CO} \) and \( p_{H_2O} \). It is not possible to directly calculate \( p_{NO} \) from the above equations, so an approximation \( (p_{NO}^*) \) is first determined. This is then used to calculate a more accurate value from which \( p_{N_2} \) can be calculated.
Figure 4.12 – Schematic of the iterative scheme of Damköhler and Edse (1943)
It should be noted that the method of Damköhler and Edse (1943) is only valid for cases when $\frac{n_C}{n_O}$ is less than unity. For these cases all the carbon can be assumed to take the form of CO$_2$ or CO.

### 4.6.2 Consideration of Atomic Nitrogen

A drawback of the method of Damköhler and Edse (1943) is the absence of atomic nitrogen (N), which prevents the chemical kinetics of NO from being solved. Therefore, the scheme has been extended to include atomic nitrogen in the product species. The updated combustion reaction is therefore given by

$$C_xH_y + \frac{a}{\phi} (O_2 + 3.76N_2) \rightarrow n_1CO_2 + n_2CO + n_3H_2O + n_4O_2$$

$$+ n_5H_2 + n_6OH + n_7H + n_8O + n_9N_2 + n_{10}NO + n_{11}N \quad (4.111)$$

The introduction of another product species requires an additional equilibrium equation.

$$\frac{1}{2}N_2 \leftrightarrow N \quad (4.112)$$

The corresponding equilibrium constant, from equation (4.94), is given as

$$K_{P7} = \frac{p_N}{\sqrt{p_{N_2}}} \quad (4.113)$$

Equations (4.109) and (4.110) are also updated as follows

$$\left(\frac{p}{N}\right)n_N = 2p_{N_2} + p_{NO} + p_N \quad (4.114)$$

$$P = p_{CO_2} + p_{CO} + p_{H_2}O + p_{O_2} + p_{H_2} + p_{OH} + p_{H} + p_{O} + p_{N_2} + p_{NO} + p_N \quad (4.115)$$

The method of substitution used to calculate the partial pressures remains unchanged from the scheme of Damköhler and Edse (1943) until the calculation of $p_{N_2}$. Then, since $p_N$ appears in both equations (4.113) and (4.114), an iterative scheme is introduced. An initial value for $p_{N_2}$ is first obtained from equation (4.109), as outlined in Figure 4.12. This is used to calculate an initial value for $p_N$ (equation (4.113)), which is
then substituted into equation (4.114) to give a new value for $p_{N_2}$. This is substituted back into equation (4.113) and the iterative process proceeds until the newly calculated values of $p_N$ and $p_{N_2}$ are within a specified accuracy.

### 4.6.3 Method of Solution

Gaydon and Wolfard (1960) described a graphical method for the iteration of the ten partial pressures. The following describes the method employed in the present work. The method requires inputs of pressure, temperature, equivalence ratio and the number of carbon and hydrogen atoms in the fuel. In this method, the value of $n_O/n_H$ depends mainly on the assumption of $p_{CO_2}/p_{CO}$ and the value of $P$ depends mainly on the assumption of $p_{H_2O}$. To begin the iterative process, the partial pressure ratio $p_{CO_2}/p_{CO}$ is given a value of 1 and it is assumed that $p_{H_2O}$ takes a value which is 10 percent of the total pressure. The partial pressures are then calculated using the method outlined in Figure 4.12 and section 4.6.2. Values of $n_O/n_H$ and $P$ are then calculated using equations (4.107), (4.108) and (4.115). These are compared with the known values of $n_O/n_H$ and $P$, given by equation (4.104) and the input pressure, to assess the accuracy of the solution. Updated values of $p_{CO_2}/p_{CO}$ and $p_{H_2O}$ are then determined simultaneously using the bisection method. Once the values agree within a specified accuracy, the iterative process is complete.

Once the partial pressures have been calculated, the mole fraction ($y_i$) of each species is calculated from the definition of the ideal gas relation.

$$y_i = \frac{p_i}{P}$$  \hspace{1cm} (4.116)

Figures 4.13 and 4.14 show the equilibrium combustion product composition for n-dodecane and methane at 50 bar for the temperature range 1500 K to 3000 K, as calculated by the method outlined above. Figure 4.13 shows the change in composition for n-dodecane-air mixtures at an equivalence ratio of 1. Figure 4.14 shows the change in composition for methane-air mixtures at equivalence ratios of 1 and 0.3. Here, an equivalence ratio of 0.3 is illustrative of premixed combustion of the gaseous charge. For an equivalence ratio of 1, the largest mole fractions are for $N_2$, $H_2O$ and $CO_2$. For the leaner methane-air mixture, species of $O_2$ and NO are also significant. The equilibrium combustion product composition is further used to calculate emissions of NOx.
Figure 4.13 – Equilibrium combustion product composition for n-dodecane (C\textsubscript{12}H\textsubscript{26})-air mixtures at $P = 50$ bar and $\phi = 1.0$ for the temperature range 1500 K – 3000 K.

Figure 4.14 – Equilibrium combustion product composition for methane (CH\textsubscript{4})-air mixtures at $P = 50$ bar and $\phi = 1.0$ and 0.3 for the temperature range 1500 K – 3000 K.
4.7 EMISSIONS FORMATION

In dual fuel engines, the main emissions produced during combustion are NO\textsubscript{x}, uHC, CO and PM. In the present work, NO\textsubscript{x} and PM, which are the most challenging of the emissions limits, are considered. Emissions of NO\textsubscript{x} consist of nitric oxide (NO) and nitrogen dioxide (NO\textsubscript{2}) (Warnatz et al., 2006). In engine modelling, the total NO\textsubscript{x} formation is generally reduced to the total formation of NO, as this is the dominant species present in the cylinder (Stone, 1999).

4.7.1 Nitric Oxide (NO)

In internal combustion engines, NO can be formed in three main ways: thermal NO, which is formed from atmospheric nitrogen via the extended Zeldovich mechanism; prompt NO, which is formed in the flame front according to the Fenimore mechanism; and by the recombination of nitrous oxide (N\textsubscript{2}O), which is significant for very lean mixtures and low temperatures.

In internal combustion engines, a major fraction of NO is formed via the thermal mechanism (Stiesch, 2003). This is a non-equilibrium process and is described using the extended Zeldovich mechanism. This consists of three reactions. The first two reactions were originally identified by Zeldovich (Heywood, 1988) and the third was added later by Lavoie et al. (1970). The reactions and their respective rate constants (Warnatz et al., 2006) are given in Table 4.2.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>( A ) ( (\text{cm}^3\cdot\text{mol}^{-1}\cdot\text{s}^{-1}) )</th>
<th>( b )</th>
<th>( E ) ( (\text{kJ}\cdot\text{mol}^{-1}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 ( \text{O} + \text{N}_2 \leftrightarrow \text{NO} + \text{N} )</td>
<td>( 3.27 \cdot 10^{12} )</td>
<td>0.3</td>
<td>0.0</td>
</tr>
<tr>
<td>2 ( \text{N} + \text{O}_2 \leftrightarrow \text{NO} + \text{O} )</td>
<td>( 6.40 \cdot 10^{5} )</td>
<td>1.0</td>
<td>26.1</td>
</tr>
<tr>
<td>3 ( \text{N} + \text{OH} \leftrightarrow \text{NO} + \text{H} )</td>
<td>( 3.80 \cdot 10^{13} )</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

These reactions describe the breakup of a nitrogen molecule by atomic oxygen and the subsequent oxidation of the atomic nitrogen (Stiesch, 2003).

For the generalised form of the above equations, the rates of reaction are given by
\[ \frac{d[A_c]}{dt} = x_c(k^+[A_a]^{x_a}[A_b]^{x_b} - k^-[A_c]^{x_c}[A_d]^{x_d}) \]  

(4.117)

where \([\]
\) denotes a concentration and \(k^+
\) and \(k^-
\) are forward and reverse rate coefficients respectively. According to equation (4.117), the rate of NO formation by the extended Zeldovich mechanism can be written as

\[ \frac{d[\text{NO}]}{dt} = k_1^+[\text{O}][\text{N}_2] + k_2^+[\text{N}][\text{O}_2] + k_3^+[\text{N}][\text{OH}] - k_1^-[\text{NO}][\text{N}] 
- k_2^-[\text{NO}][\text{O}] - k_3^-[\text{NO}][\text{H}] \]  

(4.118)

Since the rate at which atomic nitrogen oxidises (Table 4.2 – reactions 2 and 3) is much greater than the rate at which it is formed (Table 4.2 – reaction 1), the concentration of atomic nitrogen can be assumed to be quasi-steady. Hence, the rate of formation of atomic nitrogen by the extended Zeldovich mechanism can be equated to zero.

\[ \frac{d[\text{N}]}{dt} \approx 0 = k_1^+[\text{O}][\text{N}_2] - k_2^+[\text{N}][\text{O}_2] - k_3^+[\text{N}][\text{OH}] + k_1^-[\text{NO}][\text{N}] + k_2^-[\text{NO}][\text{O}] + k_3^-[\text{NO}][\text{H}] \]  

(4.119)

The concentration of atomic nitrogen can then be expressed as

\[ [\text{N}] = \frac{k_1^+[\text{O}][\text{N}_2] + k_2^-[\text{NO}][\text{O}] + k_3^-[\text{NO}][\text{H}]}{k_1^-[\text{NO}] + k_2^-[\text{O}_2] + k_3^-[\text{OH}]} \]  

(4.120)

Substituting equation (4.120) into equation (4.119) and assuming all respective species except NO are in equilibrium, the rate of NO formation can be written as

\[ \frac{d[\text{NO}]}{dt} = \frac{2R_1\{1 - ([\text{NO}]/[\text{NO}]_e)^2\}}{1 + ([\text{NO}]/[\text{NO}]_e)R_1/(R_2 + R_3)} \]  

(4.121)

where \(R_1, R_2\) and \(R_3\) are reaction rate variables given by

\[ R_1 = k_1^+[\text{O}]_e[\text{N}_2]_e = k_1^-[\text{NO}]_e[\text{N}]_e \]  

(4.122)
\[ R_2 = k_2^+ [N]_e [O_2]_e = k_2^- [NO]_e [O]_e \quad (4.123) \]

\[ R_3 = k_3^+ [N]_e [OH]_e = k_3^- [NO]_e [H]_e \quad (4.124) \]

and the subscript \( e \) denotes equilibrium.

### 4.7.2 Particulate Matter (PM)

In combustion modelling, the total formation of PM or soot is generally determined using empirical correlations, since the chemical kinetics are not yet fully understood. Total soot formation is typically described using a two-step approach in which the net soot formation rate is described as the difference between the rate of soot formation and the rate of soot oxidation

\[ \frac{dm_s}{dt} = \frac{dm_{sf}}{dt} - \frac{dm_{sox}}{dt} \quad (4.125) \]

where \( m_s \) is the mass of soot and the subscripts \( f \) and \( ox \) denote the formation and oxidation processes respectively. Soot formation is generally modelled using Arrhenius-type equations, with the models of Hiroyasu et al. (1983) and Lipkea and DeJoode (1994) widely cited. The oxidation process is modelled using either an Arrhenius-type equation (Hiroyasu et al., 1983, Lipkea and DeJoode, 1994) or the phenomenological model of Nagle and Strickland-Constable (1962), which relates carbon oxidation to surface chemistry. In the present work, the rate of soot formation is determined using the model proposed by Hiroyasu et al. (1983)

\[ \frac{dm_{sf}}{dt} = A_f m_v P_{cy}^{0.5} \exp \left( - \frac{E_{sf}}{R_u T_z} \right) \quad (4.126) \]

where \( m_v \) is the mass of evaporated fuel, \( P_{cy} \) is the in-cylinder pressure (in MPa) and \( E_{sf} \) is the soot formation activation energy. Here, the rate of soot formation is a function of the mass of unburned fuel vapour and the local in-cylinder temperature. The soot formation activation energy, \( E_{sf} \), is given as 52300 kJ.kmol\(^{-1}\) and the pre-exponential constant (\( A_f \)) is adjusted to match the engine type being studied.

The rate of soot oxidation is determined using the model proposed by Nagle and Strickland-Constable (1962). In this model, soot particles are assumed to have two
surface sites: a more reactive surface site A and a less reactive surface site B. Three
reactions are considered: (i) the oxidation of surface sites A; (ii) the oxidation of
surface sites B; and (iii) the thermal rearrangement of surface sites A to surface sites
B. The reactions and their respective reaction rates (in g-C.cm$^{-2}$s$^{-1}$) are given by
equations (4.127) to (4.129).

(i) \[ A + O_2 \rightarrow A + 2CO \]
\[ R_1 = \frac{k_{AP}p_{O_2}}{1 + k_{ZP}p_{O_2}}x_A \] (4.127)

(ii) \[ B + O_2 \rightarrow A + 2CO \]
\[ R_2 = k_{BP}p_{O_2}(1 - x_A) \] (4.128)

(iii) \[ A \rightarrow B \]
\[ R_3 = k_Tx_A \] (4.129)

The overall oxidation rate ($R_{tot}$) is given by

\[ R_{tot} = \left[ \frac{k_{AP}p_{O_2}}{1 + k_{ZP}p_{O_2}}x_A + k_{BP}p_{O_2}(1 - x_A) \right] \] (4.130)

Assuming the reaction rates of reactions (ii) and (iii) are quasi-steady ($R_2 = R_3$), the
fraction of surface site A ($x_A$) can be expressed as

\[ x_A = \left( 1 + \frac{k_T}{k_Bp_{O_2}} \right)^{-1} \] (4.131)

where $p_{O_2}$ is the partial pressure of oxygen (in atm). The rate constants used above
are given in Table 4.3.
Table 4.3 – Rate coefficients for the soot oxidation model of Nagle and Strickland-Constable (1962)

<table>
<thead>
<tr>
<th>Rate Coefficient</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_A = 20 \exp(-15100/T)$</td>
<td>$\text{g-C.cm}^{-2}\text{s}^{-1}\text{atm}^{-1}$</td>
</tr>
<tr>
<td>$k_B = 4.46 \cdot 10^{-3} \exp(-7640/T)$</td>
<td>$\text{g-C.cm}^{-2}\text{s}^{-1}\text{atm}^{-1}$</td>
</tr>
<tr>
<td>$k_T = 1.51 \cdot 10^5 \exp(-4800/T)$</td>
<td>$\text{g-C.cm}^{-2}\text{s}^{-1}$</td>
</tr>
<tr>
<td>$k_Z = 21.3 \exp(-2060/T)$</td>
<td>$\text{atm}^{-1}$</td>
</tr>
</tbody>
</table>

Considering spherical particles, the rate of soot oxidation ($\frac{dm_{s,ox}}{dt}$) is given by

$$\frac{dm_{s,ox}}{dt} = \frac{6m_s}{\rho_s D_s M_C} R_{tot}$$

(4.132)

where $\rho_s$, $D_s$ and $M_C$ are the soot particle density, soot particle diameter and molecular weight of carbon respectively. Several values for the soot particle density and diameter have been proposed in the literature. Typically, the soot density and characteristic soot particle diameter are assumed to be 2 g cm$^{-3}$ and 25 nm respectively (Stiesch, 2003).

### 4.8 NUMERICAL SOLUTION

A quasi-dimensional, multi-zone combustion model has been developed and implemented using C/C++. This is operated using a graphical user interface (GUI) designed and developed as part of the present work (Appendix D). The following is a description of the main model assumptions and the conservation and state equations. A flowchart of the computational simulation is also given.

#### 4.8.1 General Description

The combustion simulation proceeds between IVC and EVO, thereby including the compression, combustion and expansion processes of the engine. The sub processes that occur during this time include injection, atomisation, entrainment, evaporation, ignition and combustion, and pollutant formation (as described in sections 4.3 through 4.7). During the cycle, the in-cylinder properties are calculated at one degree crank angle intervals. The main model assumptions are as follows:
• The model assumes injection of n-dodecane ($C_{12}H_{26}$) into a gaseous mixture comprising air and natural gas. Air is modelled on a volume basis as a mixture of 79 percent nitrogen and 21 percent oxygen. Natural gas is modelled as 100 percent methane ($CH_4$).

• The model comprises an unburned gaseous zone, pilot fuel spray zones and a premixed burning zone. These are denoted by the subscripts $u$, $z$ and $p$ respectively. Spray zones with an ignition integral greater than or equal to one and the premixed burning zone are collectively referred to as burning zones.

• The in-cylinder pressure is considered to be uniform across the combustion chamber.

• The evaporated liquid fuel and cylinder gases are modelled as ideal gases.

• Residuals from the previous cycle are neglected.

• Reactions within the unburned zone are neglected.

• A uniform droplet distribution is assumed.

• Ignition is attributed solely to the evaporated liquid fuel.

• It is assumed that there are no chemical interactions between the evaporated liquid fuel and ingested gaseous fuel.

• The composition of the burned species is calculated assuming chemical equilibrium.

• Each zone is uniform in composition and temperature.

• Entrainment is considered to be a net mass transfer process. There is no mass transfer between the burning zones.

• Flame propagation is assumed to be spherical.

• Flame quenching is neglected.

• Blowby is neglected.

A flowchart of the combustion simulation is shown in Figure 4.15. This is an extension of the approach of Whitehouse (1986). Here, the combustion simulation is solved using a nested iterative loop. The first loop solves for the temperature constraint of the energy conservation equations. The temperatures of the model zones at the end of the computational time step are resolved using the Newton Raphson method (Press et al., 1994). The second loop solves for the cylinder volume constraint (as described in section 4.8.2). The relevant differential equations are solved using either the Euler method or the Runge-Kutta-Fehlberg scheme (Press et al., 1994).
Figure 4.15a – Flowchart for combustion simulation (continued on next page)
Figure 4.15b – Flowchart for combustion simulation (continued from previous page)
4.8.2 Conservation and State Equations

The cylinder contents are initially represented by a homogeneous single zone. Consequently, the changes in pressure and temperature of the unburned gaseous charge can be solved using the first law of thermodynamics for a closed system in combination with the ideal gas equation of state

\[ dU = dQ - dW \]  \hspace{1cm} (4.133)

\[ PV = nR_uT \]  \hspace{1cm} (4.134)

where \( dU \) is the change in internal energy, \( dQ \) is the change in heat transfer and \( dW \) is the boundary work. The internal energy of the model zones is calculated using polynomial curve fits of the specific molar enthalpy (\( \bar{h} \)) to the JANAF tables (1998) (Appendix B). Considering a reversible process, the boundary work is given by

\[ dW = PdV \]  \hspace{1cm} (4.135)

The mole number (\( n \)) of the trapped cylinder charge is determined from the ideal gas equation of state, using the in-cylinder pressure, cylinder volume and manifold temperature at IVC. The instantaneous cylinder volume (\( V_{cyl} \)) is calculated from the engine geometry as follows

\[ V_{cyl} = V_c + \frac{\pi B^2}{4} s \]  \hspace{1cm} (4.136)

where \( V_c \) is the clearance volume and \( s \) is the instantaneous stroke length relative to TDC. The clearance volume, \( V_c \), can be determined from the definition of the compression ratio (\( r_c \)). Hence,

\[ V_c = \frac{V_d}{r_c - 1} \]  \hspace{1cm} (4.137)

where \( V_d \) is the displacement volume. The instantaneous stroke, \( s \), is given by

\[ s = r(1 - \cos\varphi) + \left[l - \sqrt{(l^2 - r^2 \sin^2\varphi)}\right] \]  \hspace{1cm} (4.138)
where \(r\) is the crankshaft throw, \(\varphi\) is the crank angle and \(l\) is the connecting rod length. The instantaneous stroke, \(s\), is also used to determine the combustion chamber surface area, \(A\), employed in the heat transfer model of Annand (1963). The combustion chamber surface area, \(A\), is given by

\[
A = A_p + A_{ch} + \pi Bs
\]

where \(A_p\) and \(A_{ch}\) are the piston and cylinder head area respectively.

Equations (4.133) and (4.134) are applied until the point of spray breakup. Liquid fuel injected during this time is tracked, but is not included in the combustion simulation. Following breakup, the multi-zone model is initiated and the first law of thermodynamics for an open system is applied to all model zones. In the case of the unburned gaseous zone, mass is removed due to entrainment. Therefore, the first law is expressed as

\[
dE_u = dQ_u - dW_u - h_g dm_g
\]

where \(dE\) is the change in energy of the zone, \(h_g\) is the specific enthalpy of the unburned gaseous zone and \(dm_g\) is the mass of entrained gaseous mixture. In the case of the spray zones, there are enthalpic flows associated with the entrainment of unburned gaseous mixture and evaporation of the liquid fuel. Hence,

\[
dE_z = dQ_z - dW_z + h_g dm_{g,z} + h_{fg,z} dm_{l,ev,z}
\]

where \(h_{fg,z}\) is the latent heat of evaporation and \(dm_{l,ev,z}\) is the mass of evaporated liquid fuel. Following initiation of the premixed burning zone, unburned gaseous mixture is also entrained by the turbulent flame front. Hence, the first law for the premixed burning zone is expressed as

\[
dE_p = dQ_p - dW_p + h_g dm_{g,p}
\]

The combustion simulation iterates under the constraint that the sum of the zone volumes must be equal to the instantaneous cylinder volume \((V_{cyl})\).
If the volume constraint is not satisfied, the in-cylinder pressure is adjusted using the following expression

\[ P_{\text{cyl}} = P_{\text{cyl}} \frac{V_u + V_p + \sum V_z}{V_{\text{cyl}}} \]  

(4.144)

4.9 CONCLUDING SUMMARY

A new quasi-dimensional, multi-zone model has been developed to describe the combustion processes occurring inside a dual fuel engine during the closed part of the engine cycle. The pilot fuel spray is described using a packet model approach, which accounts for spray development and mixing, swirl, spray wall impingement, ignition and combustion. Flame development is described using an original approach in which flame growth is coupled to the burning zones in the cylinder and is simulated using a turbulent entrainment model. The model is the first to account for flame growth from the viewpoint of coalescence of enflamed zones.

Heat transfer has been extensively treated in the present work, with sub-models for convective heat transfer, heat transfer from the spray burning zones to the premixed burning zone and unburned zone, and radiative heat transfer from the spray burning zones all considered. It is proposed that this gives a much better description of the heat transfer processes occurring inside a dual fuel engine.

Dissociation of the combustion products is calculated using an iterative chemical equilibrium scheme modified to include eleven product species. The equilibrium concentrations are further used to calculate non-equilibrium emissions of NO. Emissions of soot are also considered.

The main objective during model development was to describe the combustion processes occurring inside a dual fuel engine on the basis of physical and chemical phenomena, thus limiting the number of adjustable model constants. In Chapter 5, the calibration of the model constants and validation of the quasi-dimensional model are discussed.
CHAPTER 5
MODEL CALIBRATION AND VALIDATION

5.1 INTRODUCTION

In this chapter, the calibration and validation of the quasi-dimensional dual fuel model (described in Chapter 4) are discussed. Inherent in the adopted modelling approach is the need to modify model constants to match the engine type being studied. In the present work, the model has been calibrated to match data obtained from a naturally aspirated, in-line, four-cylinder, direct injection diesel engine typical of a small genset application (Stewart, 2006).

Calibration of the model proceeded in two stages. The model was first calibrated against a baseline diesel case at 1500 rpm and 100 percent load. The model was then calibrated against a baseline dual fuel case at 1500 rpm and 100 percent load for the maximum gaseous substitution ratio for stable operation. In each case, a single-zone energy release analysis was used to provide the associated energy release diagram. The adopted approach allowed the phenomena associated with the pilot fuel injection model to be decoupled from the turbulent entrainment model during the calibration process.

The predictive capability of the model was assessed by comparing the calibrated model against experimental data taken across a range of gaseous substitution ratios at 1500 rpm under 100 and 50 percent load conditions. Here, the main aim was to accurately predict engine performance and emissions by accurately predicting the associated pressure and energy release diagrams. The main engine parameters considered in the present work are the magnitude and timing of peak in-cylinder pressure and the ignition delay period. The main emissions of interest are NO\textsubscript{x} and soot.

The chapter begins with a brief overview of the engine test facility, followed by a discussion of the experimental analysis. The calibration of the dual fuel model is then discussed, with the predictive capability of the model assessed by comparing model predictions against experimental data.
CHAPTER 5

MODEL CALIBRATION AND VALIDATION

5.2 OVERVIEW OF ENGINE FACILITY

The combustion model was calibrated and validated using data obtained in a study previously conducted at Loughborough University (Stewart, 2006). The following is an overview of the test engine, test bed facility and emissions measurement techniques employed in that work. Further details of the engine facility can be found in Stewart (2006) and Abdul-Karim (2004).

5.2.1 Test Engine

The test engine was based on a Lister-Petter naturally aspirated, in-line, four-cylinder, direct injection diesel engine with re-entrant bowl piston geometry. This type of engine is typical of a small diesel genset application. The engine details relevant to the present work are given in Table 5.1.

<table>
<thead>
<tr>
<th>Table 5.1 – Lister-Petter engine specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine type</td>
</tr>
<tr>
<td>Chamber geometry</td>
</tr>
<tr>
<td>Bore diameter</td>
</tr>
<tr>
<td>Stroke length</td>
</tr>
<tr>
<td>Connecting rod length</td>
</tr>
<tr>
<td>Compression ratio</td>
</tr>
<tr>
<td>Inlet valve closure (IVC)</td>
</tr>
<tr>
<td>Exhaust valve opening (EVO)</td>
</tr>
</tbody>
</table>

The fuel injection system was fed by a Lucas rotary fuel injection pump and SOI was controlled by the engine governor. Low flow injectors were employed in place of standard injectors to improve engine performance at larger gas substitutions. The rate of fuel supply to the engine was measured on a volumetric basis. A single injector was fitted with a hall-effect sensor to record needle lift. This was subsequently used to determine the injection duration. Further details of the injection system are given in Table 5.2. For the purpose of model calculations, the $L/D$ ratio of the nozzle was assumed to equal 4 (Chehroudi et al., 1985, Reitz and Bracco, 1979).
Table 5.2 – Injection system

<table>
<thead>
<tr>
<th>Nozzle type</th>
<th>VCO type nozzle</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nozzle opening pressure</td>
<td>240 ±5 bar</td>
</tr>
<tr>
<td>Number of nozzle holes</td>
<td>5</td>
</tr>
<tr>
<td>Nozzle hole diameter</td>
<td>0.171 mm</td>
</tr>
<tr>
<td>Spray included angle</td>
<td>145°</td>
</tr>
</tbody>
</table>

To operate the engine in dual fuel mode, the engine was modified to allow the introduction of gaseous fuel into the cylinders. The gaseous fuel, in this case methane (which is representative of natural gas), was supplied by a BOC gas bottle. The outlet from the gas bottle was first passed through a two-stage regulator before being mixed with air using a simple venturi-type gas mixer. This was situated ten pipe diameters upstream of the inlet manifold to provide adequate mixing. Gaseous fuel flow was controlled using a needle valve and the flow rate was measured using an Omega FMA 1610 mass flowmeter, which also recorded the fuel line pressure and gas temperature.

5.2.2 Test Bed Facility
The engine facility is shown schematically in Figure 5.1. The test engine was coupled to a Heenan-Dynamatic MkII eddy current dynamometer rated at 220 kW. This was controlled by a TA 2000 controller, capable of controlling engine speed and torque to within ±0.5 rpm and ±2 Nm respectively. The air flow rate to the engine was measured using a laminar viscous air flowmeter with a type 5 Cussons manometer. The intake manifold pressure was measured using a Druck PDCR 810-0799 piezo-resistive absolute pressure transducer coupled to a digital manometer.

The in-cylinder pressure and dynamic injection pressure were measured on a crank angle resolved basis. The crank angle was measured using an AVL 35401 optical encoder at 0.5 degree crank angle (°CA) increments. A TDC marker was also used to index the data acquisition. The in-cylinder pressure was measured using a Kistler 6053B60 piezo-capacitive pressure transducer. The signal from this transducer was amplified using a Kistler 5011 charge amplifier. The in-cylinder pressure data was referenced (pegged) to the intake manifold pressure at IVC. The dynamic injection pressure was measured using a Kistler 4065A piezo-resistive sensor connected to a Kistler 4617A amplifier. At each test case, data was collected over 100 consecutive cycles for the purposes of averaging.
132

The inlet manifold temperature, exhaust manifold temperature and inlet coolant temperature were measured using K-type thermocouples. The inlet coolant temperature was held constant at 75 °C throughout the experimental program.

5.2.3 Emissions Measurement
Exhaust emissions were measured using the Horiba Mexa 7100 HEGR and the AVL 415 smoke meter (Figure 5.1). The Horiba Mexa 7100 HEGR was used to measure the concentrations of five species in the exhaust – O₂, CO, CO₂, NOₓ and uHC – and the AVL 415 smoke meter was used to determine the concentration of PM. As stated previously, the main emissions of interest in the present work are NOₓ and PM. The associated measurement techniques for these emissions are described in the following sections.

5.2.3.1 Oxides of Nitrogen (NOₓ)
Emissions of NOₓ were measured using the chemiluminescence technique, which operates on the principle of emission of light. Nitric oxide (NO) reacts with ozone (O₃)
CHAPTER 5 MODEL CALIBRATION AND VALIDATION

to produce nitrogen dioxide (NO$_2$) in an activated state, and as it reverts to its normal state, light is emitted. This emission of light is proportional to the concentration of NO. NO$_x$ is primarily comprised of NO and NO$_2$. Thus, for the detection of NO$_x$, an exhaust sample containing NO and NO$_2$ is first passed through a catalyst where all the NO$_2$ is converted to NO. The total sum of NO$_x$ is therefore the sum of the NO produced from the NO$_2$ and NO originally in the exhaust.

5.2.3.2 Particulate Matter (PM)
The AVL 415 is a filter-type smoke meter used for measuring steady-state soot emissions. It operates by passing a controlled volume (0.5 litres) of sampled exhaust gas through a section of clean filter paper. This causes blackening of the filter paper, which is measured using a reflective photometer. The reflectance of the filter paper corresponds to the smoke level, which is characterised by a Filter Smoke Number (FSN). This in turn corresponds to the carbon content of the soot and can be equated to the soot concentration ($C_s$) (in mg/m$^3$)$^1$.

$$C_s = \frac{1}{0.405 \cdot 4.95 \cdot \text{FSN} \cdot \exp(0.38 \cdot \text{FSN})}$$ (5.1)

5.3 EXPERIMENTAL ANALYSIS

5.3.1 Energy Release Analysis
The energy release rate can provide important information about the progression of combustion and aid the explanation of emissions formation. In terms of engine modelling, a suitable prediction of the energy release rate can provide an insight into the underlying combustion processes without the need for experimental data.

In the present work, the net energy release rate has been used to calibrate and assess the predictive capability of the dual fuel model. Typically, the experimental net energy release rate is determined using a single-zone energy release analysis, whereby the cylinder contents are assumed to be uniform in composition and temperature. The following describes the mathematical formulation of the single-zone energy release analysis, as used in the present work.

---

$^1$ AVL (2005) Smoke value measurement with the filter-paper-method (AT1007E, Rev. 2), Austria, pp. 92.
The first law of thermodynamics for a closed system, expressed in terms of the net energy release rate ($\delta Q_n$), is given by

$$\delta Q_n = dU + \delta W$$

(5.2)

where $dU$ is the change in internal energy and $\delta W$ is the boundary work. Since $\delta W = PdV$ (for a reversible process) and $dU = mC_VdT$, equation (5.2) can be expressed as

$$\delta Q_n - PdV = mC_VdT$$

(5.3)

From the differential form of the ideal gas law ($PV = mRT$)

$$mdT = \frac{1}{R}(PdV + VdP)$$

(5.4)

the energy equation can be written as

$$\delta Q_n - PdV = \frac{C_V}{R}(PdV + VdP)$$

(5.5)

which on a crank angle basis is given by

$$\frac{dQ_n}{d\varphi} = \frac{C_V}{R} \left( P \frac{dV}{d\varphi} + V \frac{dP}{d\varphi} \right) + P \frac{dV}{d\varphi}$$

(5.6)

Since $C_p/C_V = k$ and $R = C_p - C_V$, equation (5.6) can be expressed as

$$\frac{dQ_n}{d\varphi} = \frac{1}{k - 1} \left( P \frac{dV}{d\varphi} + V \frac{dP}{d\varphi} \right) + P \frac{dV}{d\varphi}$$

(5.7)

$$\frac{dQ_n}{d\varphi} = k \frac{C_V}{R} \left( P \frac{dV}{d\varphi} + V \frac{dP}{d\varphi} \right)$$

(5.8)

In equation (5.8), $k$ is generally taken to be constant. Heywood (1988) suggests that an appropriate range of $k$ for diesel engines is 1.3 to 1.35. This is based on values of $\sim1.35$ and $\sim1.26-1.23$ for the specific heat ratios of air at the end of the compression
stroke and the burned gases in the cylinder following combustion respectively. Hence, in the present work, $k$ is considered to equal 1.33.

Caution must be exercised when comparing the experimental and predicted energy release diagrams because the single-zone energy release analysis can only provide an indication of the energy release rates in the cylinder. This is due to the description of the heterogeneous cylinder contents by a single zone. Thus, in the present chapter, the main aim is to accurately predict the experimental pressure diagram, whilst matching the trends associated with the energy release diagram.

### 5.3.2 Start of Combustion (SOC)

The SOC can be defined in a number of ways. Methods include defining the point at which there is an abrupt increase in in-cylinder pressure (Assanis et al., 2003); the point at which combustion of a specified mass of fuel has occurred (Zhou and Karim, 1994); or the point at which the net energy release rate becomes positive (Stone, 1999). Assanis et al. (2003) used the second derivative of the pressure diagram to define the SOC across a range of engine loads and speeds. Here, the maximum of the second derivative of the pressure diagram represents the maximum acceleration in the net energy release rate. Figure 5.2 shows the use of the second derivative of the pressure diagram to determine the SOC. The pressure data is taken from the present data set for diesel operation at 1500 rpm and 100 percent load. It is observed that the second derivative of the pressure diagram gives a clear indication of the SOC. This method was also applied to the predicted pressure diagram to determine the simulated SOC.
5.4 MODEL CALIBRATION AND VALIDATION

Experimental data was collected across a range of engine load and speed conditions for a number of gaseous substitution ratios (Stewart, 2006). The data was collected under steady-state operating conditions at engine speeds of 1500, 1800 and 2100 rpm. These correspond to synchronous speed, rated speed and peak torque respectively. Five engine loads were considered: 0, 25, 50, 75 and 100 percent of full load; where full load was taken to be the maximum torque that could be achieved under diesel operation at a given engine speed. The experimental conditions used in the present work are given in Table 5.3. Here, an engine speed of 1500 rpm was selected, as this is the speed at which the engine studied would most typically run. The letters C and V denote calibration and validation cases respectively. Full load conditions for an engine speed of 1500 rpm corresponded to a torque of 118 Nm.

Calibration of the dual fuel model was completed in two stages (Table 5.3). Firstly, the model was calibrated against a baseline diesel case (Ref C.1). This allowed the model constants associated with the pilot injection model to be determined. The model was then calibrated against a baseline dual fuel case (Ref C.2) to determine the constants associated with the turbulent entrainment model. This approach allowed the phenomena associated with the pilot injection model to be decoupled from the turbulent entrainment model during the calibration process. The baseline dual fuel case was selected at 100 percent load for the maximum gaseous substitution ratio for
stable operation, as this is where the main benefits associated with dual fuelling occur. Following model calibration, model validation was completed under 100 and 50 percent load conditions for a range of gaseous substitution ratios.

### Table 5.3 – Experimental conditions at 1500 rpm under 100 and 50 percent load conditions

<table>
<thead>
<tr>
<th>Ref</th>
<th>Load</th>
<th>Gaseous Energy Substitution</th>
<th>Diesel Fuel Flow Rate</th>
<th>Gaseous Fuel Flow Rate</th>
<th>Gaseous Equivalence Ratio</th>
<th>SOI (ATDC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C.1</td>
<td>100</td>
<td>0.0</td>
<td>4.401</td>
<td>0.0</td>
<td>0.0</td>
<td>-9.0</td>
</tr>
<tr>
<td>C.2</td>
<td>100</td>
<td>80.68</td>
<td>0.833</td>
<td>3.085</td>
<td>0.547</td>
<td>-8.5</td>
</tr>
<tr>
<td>V.1.1</td>
<td>100</td>
<td>24.96</td>
<td>3.271</td>
<td>0.964</td>
<td>0.167</td>
<td>-8.5</td>
</tr>
<tr>
<td>V.1.2</td>
<td>100</td>
<td>48.50</td>
<td>2.295</td>
<td>1.915</td>
<td>0.336</td>
<td>-10.0</td>
</tr>
<tr>
<td>V.1.3</td>
<td>100</td>
<td>75.00</td>
<td>1.083</td>
<td>2.879</td>
<td>0.514</td>
<td>-13.5</td>
</tr>
<tr>
<td>V.2.1</td>
<td>50</td>
<td>0.0</td>
<td>2.313</td>
<td>0.0</td>
<td>0.0</td>
<td>-9.5</td>
</tr>
<tr>
<td>V.2.2</td>
<td>50</td>
<td>45.86</td>
<td>1.404</td>
<td>1.054</td>
<td>0.178</td>
<td>-14.0</td>
</tr>
<tr>
<td>V.2.3</td>
<td>50</td>
<td>64.34</td>
<td>0.994</td>
<td>1.589</td>
<td>0.270</td>
<td>-12.5</td>
</tr>
<tr>
<td>V.2.4</td>
<td>50</td>
<td>67.97</td>
<td>0.900</td>
<td>1.692</td>
<td>0.288</td>
<td>-12.5</td>
</tr>
<tr>
<td>V.2.5</td>
<td>50</td>
<td>69.50</td>
<td>0.897</td>
<td>1.812</td>
<td>0.308</td>
<td>-12.5</td>
</tr>
<tr>
<td>V.2.6</td>
<td>50</td>
<td>71.06</td>
<td>0.880</td>
<td>1.915</td>
<td>0.328</td>
<td>-12.0</td>
</tr>
</tbody>
</table>

The gaseous equivalence ratios considered in the present work range from \( \phi = 0.167 \) to \( \phi = 0.547 \) (Table 5.3, Refs V.1.1 and C.2 respectively). At atmospheric conditions, the lean flammability limit of a methane-air mixture is approximately \( \phi \approx 0.5 \) (Figure 5.3). Egolfopoulos et al. (2007) performed a numerical study to investigate the extension of the lean flammability limit under conditions relevant to internal combustion engines. Their study showed that the lean flammability limit of methane-air mixtures is a function of both the in-cylinder pressure and unburned gas temperature. Figure 5.3 shows that for an in-cylinder pressure of 50 atm and unburned gas temperature of 700 K, the lean flammability limit is extended to an equivalence ratio of approximately \( \phi \approx 0.2 \).
In the present work, where the peak in-cylinder pressures range from 48.84 to 60.74 atm and the unburned gas temperature at TDC for motored operation is greater than 700 K, premixed combustion by flame propagation is assumed to occur for all gaseous equivalence ratios greater than $\Phi \approx 0.2$. Below $\Phi \approx 0.2$, it is postulated that the ignition energy from the diesel promotes the combustion of the gas surrounding the pilot. Therefore, premixed combustion by flame propagation is assumed to occur for all the experimental cases considered. The impact of this assumption on the prediction of the in-cylinder pressure and energy release rate for cases where $\Phi < 0.2$ is discussed in the relevant sections.

### 5.4.1 Model Calibration

This section discusses the calibration of the pilot injection and turbulent entrainment models. During the calibration process, the main aim was to match the experimental and predicted pressure diagrams and accurately predict the shape of the energy release rate. The following sections highlight the model constants employed in the calibration process and the calibration procedure adopted.

#### 5.4.1.1 Calibration of Pilot Injection Model

The pilot injection model was calibrated at a single operating point corresponding to a baseline diesel case of 1500 rpm and 100 percent load (Table 5.3, Ref C.1). The number of radial and circumferential spray zones was set to 5 and 6 respectively.
These values were obtained following a sensitivity analysis of performance and emissions predictions for different numbers of spray zones. This will be discussed further in Chapter 6.

The model constants associated with the pilot injection model modify the phenomena related to the heat transfer, entrainment and ignition processes occurring inside the cylinder. The calibration procedure employed to determine the pilot injection model constants is described in the following:

1. **Heat transfer.** To calibrate the convective heat transfer model, the experimental and predicted compression curves were matched. (The relevant constants are discussed in Chapter 4, section 4.5.1.) Here, the constant $a$ in the correlation of Annand (1963) was set to its most common value of 0.26. The value of $b$ was then adjusted until the predicted and experimental pressure diagrams matched. Thus, a value of 0.83 was selected. The temperature of the cylinder walls, $T_w$, was held constant throughout, at 450 K. The zonal heat transfer constant $\xi$ was set to 0.005 (under the condition $0 \leq \xi \leq 1$) (see Chapter 4, section 4.5.3).

2. **Rate of entrainment.** The rate of entrainment into the pilot fuel spray was calibrated by adjusting the constants controlling the conservation of initial spray momentum; the increase in entrainment towards the spray periphery; and the increase in entrainment following spray wall impingement. The calibration of these parameters is discussed in the following:

   a. **Conservation of initial spray momentum.** The factor applied to the conservation of initial spray momentum, $C_p$, (see Chapter 4, section 4.3.4.2) was determined together with the entrainment factor to match the initial pressure rise and peak value of in-cylinder pressure. A factor of 0.42 was found to give the best agreement with the experimental data.

   b. **Entrainment factor.** The shape factor for the Gaussian distribution (entrainment factor, $\alpha$) (see Chapter 4, section 4.3.3.1) was determined together with the factor applied to the conservation of initial spray momentum. It was found that a value of 30 gave the best agreement with the experimental data. Figure 5.4 shows a qualitative assessment of the development of a spray with an entrainment factor of 30. The
spray head shape is in good agreement with results presented in the literature (Cao et al., 2000).

c. **Spray Wall Impingement.** In the present work, the decrease in spray velocity following wall impingement (see Chapter 4, section 4.3.3.3) was assumed to be proportional to $t^{-0.6}$.

![Figure 5.4 – Predicted spray development during injection into nitrogen.](image)

Spray tip penetration and spray cone angle calculated from the correlations of Arai et al. (1984) and Reitz and Bracco (1979).

3. **Ignition delay.** The value of $E/R_u$ in the Arrhenius expression of Nishida and Hiroyasu (1989) (see Chapter 4, section 4.3.5) was modified to match the experimental ignition delay period. A value of 7100 K was found to give the best agreement with the experimental data.

During the calibration process, the nozzle discharge coefficient, $C_d$, was assigned a value of 0.66 (see Chapter 4, section 4.3.2). The temperature of the liquid fuel was maintained constant throughout and was assumed to take a value of 400 K. The calculation of the change in angular velocity with crank angle was initiated at IVC by
defining an initial value for the swirl ratio (see Chapter 4, section 4.3.3.2). It is favourable to obtain this from experimental data. However, in the present work, the swirl ratio for the cylinder head was unavailable. Therefore, following a sensitivity analysis, the swirl ratio at IVC was given a value of 0.5. The effect of the magnitude of this value is investigated in the following chapter.

The remainder of the model constants were set to baseline values cited in the literature (see Chapter 4). Table 5.4 shows a summary of the model constants adjusted to match the engine type studied.

<table>
<thead>
<tr>
<th>Constant</th>
<th>Model value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat transfer, (a)</td>
<td>0.26</td>
</tr>
<tr>
<td>Heat transfer, (b)</td>
<td>0.83</td>
</tr>
<tr>
<td>Heat transfer, (\xi)</td>
<td>0.005</td>
</tr>
<tr>
<td>Conservation of spray momentum, (c_b)</td>
<td>0.42</td>
</tr>
<tr>
<td>Entrainment factor, (\alpha)</td>
<td>30</td>
</tr>
<tr>
<td>Ignition delay, (E/R_u, l(K))</td>
<td>7100</td>
</tr>
</tbody>
</table>

Figure 5.5 compares the experimental and predicted in-cylinder pressure diagrams for the baseline diesel case. It is observed that the predicted pressure diagram is in good agreement with the experiment data. The experimental peak in-cylinder pressure is 52.60 bar at 7.0 degrees ATDC and the predicted peak in-cylinder pressure is 52.28 bar at 6.0 degrees ATDC. Hence, the magnitude and timing of the predicted peak in-cylinder pressure show excellent agreement with the experimental data.

A comparison of the experimental and predicted net energy release rates is shown in Figure 5.6. The fuel injection rate, derived from the total mass injected and fuel line pressure, is shown for reference. In general, the overall shape of the energy release rate is in good agreement with the experimental data. It is observed that the timing of SOC is also in good agreement. However, the magnitude of peak energy release is over-predicted relative to the experimental case. Some variation in the experimental and predicted energy release diagrams is expected, since the spatial representation of temperature and specific heats is better described by the multi-zone approach. The
Figure 5.5 – Comparison of experimental and predicted in-cylinder pressure diagrams at 1500 rpm and 100 percent load for diesel operation.

Figure 5.6 – Comparison of experimental and predicted net energy release rate diagrams at 1500 rpm and 100 percent load for diesel operation. The simulated injection rate is also shown.
shape of the energy release diagram is also affected by smoothing of the pressure diagram, which reduces the peak energy release value (Stone, 1999).

The agreement between the pressure and energy release diagrams gives confidence in the sub-models employed in the pilot injection model. The next section describes the calibration of the turbulent entrainment model.

5.4.1.2 Calibration of Turbulent Entrainment Model

The calibration of the turbulent entrainment model was completed at a single operating point corresponding to a baseline dual fuel case of 1500 rpm and 100 percent load for the maximum gaseous substitution ratio for stable operation (Table 5.3, Ref C.2).

The constants associated with the turbulent entrainment model describe the definition of the turbulence characteristics, characteristic burning time, characteristic entrainment mass and entrainment area damping factor. The calibration procedure for determining the model constants is described below. The calibration of the integral length scale, turbulence intensity and characteristic burning time were determined together to best describe the initial rate of premixed combustion by flame propagation. (The constants referred to in the following can be found in Chapter 4, section 4.4.2.)

1. **Integral length scale.** The integral length scale is considered to be proportional to the combustion chamber height, $h$, at the initiation of combustion. In the present work, the proportionality constant applied to the integral length scale, $C_L$, was considered to equal 0.05.

2. **Turbulence intensity.** The turbulence intensity is considered to be proportional to the mean piston speed, $S_p$. Here, the proportionality constant applied to the turbulence intensity, $C_{U'}$, was considered to equal 0.85.

3. **Characteristic burning time.** The factor applied to the characteristic burning time, $C_T$, was assigned a value of 0.001.

4. **Characteristic entrainment mass.** The characteristic entrainment mass, $C_m$, was used to define the peak in energy release from the premixed gaseous charge. In the present work, it was defined as the point at which greater than 12 percent of the ingested cylinder contents had been entrained.

5. **Entrainment area damping factor.** The factor applied to the entrainment area damping factor, $C_e$, was chosen to match the late combustion phase. A value of 50 was found to give the best agreement with the experimental data.
Table 5.5 shows a summary of the model constants associated with the turbulent entrainment model.

<table>
<thead>
<tr>
<th>Constant</th>
<th>Model value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Integral length scale, $C_L$</td>
<td>0.05</td>
</tr>
<tr>
<td>Turbulence intensity, $C_U'$</td>
<td>0.85</td>
</tr>
<tr>
<td>Characteristic burning time, $C_t$</td>
<td>0.001</td>
</tr>
<tr>
<td>Characteristic entrainment mass, $C_m$</td>
<td>0.88</td>
</tr>
<tr>
<td>Entrainment area damping factor, $C_e$</td>
<td>50</td>
</tr>
</tbody>
</table>

Initially, the model constants associated with the pilot injection model were held constant during the calibration of the turbulent entrainment model. However, it was found that for smaller diesel flow rates, the model was unable to describe the spray mixing process adequately. Therefore, the rate of entrainment into the pilot fuel spray was adjusted (Cui et al., 2001, Dent and Mehta, 1981). In the present work, the factor applied to the conservation of initial spray momentum was modified. This can be attributed to difficulties in describing the injection rate, particularly for small pilot fuel quantities. Thus, the factor applied to the conservation of initial spray momentum was assigned a value of 0.7.

Figure 5.7 compares the experimental and predicted in-cylinder pressure diagrams for the dual fuel calibration case. The experimental and predicted in-cylinder pressures are in good general agreement, with the experimental peak in-cylinder pressure occurring at 53.55 bar and 10.0 degrees ATDC, and the predicted peak in-cylinder pressure occurring at 51.01 bar and 10.0 degrees ATDC.

Figure 5.8 compares the net energy release rate calculated from the experimental in-cylinder pressure diagram against the predicted net energy release rate. The derived fuel injection rate is also shown. The overall shape of the predicted energy release rate is in good agreement with the experimental data. It is also observed that the experimental and predicted SOC are in good agreement.
Figure 5.7 – Comparison of experimental and predicted in-cylinder pressure diagrams at 1500 rpm and 100 percent load for a gaseous energy substitution of 80.68 percent.

Figure 5.8 – Comparison of experimental and predicted net energy release rate diagrams at 1500 rpm and 100 percent load for a gaseous energy substitution of 80.68 percent. The simulated injection rate is also shown.
Figure 5.9 shows the main components of energy release for the dual fuel calibration case. The energy release in a dual fuel engine is comprised of three components: the combustion of the premixed gaseous charge; the combustion of the prepared fuel vapour; and the combustion of the entrained gaseous fuel. For the dual fuel calibration case, it is observed that the main source of energy release is from the premixed gaseous charge, with the pilot primarily acting as an ignition source. The figure also shows the rapid initial increase in energy release from the premixed charge before the entrainment of a characteristic mass, after which flame growth is described by an exponential decay. It is noted that the magnitude of energy release from the entrained gaseous fuel is relatively small.

![Figure 5.9](image_url)

Figure 5.9 – Constituent components of dual fuel energy release at 1500 rpm and 100 percent load for a gaseous energy substitution of 80.68 percent

The agreement between the experimental and predicted pressure and energy release diagrams gives confidence in the sub-models employed in the turbulent entrainment model.

### 5.4.2 Model Validation

The validation of the combustion model was completed by comparing the calibrated model against experimental data taken at 1500 rpm under 100 and 50 percent load conditions for a range of gaseous substitution ratios. The capability of the model was assessed by comparing the experimental and predicted pressure and net energy release diagrams, and the trends for emissions of NO and soot. The magnitude and
timing of peak in-cylinder pressure and the ignition delay period were further used to assess the accuracy of the model predictions.

As with the calibration cases, the factor applied to the conservation of initial spray momentum was adjusted for different diesel fuel flow rates to match the experimental and predicted pressure diagrams. Figure 5.10 shows the factors applied to the conservation of initial spray momentum for the diesel fuel flow rates employed in the present work. It is observed that there is a linear relationship between the rate of entrainment and the diesel fuel flow rate for each of the load cases. This is associated with the lower fuel line pressures and injection rates observed for smaller pilot fuel quantities. These affect the magnitude of initial spray momentum, which has an important effect on all subsequent in-cylinder processes, including prolonging the physical and chemical preparation of the fuel and reducing the rate of mixing and combustion. It is noted that lower factors were assigned to the diesel fuel flow rates at 100 percent load. It is postulated that this is due to the greater gaseous equivalence ratios employed at these conditions, which lead to a reduction in the available air for combustion in the pilot. The remaining constants set in sections 5.4.1.1 and 5.4.1.2 were held constant throughout the validation process.

![Figure 5.10](image)

**Figure 5.10** – Factor applied to conservation of initial spray momentum as a function of diesel fuel flow rate at 100 and 50 percent load
5.4.2.1 Pressure and Energy Release Diagrams

Figures 5.11 to 5.16 show the experimental and predicted pressure and net energy release diagrams for the range of gaseous substitution ratios studied at 100 percent load. It is observed that the experimental and predicted pressure diagrams are in good general agreement. The overall shape of the energy release rates is also in good agreement. At lower gaseous substitution ratios, where the main source of energy release is from the pilot, the energy release diagram is typical of that observed for diesel operation. At larger gaseous substitution ratios, premixed gaseous combustion becomes more prominent, as for the dual fuel calibration case (Figure 5.8). It is observed that at higher gaseous substitutions, the model is unable to account for the agglomeration of the energy release from the pilot and premixed gaseous charge. This is attributed to the inability of the model to capture the energy release in the reactive boundary surrounding the pilot fuel spray. However, as mentioned previously, the shapes of the energy release rates are in good general agreement, giving confidence in the overall prediction of the energy release. For a gaseous energy substitution of 24.96 percent (Figures 5.11 and 5.12), where the gaseous equivalence ratio is less than $\phi \approx 0.2$, the assumption of flame propagation has little effect on the predictive capability of the model, as the pilot fuel is the main source of energy release.
Figure 5.11 – Comparison of experimental and predicted in-cylinder pressure diagrams at 1500 rpm and 100 percent load for a gaseous energy substitution of 24.96 percent.

Figure 5.12 – Comparison of experimental and predicted net energy release rate diagrams at 1500 rpm and 100 percent load for a gaseous energy substitution of 24.96 percent. The simulated injection rate is also shown.
CHAPTER 5 MODEL CALIBRATION AND VALIDATION

Figure 5.13 – Comparison of experimental and predicted in-cylinder pressure diagrams at 1500 rpm and 100 percent load for a gaseous energy substitution of 48.50 percent.

Figure 5.14 – Comparison of experimental and predicted net energy release rate diagrams at 1500 rpm and 100 percent load for a gaseous energy substitution of 48.50 percent. The simulated injection rate is also shown.
Figure 5.15 – Comparison of experimental and predicted in-cylinder pressure diagrams at 1500 rpm and 100 percent load for a gaseous energy substitution of 75.00 percent.

Figure 5.16 – Comparison of experimental and predicted net energy release rate diagrams at 1500 rpm and 100 percent load for a gaseous energy substitution of 75.00 percent. The simulated injection rate is also shown.
Table 5.6 compares the experimental and predicted values for the magnitude and timing of peak in-cylinder pressure for the range of gaseous substitution ratios studied at 100 percent load. The baseline diesel and dual fuel calibration cases are included for comparison. In general, the magnitudes and timings of peak in-cylinder pressure are in good agreement for the range of gaseous substitutions studied. However, the magnitude of peak in-cylinder pressure is under-predicted for both the 75.00 and 80.68 percent gaseous energy substitution cases (Refs V.1.3 and C.2) respectively.

Table 5.6 – Comparison of experimental and predicted values for the magnitude and timing of peak in-cylinder pressure at 1500 rpm and 100 percent load for a range of gaseous energy substitutions

<table>
<thead>
<tr>
<th>Ref</th>
<th>Experimental</th>
<th>Predicted</th>
<th>Percentage Difference</th>
<th>Experimental</th>
<th>Predicted</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>/(/bar)</td>
<td>%</td>
<td></td>
<td>/(^°CA)</td>
<td></td>
</tr>
<tr>
<td>C.1</td>
<td>52.60</td>
<td>52.28</td>
<td>-0.61</td>
<td>7.0</td>
<td>6.0</td>
</tr>
<tr>
<td>C.2</td>
<td>53.55</td>
<td>51.01</td>
<td>-4.74</td>
<td>10.0</td>
<td>10.0</td>
</tr>
<tr>
<td>V.1.1</td>
<td>52.41</td>
<td>52.51</td>
<td>0.19</td>
<td>7.0</td>
<td>7.0</td>
</tr>
<tr>
<td>V.1.2</td>
<td>56.38</td>
<td>55.65</td>
<td>-1.29</td>
<td>6.5</td>
<td>7.0</td>
</tr>
<tr>
<td>V.1.3</td>
<td>61.54</td>
<td>58.20</td>
<td>-5.43</td>
<td>6.5</td>
<td>7.0</td>
</tr>
</tbody>
</table>

\[
\text{Percentage Difference} \text{ (%) } = \left( \frac{P_{\text{max, Predicted}} - P_{\text{max, Experimental}}}{P_{\text{max, Experimental}}} \right) \cdot 100
\]

Figure 5.17 shows the prediction of the ignition delay period for the range of gaseous substitutions studied at 100 percent load. The SOI was determined from the recorded needle lift and the SOC was determined using the second derivative of the pressure diagram, as outlined in section 5.3.2. Overall, the predicted ignition delays show excellent agreement with the values determined from the experimental data. This is particularly encouraging given that the ignition delay was calculated using a correlation developed for diesel engines. It is noted that the ignition delay period is under-predicted for the 75.00 percent gaseous energy substitution case.
Figure 5.17 – Ignition delay period at 1500 rpm and 100 percent load for a range of gaseous energy substitutions

Figures 5.18 to 5.29 compare the experimental and predicted pressure and net energy release diagrams for the range of gaseous substitution ratios studied at 50 percent load. It is observed that the experimental and predicted pressure diagrams are in good agreement. The shape of the energy release rates is also in good general agreement. It is observed that the magnitudes of predicted energy release are over-predicted relative to the experimental data. As mentioned previously, this is attributed to smoothing of the pressure diagram. It is noted that the premixed gaseous combustion phase is over-predicted at all but the highest gaseous substitution ratio. However, the model is able to satisfactorily predict an energy release typical of that observed for diesel operation for all the cases studied. Similarly to the 100 percent load case, at a gaseous energy substitution of 45.86 percent (Figures 5.20 and 5.21), where the gaseous equivalence ratio is less than $\phi \approx 0.2$, the assumption of flame propagation has little effect on the predictive capability of the model, as the pilot fuel is the main source of energy release.
Figure 5.18 – Comparison of experimental and predicted in-cylinder pressure diagrams at 1500 rpm and 50 percent load for diesel operation.

Figure 5.19 – Comparison of experimental and predicted net energy release rate diagrams at 1500 rpm and 50 percent load for diesel operation. The simulated injection rate is also shown.
Figure 5.20 – Comparison of experimental and predicted in-cylinder pressure diagrams at 1500 rpm and 50 percent load for a gaseous energy substitution of 45.86 percent.

Figure 5.21 – Comparison of experimental and predicted net energy release rate diagrams at 1500 rpm and 50 percent load for a gaseous energy substitution of 45.86 percent. The simulated injection rate is also shown.
Figure 5.22 – Comparison of experimental and predicted in-cylinder pressure diagrams at 1500 rpm and 50 percent load for a gaseous energy substitution of 64.34 percent.

Figure 5.23 – Comparison of experimental and predicted net energy release rate diagrams at 1500 rpm and 50 percent load for a gaseous energy substitution of 64.34 percent. The simulated injection rate is also shown.
Figure 5.24 – Comparison of experimental and predicted in-cylinder pressure diagrams at 1500 rpm and 50 percent load for a gaseous energy substitution of 67.97 percent.

Figure 5.25 – Comparison of experimental and predicted net energy release rate diagrams at 1500 rpm and 50 percent load for a gaseous energy substitution of 67.97 percent. The simulated injection rate is also shown.
**Figure 5.26** – Comparison of experimental and predicted in-cylinder pressure diagrams at 1500 rpm and 50 percent load for a gaseous energy substitution of 69.50 percent.

**Figure 5.27** – Comparison of experimental and predicted net energy release rate diagrams at 1500 rpm and 50 percent load for a gaseous energy substitution of 69.50 percent. The simulated injection rate is also shown.
Figure 5.28 – Comparison of experimental and predicted in-cylinder pressure diagrams at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent.

Figure 5.29 – Comparison of experimental and predicted net energy release rate diagrams at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent. The simulated injection rate is also shown.
The main components of energy release at 50 percent load for a gaseous energy substitution of 71.06 percent are shown in Figure 5.30. Here, the energy release from the liquid fuel and premixed charge are similar in magnitude. Furthermore, relative to the dual fuel calibration case, the initial increase in energy release from the premixed charge is reduced. This is due to a reduction in combustion volume, as a result of a smaller pilot fuel quantity and leaner premixed charge, which leads to slower propagation rates. Again, it is noted that the magnitude of energy release from the entrained gaseous fuel is relatively small.

![Graph showing energy release rate](#)

**Figure 5.30** – Constituent components of dual fuel energy release at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent

Table 5.7 compares the experimental and predicted values for the magnitude and timing of peak in-cylinder pressure for the range of gaseous substitutions studied at 50 percent load. It is observed that the magnitudes and timings of peak in-cylinder pressure are in good general agreement. In general, the timing of the predicted peak in-cylinder pressure is slightly later than that observed for the experimental data. This is due to the over-prediction of the premixed gaseous combustion phase.

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160
Table 5.7 – Comparison of experimental and predicted values for the magnitude and timing of peak in-cylinder pressure at 1500 rpm and 50 percent load for a range of gaseous energy substitutions

<table>
<thead>
<tr>
<th>Ref</th>
<th>Experimental (P_{\text{max}}) (bar)</th>
<th>Predicted (P_{\text{max}}) (bar)</th>
<th>Percentage Difference</th>
<th>Timing of (P_{\text{max}}) (ATDC)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Experimental Predicted</td>
</tr>
<tr>
<td>V.2.1</td>
<td>49.74</td>
<td>49.91</td>
<td>0.34</td>
<td>5.0</td>
</tr>
<tr>
<td>V.2.2</td>
<td>52.76</td>
<td>52.66</td>
<td>-0.19</td>
<td>3.0</td>
</tr>
<tr>
<td>V.2.3</td>
<td>50.82</td>
<td>51.24</td>
<td>0.83</td>
<td>4.5</td>
</tr>
<tr>
<td>V.2.4</td>
<td>49.49</td>
<td>49.33</td>
<td>-0.12</td>
<td>4.5</td>
</tr>
<tr>
<td>V.2.5</td>
<td>50.53</td>
<td>51.04</td>
<td>1.01</td>
<td>4.5</td>
</tr>
<tr>
<td>V.2.6</td>
<td>51.40</td>
<td>49.95</td>
<td>-2.82</td>
<td>5.0</td>
</tr>
</tbody>
</table>

\[
\text{Percentage Difference (\%)} = \left(\frac{P_{\text{max, predicted}} - P_{\text{max, experimental}}}{P_{\text{max, experimental}}}\right) \times 100
\]

A comparison of the experimental and predicted ignition delays for the range of gaseous substitutions studied at 50 percent load is shown in Figure 5.31. It is observed that the values are in good general agreement with the experimental data. It is noted that the ignition delay period is under-predicted by 1.5 degrees crank angle for the 48.56 percent gaseous energy substitution case. The under-prediction of the ignition delay at this case is comparable to the under-prediction of the ignition delay for the 100 percent load case at 75.00 percent gaseous energy substitution. This is attributed to the earlier injection timings employed at these conditions, -13.5 degrees ATDC at 100 percent load and -14.0 degrees ATDC at 50 percent load respectively. Hence, at advanced injection timings, the prediction of the ignition delay model is less satisfactory. It is postulated that this is due to increased periods of pre-ignition reaction chemistry between the pilot and gaseous fuel during the ignition delay period that the ignition model does not consider.
5.4.2.2 Emissions of Nitric Oxide and Soot

Figures 5.32 to 5.35 compare the experimental and predicted trends for NO and soot at 1500 rpm under 100 and 50 percent load conditions for the range of gaseous substitutions studied. The trends for emissions of NO are shown in Figures 5.32 and 5.34. Here, the magnitudes of predicted NO for the diesel cases at 100 and 50 percent load have been increased by factors of 6.5 and 2.8 respectively to match the experimental data. The factor applied to the 50 percent load case is less than that applied to the 100 percent load case due to the increased factor applied to the conservation of initial spray momentum. This leads to greater entrainment rates and therefore higher temperatures and greater burned species in the cylinder, promoting NO formation. It is observed that the trend for emissions of NO with gaseous energy substitution is in good agreement for the 50 percent load case. However, at 100 percent load, the trend for emissions with gaseous energy substitution is not well predicted. This is attributed to the inability of the model to capture emissions formation in the reactive boundary surrounding the pilot fuel spray. Here, increased gaseous equivalence ratios lead to a relative increase in the local temperature around the fuel spray. Coupled with the high oxygen availability, as a result of the lean nature of the gaseous mixture, conditions for NO formation are promoted.
Figure 5.32 – Comparison of NO emissions at 1500 rpm and 100 percent load for a range of gaseous energy substitutions

Figure 5.33 – Comparison of soot emissions at 1500 rpm and 100 percent load for a range of gaseous energy substitutions
Figure 5.34 – Comparison of NO emissions at 1500 rpm and 50 percent load for a range of gaseous energy substitutions

Figure 5.35 – Comparison of soot emissions at 1500 rpm and 50 percent load for a range of gaseous energy substitutions
Figures 5.33 and 5.35 show the prediction of soot at 100 and 50 percent load for the range of gaseous substitutions studied. In the present work, the density and diameter of soot in the oxidation model of Nagle and Strickland-Constable (1962) (see Chapter 4, section 4.7.2) were set to their usual values of 2.0 g.cm\(^{-3}\) and 25 nm respectively. The soot formation constant, \(A_f\), (see Chapter 4, section 4.7.2) was then adjusted to match the final soot concentrations for diesel operation at 100 and 50 percent load. The values of the soot formation constant for the 100 and 50 percent load cases were taken to be 96.0 and 12.0 respectively. It is observed that the trend for emissions of soot with gaseous energy substitution is in good agreement with the experimental data. However, the final magnitudes of soot concentration for dual fuel operation are over-predicted relative to the experimental data.

The predicted trends for NO and soot at 50 percent load give confidence in the predictive capability of the emissions models at that load. Figure 5.36 shows the production of NO and soot at 50 percent load for a gaseous energy substitution of 71.06 percent. The trends for the production of NO and soot are in good agreement with the literature. The production of soot precedes the formation of NO due to the rich conditions present in the spray early in the combustion process. Furthermore, the NO composition freezes during the expansion stroke due to reduced local temperatures as a result of expansion and mixing of the combustion products with cooler surrounding gas. It is noted that, similarly to diesel combustion, NO formation takes place within 20 degrees crank angle from the SOC, as reported by Heywood (1988).

The predicted zonal in-cylinder temperatures for the 71.06 percent gaseous energy substitution case are shown in Figure 5.37. Here, \(T_{\text{avg}}\) is the mass average cylinder temperature, \(T_u\) is the unburned zone temperature, \(T_{\text{spry,avg}}\) is the mass average spray temperature, \(T_p\) is the premixed zone temperature and \(T_{\text{max}}\) is the maximum instantaneous zone temperature. The unburned zone temperature increases during compression and peaks shortly after TDC as a result of expansion of the spray zones following ignition, before decreasing during the expansion process. Following the ignition delay period, the mass average spray temperature and maximum instantaneous zone temperature increase rapidly, with the maximum zone temperature equal to 2586 K. The inception of the premixed burning zone occurs following the ignition delay of the pilot. It is noted that the lean nature of the premixed gaseous charge results in combustion temperatures that are below those critical for NO formation (~2000 K (Heywood, 1988)). Hence, it can be concluded that little NO is formed in the premixed burning zone.
Figure 5.36 – Production of NO and soot at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent

Figure 5.37 – Predicted zone temperatures at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent
5.5 CONCLUDING SUMMARY

In this chapter, the calibration and validation of the quasi-dimensional dual fuel model were discussed. The model was calibrated and validated against experimental data taken from a small diesel genset operating at 1500 rpm under 100 and 50 percent load conditions for a range of gaseous substitution ratios.

Model calibration was completed for both diesel and dual fuel modes of operation at 1500 rpm and 100 percent load. This approach allowed the phenomena associated with the pilot injection model to be decoupled from the turbulent entrainment model during the calibration process. It was found that the factor controlling the conservation of initial spray momentum had to be adjusted throughout model calibration and validation to account for difficulties describing the initial spray momentum. This was attributed to the lower fuel line pressures observed for smaller pilot fuel quantities.

Comparisons of the experimental and predicted pressure and net energy release diagrams are in good agreement for the engine loads and range of gaseous substitution ratios studied. Moreover, the prediction of the magnitude and timing of peak in-cylinder pressure and ignition delay period give confidence in the breakup, entrainment, evaporation, ignition and combustion sub-models. Furthermore, the prediction of the late combustion phase gives confidence in the description of the flame area by an exponential decay following the entrainment of a characteristic mass. It is also noted that the description of the flame area from the viewpoint of coalescence of enflamed zones successfully describes the greater rates of premixed gaseous combustion observed for larger pilot fuel quantities.

Predictions for emissions of NO were in good agreement for the range of gaseous substitution ratios studied at 50 percent load. However, at 100 percent load, the model was unable to predict NO formation with increasing gaseous substitution. Further work is therefore required to accurately describe NO formation at high load conditions. The model revealed that emissions of NO are primarily associated with the pilot fuel spray, where in-cylinder temperatures are high. Emissions from the premixed burning zone are small due to the lean nature of the premixed gaseous charge, which leads to reduced combustion temperatures. Trends for emissions of soot were in good agreement with the experimental data. However, soot concentrations were over-predicted for dual fuel operation.
In summary, the predictive capability of the model is encouraging, particularly given the complexity of the combustion processes occurring inside a dual fuel engine. In the following chapter, the model sensitivity will be discussed. This will highlight the underlying physical mechanisms which have a major influence on the dual fuel combustion processes.
6.1 INTRODUCTION

In this chapter, a sensitivity analysis has been conducted to investigate the underlying physical mechanisms influencing the performance and emissions of a dual fuel engine. The aim of the sensitivity analysis is to provide an improved understanding of the model inputs/constants controlling the physical phenomena occurring inside the cylinder. The main objective is to quantify the effect of the model inputs/constants, so that the main controlling parameters in the model can be identified.

The sensitivity analysis was performed using the dual fuel operating case at 50 percent load with a gaseous energy substitution of 71.06 percent (Table 5.3, Ref V.2.6). This case was selected due to its agreement with both performance and emissions data. The model inputs selected for analysis include the swirl ratio and in-cylinder temperature at IVC. The model constants selected for analysis include those controlling the rate of entrainment into the pilot fuel spray, the turbulence characteristics in the cylinder and the characteristic burning time behind the flame front. The effect of the number of radial and circumferential spray zones is also considered. The effect of these inputs/constants on the combustion processes is considered by comparing the corresponding pressure diagrams and considering the effect of the model inputs/constants on the magnitude and timing of peak in-cylinder pressure, the ignition delay period, and emissions of NO and soot. The effect of varying the model inputs/constants is quantified by comparing the relative changes in the combustion parameters. In this way, the main physical mechanisms affecting the performance and emissions of a dual fuel engine are identified.

6.2 SENSITIVITY ANALYSIS

The sensitivity analysis, as presented in the following sections, was completed alongside the calibration and validation work. It is presented here to illustrate the main inputs/constants influencing the prediction of performance and emissions in a dual fuel engine. The sensitivity analysis is divided into three sections: the first investigates the sensitivity of the model inputs; the second investigates the effect of the constants controlling the rate of entrainment into the pilot fuel spray; and the third investigates
the main constants controlling the rate of entrainment and burning in the premixed burning zone.

6.2.1 Effect of Input Parameters
In this section, the effects of the model inputs critical to the description of the combustion processes in a dual fuel engine are investigated. Here, three parameters are of interest. The first set of parameters specifies the total number of radial and circumferential spray zones used in the description of the spray geometry. Previous studies have shown that the total number of spray zones has an important influence on the prediction of emissions in the cylinder (Jung and Assanis, 2001). The second parameter of interest is the definition of the swirl ratio at IVC. As stated in Chapter 5, in the present work, the swirl ratio at IVC is set to 0.5. The effect of the magnitude of this value on the model predictions is discussed further. The third parameter under investigation is the in-cylinder temperature at IVC. The effect of these parameters on the prediction of performance and emissions in a dual fuel engine are considered in the following sections.

6.2.1.1 Effect of Number of Spray Zones
The combustion processes in the pilot fuel spray are modelled on a zonal basis (see Chapter 4, section 4.3.1), with the total number of zones in the radial and circumferential directions defined by model inputs. In this section, the sensitivity of the model predictions to the number of radial and circumferential spray zones is investigated. Here, the zonal parameter under consideration is varied, whilst the other is fixed at the baseline value. Figure 6.1 shows that the number of radial spray zones has minimal effect on the prediction of the pressure diagram, with peak in-cylinder pressures varying by only 0.31 percent across the range of zones studied. It is noted that the initial pressure rise is more consistently described when greater than or equal to 5 radial spray zones are employed. The effect of the number of circumferential spray zones on the pressure diagram is negligible, as shown in Figure 6.2.

Figures 6.3 and 6.4 show the effect of the number of radial and circumferential spray zones on the prediction of emissions of NO and soot. It is noted that the description of the spray by three dimensions gives little variation in the prediction of emissions. Hence, in the present model, the numbers of radial and circumferential spray zones were selected to be 5 and 6 respectively. This gives a suitable representation of the spray geometry, whilst retaining the computational efficiency of the model.
**Figure 6.1** – Effect of number of radial spray zones on the dual fuel pressure diagram at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent

**Figure 6.2** – Effect of number of circumferential spray zones on the dual fuel pressure diagram at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent
CHAPTER 6 SENSITIVITY ANALYSIS

Figure 6.3 – Effect of number of radial spray zones on emissions of NO and soot for dual fuel operation at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent

Figure 6.4 – Effect of number of circumferential spray zones on emissions of NO and soot for dual fuel operation at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent
6.2.1.2 Effect of Swirl Ratio

The effect of swirl is to decrease the pilot fuel spray penetration and deflect the spray in the tangential direction. This has an important influence on the utilization of the gaseous charge inside the cylinder. In this section, the effect of the initial value of the swirl ratio, $R_s$, at IVC is investigated. Initial values of 0.00, 0.25, 0.50, 0.75 and 1.00 are studied, where 0.50 is the baseline constant.

Figure 6.5 shows the effect of the initial value of the swirl ratio on the dual fuel pressure diagram. It is observed that the initial value of the swirl ratio has no effect on the ignition delay period. Moreover, during the early stages of combustion, the initial value of the swirl ratio has negligible effect on the initial rate of pressure rise. The main effect of increasing the initial value of the swirl ratio is to increase the peak in-cylinder pressure. This is attributed to the increased mass of air entrained into the pilot fuel spray during the ignition delay period, which results in a larger magnitude of energy release during the premixed combustion phase. It is also noted that the initial value of the swirl ratio has no effect on the timing of peak in-cylinder pressure.

![Figure 6.5](image_url) – Effect of initial value of swirl ratio, $R_s$, at IVC on the dual fuel pressure diagram at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent

Figure 6.6 shows the effect of increasing the initial value of the swirl ratio on predictions of NO and soot. It is observed that emissions of NO increase with the initial value of the swirl ratio. This is attributed to the greater mass of burned species.
in the spray, coupled with correspondingly higher spray temperatures. The figure also reveals that emissions of soot decrease with the initial value of the swirl ratio. This is attributed to a reduction in soot formation, caused by the greater consumption of diesel fuel vapour, and greater soot oxidation, as a result of higher spray temperatures and increased oxygen availability.

Figure 6.6 – Effect of initial value of swirl ratio, $R_s$, at IVC on emissions of NO and soot at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent

6.2.1.3 Effect of In-cylinder Temperature at Inlet Valve Closure

The effect of increasing the in-cylinder temperature at IVC, $T_{cyLIVC}$, is to modify the heat transfer processes occurring inside the cylinder. Higher in-cylinder temperatures at IVC lead to less heat transfer from the surrounding surfaces to the cylinder contents, thus lowering in-cylinder pressures and temperatures towards the end of the compression stroke, as shown in Figure 6.7. It is observed that the effect of increasing the in-cylinder temperature at IVC is to promote the rate of initial pressure rise. Increased temperatures also promote the rate of entrainment behind the flame front, which advances the entrainment of the characteristic mass (see Chapter 4, section 4.4.2). Ultimately, lower quantities of gaseous fuel behind the flame front lead to lower in-cylinder pressures.

Figure 6.8 shows the effect of the in-cylinder temperature at IVC on emissions of NO and soot. It is observed that there is a step change in emissions predictions for in-
Figure 6.7 – Effect of in-cylinder temperature at IVC, $T_{cyl,IVC}$, on the dual fuel pressure diagram at 1500 rpm and 50 percent load for a fixed gaseous equivalence ratio of $\Phi = 0.328$.

Figure 6.8 – Effect of in-cylinder temperature at IVC, $T_{cyl,IVC}$, on emissions of NO and soot at 1500 rpm and 50 percent load for a fixed gaseous equivalence ratio of $\Phi = 0.328$. 
cylinder temperatures of 315 K and 320 K. This is attributed to the lower in-cylinder pressures and thus temperatures observed for these cases, which reduce the total formation of NO and hinder the oxidation of soot.

6.2.2 Effect of Parameters Controlling the Rate of Entrainment into the Pilot Fuel Spray

One of the most important aspects of spray modelling is the calculation of the entrainment rate, as this has an important influence on the subsequent combustion processes occurring inside the cylinder. In a dual fuel engine, this is further complicated by the entrainment of a gaseous fuel-air mixture. In this section, the effects of the factor controlling the conservation of initial spray momentum, $C_b$, and the entrainment factor, $\alpha$, are considered. These factors control the overall rate of entrainment into the pilot fuel spray and the rate of entrainment across the radial cross-section of the spray respectively. The factor controlling the conservation of initial spray momentum is varied in increments of 0.05 in the range 0.90 to 1.10, where 1.00 is the baseline constant. The entrainment factor is varied in increments of 5 in the range 20 to 40, where 30 is the baseline constant.

Figure 6.9 shows the effect of the factor controlling the conservation of initial spray momentum on the combustion processes in a dual fuel engine. It is observed that an increase in the factor controlling the conservation of initial spray momentum results in a slower rate of initial pressure rise, after which the rate of pressure rise increases due to the increased availability of air. In general, the factor controlling the conservation of initial spray momentum also leads to higher values of peak in-cylinder pressure. This is attributed to greater rates of entrainment into the pilot fuel spray during the ignition delay period, which lead to an increase in energy release during the premixed combustion phase. The greater rates of entrainment into the pilot fuel spray also lead to a greater flame surface area from which flame propagation can develop, further increasing in-cylinder pressure. It is further observed that, in general, the factor controlling the conservation of initial spray momentum has no effect on the timing of peak in-cylinder pressure. For a factor of 0.9, the trends for the magnitude and timing of peak in-cylinder pressure vary from those described above. This is due to slower entrainment rates, which prolong the entrainment of the characteristic mass. This leads to an increase in the time available for the flame front to propagate freely through the premixed charge. This results in an increase in the initial energy release from the premixed charge, thus leading to higher values of peak in-cylinder pressure.
Moreover, since the peak in premixed gaseous combustion occurs later than the premixed combustion spike, the timing of peak in-cylinder pressure is retarded.

![Cylinder Pressure vs Crank Angle](image)

**Figure 6.9** – Effect of factor controlling conservation of initial spray momentum, $C_b$, on the dual fuel pressure diagram at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent

Figure 6.10 shows the effect of the entrainment factor on the dual fuel combustion process. It is observed that the entrainment factor has no effect on the ignition delay period. However, as the entrainment factor is increased, the initial rate of pressure rise decreases. This is attributed to a relative increase in air-fuel ratio towards the fuel spray periphery. This extends the local ignition delay, thus prolonging the first phase of energy release. Similarly to the factor controlling the conservation of initial spray momentum, the effect of increasing the entrainment factor is to increase the rate of entrainment into the pilot fuel spray. This leads to greater availability of air, which increases the rate of burning in the pilot, thus increasing peak in-cylinder pressures. It is also noted that at all but the highest value ($\alpha = 40$), the entrainment factor has no effect on the timing of peak in-cylinder pressure.
Figure 6.10 – Effect of entrainment factor, $\alpha$, on the dual fuel pressure diagram at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent

The effect of the factor controlling the conservation of initial spray momentum and entrainment factor on the prediction of emissions is shown in Figures 6.11 and 6.12. As discussed previously, the emissions of interest – NO and soot – are primarily formed in the pilot fuel spray. Hence, the rate of entrainment into the fuel spray has an important influence on emissions formation in a dual fuel engine.

It is observed that emissions of NO increase with both the factor controlling the conservation of initial spray momentum and the entrainment factor. This is due to an increase in the mass of burned species in the spray and the spray temperature. Moreover, it is observed that emissions of soot decrease with both the factor controlling the conservation of initial spray momentum and the entrainment factor. This is attributed to reduced soot formation, caused by the greater consumption of diesel fuel vapour, and greater soot oxidation, as a result of higher in-cylinder temperatures and greater oxygen availability.
Figure 6.11 – Effect of factor controlling conservation of initial spray momentum, $C_b$, on emissions of NO and soot for dual fuel operation at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent

Figure 6.12 – Effect of entrainment factor, $\alpha$, on emissions of NO and soot for dual fuel operation at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent
6.2.3 Effect of Parameters Controlling the Rate of Entrainment and Burning in the Premixed Burning Zone

The description of the development of the premixed burning zone is important in defining the dual fuel combustion process. In the present work, this is described using a turbulent entrainment model (see Chapter 4, section 4.4.1). There are two important aspects in the turbulent entrainment model: the calculation of the unburned mass entrained behind the flame front and the rate of burning behind the flame front. In the present work, the integral length scale, turbulence intensity and characteristic burning time have been identified as being important to these processes. The following sections describe the effect of these parameters on the prediction of performance and emissions in a dual fuel engine.

6.2.3.1 Effect of Integral Length Scale

The integral length scale, $L$, describes the size of the turbulent eddies entrained by the flame front. In combustion modelling, the integral length scale at the initiation of combustion is typically assumed to be proportional to the instantaneous combustion chamber height. In this section, the effect of the proportionality constant controlling the initial value of the integral length scale, $C_L$, is studied. The proportionality constant is varied in the range 0.05 to 0.40. The baseline value is taken to be 0.05, as described in Chapter 5.

The effect of the size of the integral length scale at the initiation of combustion on the dual fuel pressure diagram is shown in Figure 6.13. It is observed that the size of the integral length scale at the initiation of combustion has little effect on the pressure diagram. This is due to the size of the constant controlling the characteristic burning time ($C_T = 0.001$). Here, the present modelling approach assumes that the majority of unburned gas entrained behind the flame front burns to completion as it crosses the flame front. Thus, the integral length scale has little effect on burning behind the flame front.

Figure 6.14 shows the effect of the size of the integral length scale at the initiation of combustion on emissions formation in a dual fuel engine. As a result of the current modelling approach, the integral length scale has little effect on emissions of NO and soot.
Figure 6.13 – Effect of integral length scale proportionality constant, $C_L$, on the dual fuel pressure diagram at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent.

Figure 6.14 – Effect of integral length scale proportionality constant, $C_L$, on emissions of NO and soot for dual fuel operation at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent.
6.2.3.2 Effect of Turbulence Intensity

The turbulence intensity, $U'$, describes the speed at which the vortex tubes in a turbulent mixture oscillate. In combustion modelling, the turbulence intensity at the initiation of combustion is assumed to be proportional to the mean piston speed. In this section, the effect of the proportionality constant controlling the initial value of the turbulence intensity, $C_{U'}$, is investigated. The proportionality constant is varied in the range 0.75 to 0.95 in increments of 0.05, where 0.85 is the baseline constant.

The effect of the size of the turbulence intensity at the initiation of combustion on the dual fuel pressure diagram is shown in Figure 6.15. It is observed that the rate of initial pressure rise increases with increasing turbulence intensity. This is due to the greater rate of entrainment of unburned mass behind the flame front, which promotes combustion. The corresponding growth in the entrainment area also results in greater entrainment rates. This contributes to an increase in energy release from the premixed burning zone, which leads to higher in-cylinder pressures. For $C_{U'} = 0.75$, decreased entrainment rates lead to a prolonged period in which the flame front can propagate freely. This increases the peak in-cylinder pressure relative to that observed for $C_{U'} = 0.80$ and $C_{U'} = 0.85$ and retards the timing of peak in-cylinder pressure.

![Figure 6.15 – Effect of turbulence intensity proportionality constant, $C_{U'}$, on the dual fuel pressure diagram at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent](image-url)
Figure 6.16 shows the effect of the size of the turbulence intensity at the initiation of combustion on emissions formation in a dual fuel engine. It is noted that, with the exception of $C_{U'} = 0.75$, emissions of NO increase with increasing turbulence intensity. This is due to higher spray temperatures, as a result of the compression of the pilot fuel spray by the expansion of the premixed combustion products. Furthermore, it is observed that emissions of soot decrease with increasing turbulence intensity due to higher spray temperatures, which promote soot oxidation. Emissions of NO and soot for $C_T = 0.75$ are in contrast to the observed trends due to the higher in-cylinder pressures observed for this case.

**Figure 6.16** – Effect of turbulence intensity proportionality constant, $C_{U'}$, on emissions of NO and soot for dual fuel operation at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent

### 6.2.3.3 Effect of Characteristic Burning Time

In this section, the effect of the constant controlling the characteristic burning time, $C_T$, is investigated. This controls the characteristic time for burning across the Taylor microscale. In the present study, values of 0.001, 0.01 and 0.1 are considered.

Figure 6.17 shows the effect of the characteristic burning time on the dual fuel pressure diagram. It is observed that the effect of decreasing the burning time is to increase the rate of initial pressure rise. The decrease in burning time also leads to
higher peaks in in-cylinder pressure. However, it is noted that the characteristic burning time has no effect on the timing of peak in-cylinder pressure. Figure 6.17 highlights the rapid rate of burning required behind the flame front for the pressure diagram to match the baseline experimental data.

![Diagram showing the effect of characteristic burning time on cylinder pressure](image)

**Figure 6.17** – Effect of constant controlling characteristic burning time, $c_\tau$, on the dual fuel pressure diagram at 1500 rpm and 50 percent load for a gaseous energy substitution of 71.06 percent

The effect of the constant controlling the characteristic burning time on emissions in a dual fuel engine is shown in Figure 6.18. It is observed that the effect of increasing the burning time is to decrease emissions of NO. This is due to a reduction in the compression of the spray zones by the premixed burning zone, which leads to lower spray temperatures. Furthermore, it is observed that emissions of soot increase with the characteristic burning time. This is also attributed to reduced spray temperatures, which hinder soot oxidation.
6.3 DISCUSSION

In the following, the variation of the model inputs/constants is quantified by considering their effect on the magnitude and timing of peak in-cylinder pressure, the ignition delay period and emissions of NO and soot. The relative effect of the model inputs/constants on the parameters considered is expressed as

\[
\Delta X_{0,\text{rel}}(\%) = \left(\frac{X_i - X_0}{X_0}\right) \cdot 100
\]

(6.1)

where \(X_i\) is the value under consideration and \(X_0\) is the baseline value. The model inputs/constants employed for analysis are identical to those used in the previous section.

Figure 6.19 quantifies the effect of the model inputs/constants on the magnitude of peak in-cylinder pressure (\(P_{\text{max}}\)). It is observed that the in-cylinder temperature at IVC has a strong influence on this parameter. Moreover, the swirl ratio, factor controlling the conservation of initial spray momentum and proportionality constant controlling the
size of the turbulence intensity at the initiation of combustion are identified as having an important effect. It is noted that an increase in the in-cylinder temperature at IVC from 300 K to 320 K results in a 6.00 percent decrease in the magnitude of peak in-cylinder pressure. As discussed in section 6.2.1.3, this is due to reduced heat transfer from the surrounding surfaces to the cylinder contents during the compression stroke, which leads to lower pressures and temperatures at the SOC. The effect of the swirl ratio and factor controlling the conservation of initial spray momentum is to promote greater rates of entrainment into the pilot fuel spray, which subsequently lead to greater rates of burning. It is noted that the entrainment factor has a less significant effect on the magnitude of peak in-cylinder pressure than the factor controlling the conservation of initial spray momentum. This is because the factor controlling the conservation of initial spray momentum leads to a greater variation in oxygen availability across the spray. It is observed that the proportionality constant controlling the size of the turbulence intensity at the initiation of combustion has a greater effect than the inputs/constants controlling the rate of entrainment into the pilot fuel spray. It is postulated that this is due to compression of the spray zones by the expansion of

Figure 6.19 – Relative effect of model inputs/ constants \( (R_s, T_{cy}, IVC, C_b, \alpha, C_L, C_U', \text{ and } C_t) \) on the magnitude of peak in-cylinder pressure \( (P_{max}) \)
the premixed combustion products. The figure also shows that the integral length scale has no effect on the magnitude of peak in-cylinder pressure (as discussed in section 6.2.3.1). It is noted that for a characteristic burning time of $C_T = 0.1$, a 6.08 percent decrease in the prediction of the magnitude of peak in-cylinder pressure is observed, highlighting the need for rapid burning behind the flame front to match the experimental pressure diagram.

The effect of the model inputs/ constants on the timing of peak in-cylinder pressure is revealed in Table 6.1. Here, the inputs/ constants that affect the timing of peak in-cylinder pressure are the in-cylinder temperature at IVC, factor controlling the conservation of initial spray momentum, entrainment factor and proportionality constant controlling the size of the turbulence intensity at the initiation of combustion. In general, the timing of the magnitude of peak in-cylinder pressure is affected by the entrainment of the characteristic mass. The later this occurs, the greater the energy release from the premixed gaseous charge and the later the timing of peak in-cylinder pressure. In the case of the turbulence intensity, an increase in the proportionality constant retards the timing of peak in-cylinder pressure due to the increase in energy release from the premixed burning zone as a result of greater entrainment rates behind the flame front. Table 6.1 also reveals that the model inputs/ constants have no effect on the ignition delay period for the ranges investigated. It should be noted that the constants controlling the size of the integral length scale and turbulence intensity at the initiation of combustion, and the characteristic burning time have no effect on the ignition delay period, since premixed combustion follows the ignition event.

The effect of the model inputs/ constants on the prediction of NO is shown in Figure 6.20. It is observed that both the swirl ratio and factor controlling the conservation of initial spray momentum have a strong influence on emissions of NO. The figure also reveals the importance of the entrainment factor. Hence, the inputs/ constants controlling the rate of entrainment into the pilot fuel spray have a strong influence on emissions of NO. This is because of their effect on oxygen availability, which promotes combustion and increases in-cylinder temperatures. The proportionality constant controlling the size of the turbulence intensity at the initiation of combustion is less important, however, for larger gaseous equivalence ratios, it is postulated that this effect will increase as the spray zones are compressed by the expansion of the premixed combustion products. It is noted that similarly to the magnitude of peak in-cylinder pressure, the entrainment factor has a less significant
Table 6.1 – Effect of model inputs/constants ($R_S$, $T_{cyl,IVC}$, $C_b$, $\alpha$, $C_L$, $C_{U'}$ and $C_r$) on the timing of peak in-cylinder pressure and the ignition delay period

<table>
<thead>
<tr>
<th>Constant</th>
<th>Value</th>
<th>Timing of $P_{max}$</th>
<th>Ignition Delay</th>
</tr>
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<tr>
<td></td>
<td></td>
<td>(°CA)</td>
<td>(°CA)</td>
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<tr>
<td>$R_S$</td>
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<tr>
<td></td>
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<td>0.50*</td>
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</tr>
<tr>
<td></td>
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<td>7</td>
</tr>
<tr>
<td></td>
<td>1.00</td>
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<td>7</td>
</tr>
<tr>
<td>$T_{cyl,IVC}$</td>
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<td>6</td>
<td>7</td>
</tr>
<tr>
<td></td>
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<td>320</td>
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<tr>
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<td></td>
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<tr>
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<td>7</td>
</tr>
<tr>
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<td>5</td>
<td>7</td>
</tr>
</tbody>
</table>

*Baseline constant
(1) Error ±0.5 °CA
effect on emissions of NO than the factor controlling the conservation of initial spray momentum. It is also noted that the effect of the in-cylinder temperature at IVC is relatively small in comparison to the other model inputs/ constants.

![Figure 6.20](image)

**Figure 6.20** – Relative effect of model inputs/ constants ($R_s$, $T_{cyIVC}$, $C_b$, $\alpha$, $C_L$, $C_U'$ and $C_t$) on emissions of NO

The effect of the model inputs/ constants on emissions of soot is shown in Figure 6.21. Here, the most important inputs/ constants affecting emissions of soot are the swirl ratio and the factor controlling the conservation of initial spray momentum. Hence, similarly to emissions of NO, the oxygen availability has a dominant effect on the total formation of soot. Again, it is shown that the effect of the entrainment factor is less significant than the factor controlling the conservation of initial spray momentum. It is noted that total soot formation is not a linear function of the swirl ratio, with soot formation decreasing rapidly for higher swirl ratios. This is attributed to increased spray temperatures caused by greater rates of burning and increased oxygen availability, which both promote soot oxidation.
Figure 6.21 – Relative effect of model inputs/constants ($R_s$, $T_{cyIVC}$, $C_b$, $\alpha$, $C_L$, $C_U'$ and $C_\tau$) on emissions of soot

6.4 CONCLUDING SUMMARY

A sensitivity analysis has been performed to identify the underlying physical mechanisms affecting the performance and emissions of a dual fuel engine. The study considered the model inputs/constants critical to the calibration of the model. The effect of these inputs/constants on the magnitude and timing of peak in-cylinder pressure, the ignition delay period, and emissions of NO and soot was then considered. The following conclusions can be drawn from the current chapter:

- The magnitude of peak in-cylinder pressure is strongly influenced by the swirl ratio, factor controlling the conservation of initial spray momentum, entrainment factor and proportionality constant controlling the size of the turbulence intensity at the initiation of combustion. Hence, the magnitude of peak in-cylinder pressure is a strong function of the oxygen availability in both the pilot fuel spray and the premixed burning zone. The in-cylinder temperature at IVC...
also has an important influence on the prediction of the magnitude of peak in-cylinder pressure.

- The inputs/constants controlling the rate of entrainment into the pilot fuel spray – the swirl ratio, factor controlling the conservation of initial spray momentum and entrainment factor – have an important effect on the prediction of emissions of NO. The turbulence intensity is also of importance and it is postulated that its effect would be greater for greater gaseous equivalence ratios.

- Emissions of soot are a strong function of the oxygen availability in the pilot fuel spray. Hence, the swirl ratio, factor controlling the conservation of initial spray momentum and entrainment factor have an important effect on total soot formation. In particular, it is noted that increasing the swirl ratio has a strong influence on the oxidation of soot.

- The entrainment factor, which controls the rate of entrainment across the radial cross-section of the spray, is less important in the prediction of the magnitude of peak in-cylinder pressure and emissions of NO and soot than the factor controlling the conservation of initial spray momentum, which controls the rate of entrainment into the entire spray.

In conclusion, the sensitivity analysis provides detailed insight into the effect of the model inputs/constants on model predictions. This has provided a better understanding of the relationships between the model inputs/constants and the physical mechanisms controlling the performance and emissions in a dual fuel engine. Furthermore, the figures revealing the relative effect of the model inputs/constants on the magnitude of peak in-cylinder pressure and emissions of NO and soot provide a solid foundation for the calibration of the model against different engine types in the future.
7.1 CONCLUSIONS

A new quasi-dimensional, multi-zone model has been developed to describe the combustion processes occurring inside a dual fuel engine during the closed part of the engine cycle. The model is based on the current conceptual understanding of dual fuel combustion, in which the combustion of a pilot fuel spray controls the subsequent burning of a premixed gaseous charge, and employs a novel approach to describing the development of premixed gaseous combustion during and after the ignition of the pilot. The pilot fuel spray is described using a packet model approach, which accounts for spray development and mixing, swirl, spray wall impingement, ignition and combustion. Flame development is described using an original approach in which flame growth is coupled to the burning zones in the cylinder and is described using a turbulent entrainment model. Burning zones within the spray act as flame kernels from which flame fronts develop. In an original approach, the burning zones are adiabatically mixed and a single spherical flame front is assumed to propagate at the turbulent burning velocity. The premixed charge crossing this flame front is added to a separate premixed burning zone. On subsequent steps, all burning zones are lumped together to determine the flame front surface from which propagation develops. The model is the first to account for flame growth from the viewpoint of coalescence of enflamed zones.

Dissociation of the combustion products is accounted for using the method of Damköhler and Edse (1943) (as described by Gaydon and Wolfhard (1960)), which has been modified to include eleven product species. This method was implemented using an algorithm developed as part of the present work. The equilibrium scheme was further used to determine non-equilibrium emissions of NO. These were calculated using the extended Zeldovich mechanism. Emissions of soot were calculated using a simple two-step approach which accounts for soot formation and soot oxidation. Soot formation was modelled using the Arrhenius-type equation of Hiroyasu et al. (1983) and soot oxidation was modelled using the approach of Nagle and Strickland-Constable (1962). Emissions of soot were attributed solely to the spray zones and the instantaneous soot density of each zone was incorporated into a radiative heat transfer model.
The main objective of the present work was to describe the processes occurring inside the cylinder on the basis of physical and chemical phenomena, thus reducing the number of adjustable model constants. The model constants were calibrated against diesel and dual fuel modes of operation for experimental data obtained from a naturally aspirated, in-line, four-cylinder, direct injection diesel engine operating with methane as the gaseous fuel. The predictive capability of the model was assessed by comparing the calibrated model against experimental data at 1500 rpm under 100 and 50 percent load conditions for a range of gaseous substitution ratios.

A sensitivity analysis highlighted the underlying physical mechanisms affecting the dual fuel combustion processes.

The key findings of the work are summarised below:

1. A predictive engine model has been successfully developed to simulate the in-cylinder pressures and rates of energy release in a dual fuel engine. Trends for engine-out emissions are also in reasonable agreement with experimental data.

2. The factor controlling the conservation of initial spray momentum was adjusted throughout model calibration and validation to account for difficulties in describing the initial spray momentum. A linear relationship was observed between the factor applied to the conservation of initial spray momentum and the diesel fuel flow rate. Furthermore, it was also observed that the gaseous equivalence ratio had a role in the value of the factor applied to the conservation of initial spray momentum.

3. To match the experimentally derived energy release diagram for the baseline dual fuel case, a rapid initial increase in energy release was required from the premixed charge. Thus, the turbulent flame front was initially assumed to propagate freely across the cylinder. Then, following the entrainment of a characteristic mass, the entrainment area was described by an exponential decay. At higher gaseous equivalence ratios, this is indicative of a reduced flame area due to the coalescence of individual flame fronts. At lower gaseous equivalence ratios this is attributed to bulk quenching.
4. Model predictions were compared against experimental data obtained at 1500 rpm under 100 and 50 percent load conditions for a range of gaseous substitution ratios. The general agreement between the pressure and energy release diagrams, and the prediction of the magnitude and timing of peak in-cylinder pressure and ignition delay give confidence in the breakup, entrainment, evaporation, ignition and combustion sub-models. The prediction of the late combustion phase also gives confidence in the description of the flame area by an exponential decay following the entrainment of a characteristic mass. For larger gas substitutions, it was noted that the model was unable to account for the agglomeration of energy release from the pilot fuel spray and premixed gaseous charge. This is attributed to the inability of the model to capture energy release in the reactive boundary surrounding the pilot fuel spray.

5. Emissions of both NO and soot were calibrated to match experimental data for diesel operation at 1500 rpm under 100 and 50 percent load conditions. Trends for emissions of NO and soot were then compared. At 50 percent load, the trend for emissions of NO with gaseous energy substitution was in good agreement with the experimental data. However, at 100 percent load, emissions of NO were not well predicted. Trends for emissions of soot were in good agreement for both the 100 and 50 percent load cases. However, the predicted soot concentrations were over-predicted for dual fuel operating conditions.

6. The main limitations of the model are as follows: the prediction of emissions of NO at high load conditions and the over-prediction of emissions of soot for dual fuel operation. The poor prediction of NO at high loads is attributed to the inability of the model to capture the reactive region surrounding the pilot fuel spray. Therefore, further work is required to describe the combustion processes occurring in this region. The over-prediction of emissions of soot for dual fuel operation highlights a limitation of the present model in describing soot formation for the range of pilot quantities investigated. Again, this is attributed to the inability of the model to capture the reactive region around the pilot fuel spray.

7. The sensitivity analysis revealed the importance of the model inputs/ constants controlling the rate of entrainment into the pilot fuel spray. In particular, the
swirl ratio and factor controlling the conservation of initial spray momentum had an important effect on the magnitude of peak in-cylinder pressure. The proportionality constant controlling the size of the turbulence intensity at the initiation of combustion was also found to have a strong influence on the magnitude of peak in-cylinder pressure. Moreover, it was found that the swirl ratio and factor controlling the conservation of initial spray momentum had an important influence on emissions formation.

In summary, a new quasi-dimensional, multi-zone combustion model has been developed for performance and emissions predictions in a dual fuel engine. The predictive capability of the model is very encouraging, particularly given the complexity of the combustion processes occurring inside a dual fuel engine.

7.2 RECOMMENDATIONS FOR FURTHER WORK

A new quasi-dimensional, multi-zone combustion model has been successfully developed to describe performance and emissions trends in a dual fuel engine. To further improve the predictive capability of the model, a number of improvements are suggested. The main focus here is on improving the simplifying assumptions made during model development. The sub-models considered include: the calculation of the ignition delay period; the assumption of the premixed burning zone as a single zone; and the prediction of NOx using the extended Zeldovich mechanism.

- **Ignition delay.** In the present work, the ignition delay was determined using a correlation developed for diesel engines, which was found to give good agreement with the experimental work. To better understand the ignition process, the effect of the gaseous fuel on ignition needs to be considered. Several phenomenological models have been developed to predict the ignition delay of multi-component mixtures (Kavtaradze et al., 2005, Vasil'ev, 2007). The suitability of these models for dual fuel combustion modelling needs to be investigated.

- **Premixed burning zone.** In the present work, the premixed burning zone is represented by a single zone. To better describe the stratification of temperature and burned species composition in the premixed burning zone, the zone could be sequentially divided at each computational time step. This
would account for higher temperatures in the zones formed earlier in the combustion process, thus leading to a better description of emissions formation.

- **Emissions of NO$_x$.** In the present work, emissions of NO$_x$ were modelled using the extended Zeldovich mechanism. In their single-zone model, Mansour et al. (2001) employed both the extended Zeldovich mechanism and a chemical kinetic scheme to describe the formation of NO$_x$ in a dual fuel engine. The study found that the description of NO$_x$ was better modelled by the chemical kinetic scheme. It is probable that a similar scheme applied to the multi-zone approach would lead to a better description of the formation of NO$_x$.

The dual fuel engine is faced with a number of challenges. These are mainly associated with the method of load control. At higher loads, the gaseous substitution employed to achieve maximum power is limited by knock, whereas at lower loads, the lean nature of the premixed charge leads to partial burning and misfire. This in turn leads to increased emissions of CO and uHC. The following highlights sub-models that can be implemented to further improve the understanding of these issues.

- **Knock.** One of the drawbacks of dual fuel combustion is the occurrence of knock under high load conditions. In the future, a knock model could be implemented into the model to give an indication of operating conditions which would lead to knock, thus giving a tool which could define safe operating limits for a given dual fuel engine.

- **Emissions of CO and uHC.** In the present work, emissions of CO and uHC were not considered. In the dual fuel engine modelling literature, emissions of CO have been successfully predicted using detailed chemical kinetics. This type of approach could be introduced to the current model in the future. Emissions of uHC could be determined using a phenomenological approach, although the prediction of this type of emission is difficult.

In the future, the model could also be extended to investigate the full engine cycle.

- **Full engine cycle.** The predictive capability of the model may be further improved by modelling the full engine cycle, thereby including the intake and
exhaust processes. This would give a better prediction of the mass of gas ingested into the cylinder, leading to a more accurate description of the subsequent combustion processes. This method could be further extended to include turbocharged air systems.
REFERENCES


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<td>658.00</td>
<td>Green and Perry (2008), pp. 2-100</td>
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<td>Vapour Isobaric Specific Molar Heat /kJ.kmol(^{-1})</td>
<td>(\bar{C}_{P,V} = -9.328 + 1.149 \cdot T - 6.347 \cdot 10^{-4} \cdot T^2 + 1.359 \cdot 10^{-7} \cdot T^3)</td>
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<td>-</td>
<td>Reid et al. (1987), pp. 728</td>
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<td>658.00</td>
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<tr>
<td>Vapour Thermal Conductivity /W.m(^{-1})K(^{-1})</td>
<td>(k_v = 5.719 \cdot 10^{-6} \cdot T^{1.4699} / (1 + 579.4/T))</td>
<td>489.47</td>
<td>1000.00</td>
<td>Green and Perry (2008), pp. 2-435</td>
</tr>
<tr>
<td>Liquid Dynamic Viscosity /cP(^{(2)})</td>
<td>(\mu_l = \exp(-4.562 + 1.454 \cdot 10^3/T))</td>
<td>268.00</td>
<td>493.00</td>
<td>Reid et al. (1987), pp. 452</td>
</tr>
<tr>
<td>Vapour Dynamic Viscosity /Pa.s</td>
<td>(\mu_v = 6.344 \cdot 10^{-8} \cdot T^{0.8287} / (1 + 219.5/T))</td>
<td>263.57</td>
<td>1000.00</td>
<td>Green and Perry (2008), pp. 2-423</td>
</tr>
</tbody>
</table>

\(T_r = T/T_c\), where \(T_c\) is the critical temperature given as 658 K (Green and Perry, 2008). (1) To convert liquid molar density, in mol.dm\(^{-3}\), to kg.m\(^{-3}\) multiply by the molecular weight of n-dodecane \((M_{C_{12}H_{26}} = 170.34 \text{ kg.kmol}^{-1}\) (Reid et al., 1987)). (2) To convert liquid viscosity, in cP, to Pa.s divide by 1·10\(^3\).

Table A.2 – Curve fit coefficients for the specific molar enthalpy ($\tilde{h}$) and isobaric specific molar heat ($\tilde{C}_p$) of diesel (C$_{10.8}$H$_{18.7}$) vapour

\[
\tilde{h}(kJ.kmol^{-1}) = 4184(AT + BT^2/2 + CT^3/3 + DT^4/4 - E/T + F + G)
\]
\[
\tilde{C}_p(kJ.kmol^{-1}K^{-1}) = 4.184(A + BT + CT^2 + DT^3 + E/T^2)
\]


Table A.3 – Curve fit coefficients for the specific molar enthalpy ($\tilde{h}$) and isobaric specific molar heat ($\tilde{C}_p$) to the JANAF tables (1998) for gaseous methane (CH$_4$)

\[
\tilde{h}(kJ.kmol^{-1}) = \tilde{h}_f + A + BT + CT^2 + DT^3 + ET^4 + FT^5
\]
\[
\tilde{C}_p(kJ.kmol^{-1}K^{-1}) = B + 2CT + 3DT^2 + 4ET^3 + 5FT^4
\]

**Liquid Isobaric Specific Heat**

The method for calculating the liquid isobaric specific heat ($C_{p,l}$) (in kJ.kg$^{-1}$K$^{-1}$) of n-dodecane ($C_{12}H_{26}$) was taken from Kouremenos et al. (1990).

$$C_{p,l} = 4.188(C_{p1} + 12C_{p2}) \quad (A.1)$$

$$C_{p1} = 0.84167 - 1.4704 \cdot T + 1.67165 \cdot T^2 - 0.59198 \cdot T^3 \quad (A.2)$$

$$C_{p2} = -0.003826 - 0.000747 \cdot T + 0.041126 \cdot T^2 - 0.01395 \cdot T^3 \quad (A.3)$$

$T = T_l/T_b$, where $T_b (= 489.5 \text{ K})$ is the normal boiling point of n-dodecane ($C_{12}H_{26}$) obtained from Reid et al. (1987). Kouremenos et al. (1990) state that this method gives average errors of 2 percent.

**Dynamic Viscosity and Thermal Conductivity of Gaseous Mixtures**

The dynamic viscosity and thermal conductivity of a gaseous mixture are not linear functions of mole fraction. Reid et al. (1987) draw attention to the following method (Wilke, 1950) for determining the dynamic viscosity of gaseous mixtures ($\mu_m$)

$$\mu_m = \sum_i \left( \frac{y_i \mu_i}{\sum_j y_j \Phi_{ij}} \right) \quad (A.4)$$

$$\Phi_{ij} = \frac{1 + \left( \mu_i/\mu_j \right)^{0.5} \left( M_j/M_i \right)^{0.25}}{\left( 1 + M_i/M_j \right)^{0.5}} \quad (A.5)$$

where $y$, $\mu$ and $M$ are the mole fraction, dynamic viscosity and molecular weight of gaseous mixture components $i$ and $j$ respectively. The term $\Phi_{ji}$ can be found from

$$\Phi_{ji} = \frac{\mu_j M_i}{\mu_i M_j} \Phi_{ij} \quad (A.6)$$

In a form analogous to the Wilke method, an expression for the thermal conductivity of a gaseous mixture ($k_m$) can be written as
\[ \bar{k}_m = \sum_i \left( \frac{y_i \bar{k}_i}{\sum_j y_j A_{ij}} \right) \]  
\[ (A.7) \]

Mason and Saxena (1958) showed that

\[ A_{ij} = \Phi_{ij} \]  
\[ (A.8) \]

Thus, the thermal conductivity of a gaseous mixture can be determined using the dynamic viscosities of the gaseous mixture components. Expressions for determining the vapour thermal conductivity and vapour dynamic viscosity of selected species are given below.

**Table A.4** – Curve fit coefficients for the vapour thermal conductivity \( (\bar{k}_v) \) and vapour dynamic viscosity \( (\mu_v) \) of methane (CH\textsubscript{4}), oxygen (O\textsubscript{2}) and nitrogen (N\textsubscript{2})

\[ \bar{k}_v (\text{W.m}^{-1}\text{K}^{-1}) = AT^B/(1 + C/T + D/T^2) \]
\[ \mu_v (\text{Pa.s}) = AT^B/(1 + C/T + D/T^2) \]

<table>
<thead>
<tr>
<th>Property</th>
<th>( A )</th>
<th>( B )</th>
<th>( C )</th>
<th>( D )</th>
<th>( T_{\text{min}} )</th>
<th>( T_{\text{max}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH\textsubscript{4}</td>
<td>( \bar{k}_v )</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>( \mu_v )</td>
<td>5.2546E-7</td>
<td>0.59006</td>
<td>105.67</td>
<td>-</td>
<td>90.69</td>
</tr>
<tr>
<td>O\textsubscript{2}</td>
<td>( \bar{k}_v )</td>
<td>4.4994E-4</td>
<td>0.7456</td>
<td>56.699</td>
<td>-</td>
<td>80.00</td>
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<tr>
<td></td>
<td>( \mu_v )</td>
<td>1.101E-6</td>
<td>0.5634</td>
<td>96.3</td>
<td>-</td>
<td>54.35</td>
</tr>
<tr>
<td>N\textsubscript{2}</td>
<td>( \bar{k}_v )</td>
<td>3.3143E-4</td>
<td>0.7722</td>
<td>16.323</td>
<td>373.72</td>
<td>63.15</td>
</tr>
<tr>
<td></td>
<td>( \mu_v )</td>
<td>6.5592E-7</td>
<td>0.6081</td>
<td>54.714</td>
<td>-</td>
<td>63.15</td>
</tr>
</tbody>
</table>


The method for determining the vapour thermal conductivity of methane (CH\textsubscript{4}) was taken from Reid et al. (1987) and is valid for the temperature range 273 K – 1270 K.

\[ \bar{k}_{v,\text{CH}_4} (\text{W.m}^{-1}\text{K}^{-1}) = -1.869 \times 10^{-3} + 8.727 \times 10^{-5} \cdot T + 1.179 \times 10^{-7} \cdot T^2 - 3.614 \times 10^{-11} \cdot T^3 \]  
\[ (A.9) \]
Surface Tension

The surface tension ($\sigma$) (in mN.m$^{-1}$) of n-dodecane (C$_{12}$H$_{26}$) was calculated using a method recommended by Reid et al. (1987)

$$\sigma = ([P] \rho_{l,b})^4 \left( \frac{1 - T_r}{1 - T_{b,r}} \right)^{4n}$$  \hspace{1cm} (A.10)

where,

- $P = \text{parachor, cm}^3\text{g}^{0.25}\text{s}^{-0.5}\text{mol}^{-1}$
- $\rho_{l,b} = \text{molar liquid density at the normal boiling point, mol.cm}^{-3}$
- $T_r = T/T_c$, where $T_c$ is the critical temperature
- $T_{b,r} = T_b/T_c$, where $T_b$ is the normal boiling point

For hydrocarbons, the exponent, $n$, is given as 0.29. The parachor, $P$, is a temperature-independent parameter and was calculated from Reid et al. (1987). The molar liquid density at the normal boiling temperature, $\rho_{l,b}$, was determined from the formula for liquid density given in Table A.1. Values for $T_c (= 658$ K) and $T_b (= 489.5$ K) were taken from Green and Perry (2008) and Reid et al. (1987) respectively. The final expression for the surface tension of n-dodecane (C$_{12}$H$_{26}$) is given by

$$\sigma = (1.78)^4 \left( \frac{1 - T_r}{1 - T_{b,r}} \right)^{1.16}$$  \hspace{1cm} (A.11)

Reid et al. (1987) state that this method normally gives errors less than 5 to 10 percent.

Mass Diffusivity

The mass diffusivity for the fuel vapour-gas mixture ($D_{v,g}$) (in cm$^2$.s$^{-1}$) was calculated using a method recommended by Reid et al. (1987) for diffusion in homogeneous gas mixtures

---

APPENDIX A LIQUID AND GASEOUS PROPERTIES
\[ D_{v,g} = \left( \sum_j \frac{y_j}{D_{ij}} \right)^{-1} \]  
\hspace{1cm} (A.12)

where,

\[ y_j = \text{mole fraction of gaseous mixture component } j \]
\[ D_{ij} = \text{binary diffusion coefficient of component } i \text{ into component } j, \text{ cm}^2.\text{s}^{-1} \]

The mass diffusivities for the binary systems \((D_{ij})\) were calculated using the method of Fuller et al. (1969) as recommended by Reid et al. (1987)

\[ D_{ij} = \frac{0.0017 T^{1.75} M_{ij}^{0.5}}{P \left[ (\sum_v v_i^{1/3}) + (\sum_v v_j^{1/3}) \right]^2} \]  
\hspace{1cm} (A.13)

where,

\[ T = \text{temperature, K} \]
\[ P = \text{pressure, bar} \]
\[ M_i, M_j = \text{molecular weights of } i \text{ and } j, \text{ kg.kmol}^{-1} \]
\[ M_{ij} = 2 \left[ 1/M_i + 1/M_j \right]^{-1} \]
\[ \sum_v = \text{sum of atomic diffusion volumes for each component} \]

The molecular weights were taken from the JANAF tables (1998) and Reid et al. (1987), and the atomic diffusion volumes were determined from Reid et al. (1987). The final expressions for the fuel vapour-air diffusivity and fuel vapour-methane diffusivity are given by

\[ D_{v,\text{air}} = \frac{6.07 \cdot 10^{-4} T^{1.75}}{P} \]  
\hspace{1cm} (A.14)

\[ D_{v,\text{CH}_4} = \frac{6.40 \cdot 10^{-5} T^{1.75}}{P} \]  
\hspace{1cm} (A.15)
References


Internal Energy and Specific Heat of an Ideal-Gas Mixture

The internal energy \( U = n(h - R_u T) \) of an ideal-gas mixture can be calculated from its composition and temperature (\( T \)) using polynomial curve fits of the individual components specific molar enthalpy (\( h_i \)) to the JANAF tables (1998).

\[
\bar{h} = \sum_i y_i h_i(T)
\]  

(B.1)

The isobaric specific molar heat (\( \bar{C}_p \)) of an ideal-gas mixture is determined from the following thermodynamic relation \( \bar{C}_p = d\bar{h}/dT \). Thus,

\[
\bar{C}_p = \sum_i y_i \frac{\bar{h}_i(T)}{dT}
\]

(B.2)

Coefficients for determining the specific molar enthalpy and isobaric specific molar heat of the gas species employed in the present work are given in Table B.1. The specific molar enthalpy and isobaric specific molar heat of the liquid fuel vapour can be calculated using the expressions given for diesel in Appendix A, Table A.2.

References

Table B.1 – Curve fit coefficients for the specific molar enthalpy ($\bar{h}$) and isobaric specific molar heat ($\bar{C}_p$) to the JANAF tables (1998) for selected gas species

\[ \bar{h}(kJ\cdot kmol^{-1}) = \bar{h}_f^0 + AT + CT^2 + DT^3 + ET^4 + FT^5 \]
\[ \bar{C}_p(kJ\cdot kmol^{-1} \cdot K^{-1}) = B + 2CT + 3DT^2 + 4ET^3 + 5FT^4 \]

<table>
<thead>
<tr>
<th>Species</th>
<th>T range / (K)</th>
<th>$\bar{h}_f^0$</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
</tr>
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<tbody>
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</table>

$\bar{h}_f^0$ is the enthalpy of formation (in kJ.kmol$^{-1}$) at a reference temperature of 298.15 K.
APPENDIX C
EQUILIBRIUM CONSTANTS

Table C.1 – Curve fit coefficients for the evaluation of $\log_{10} K_p$. Valid for the temperature range 600 K – 4000 K. Pressure units are in bar.

\[ \log_{10} K_p = A \ln(T) + \frac{B}{T} + C + DT + ET^2 \]

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$A$</th>
<th>$B$</th>
<th>$C$</th>
<th>$D$</th>
<th>$E$</th>
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<tbody>
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<td>$CO_2 \leftrightarrow CO + \frac{1}{2} O_2$</td>
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<tr>
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<tr>
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<tr>
<td>$\frac{1}{2} N_2 + \frac{1}{2} O_2 \leftrightarrow NO$</td>
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</table>

$T$ is the temperature in kK.
APPENDIX D

OVERVIEW OF GRAPHICAL USER INTERFACE

The quasi-dimensional dual fuel model is run using a graphical user interface (GUI) designed and developed as part of the present work (Figure D.1). This was implemented using the C# programming language. The main advantage of the GUI is its ability to complete multiple runs. Owing to the fast computational runtimes offered by the model, this allows systematic studies to be completed quickly and effectively.

The model inputs are organised into tabs under the headings of engine details, simulation details and advanced settings, with the advanced settings providing access to the model constants. The input fields are populated either manually or automatically using a standard text based input file (*.dat). Any combination of model inputs can also be saved to a standard input file for future use. A batch file (*.cvs (tab delimited)) allows multiple runs to be loaded without the need to populate the input fields.

Before runtime, simple error checking is employed to ensure that the field contents are in the correct format. Then during runtime, the GUI gives feedback on the current position of the calculation procedure, and for multiple runs, the current batch or run number. Upon completion, the user is notified of the location of the output files, where the output files are organised into folders under a file path defined by the user on the front page of the GUI.

Model outputs are provided in two *.cvs files. The first gives a summary of the main parameters of interest and the second presents the crank angle resolved data. The standard input file is saved alongside the output files for future reference.
Figure D.1 – Overview of GUI