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CFD MODELLING OF NATURAL GAS COMBUSTION
IN SPARK IGNITED ENGINES

by

Aruna Susantha Palipana
CFD MODELLING OF NATURAL GAS COMBUSTION
IN SPARK IGNITED ENGINES

Aruna Susantha Palipana

A Doctoral Thesis
Submitted in partial fulfilment of the requirements
for the award of the degree of
Doctor of Philosophy

Department of Mechanical Engineering
Loughborough University

June, 2000
Dedicated

to my parents - Mr. & Mrs. P.B. Palipana, two brothers - Lasantha and Hemantha, Wife - Gayani and my sweet little son - Lahiru

(They all sacrificed many things because of my higher education)

and

to all my teachers
Abstract

Natural gas is gaining popularity as a fuel for automobile applications. In order to procure all the benefits of using natural gas, dedicated engines optimised for this fuel are needed. It is necessary to validate multi-dimensional models of combustion of natural gas in SI engines as such models provide a powerful tool in designing engines and optimising them for this fuel and for studying the emission of pollutants.

The multi-dimensional CFD code, KIVA-II, has been used in this study, with necessary modifications and additions. Several combustion models commonly used for SI engine modelling in CFD environments were evaluated. It was concluded that flamelet combustion models are more suitable for engine combustion modelling as engine combustion, in almost all cases, lies within the flamelet regime of combustion. One such flamelet model, the Fractal Flame Model (FFM), was improved, implemented and validated for simulating the turbulent phase of the combustion process in a spark ignited, natural gas fuelled engine. The model validation was done by comparing predictions with experimental data for the base line case. This validated model was then used to study the effects of engine operating parameters and combustion chamber geometry on engine performance and emissions thus providing a suitable analytical background for the designing of dedicated engines optimised for natural gas. This parametric study was performed over a range of air/fuel ratios, with ignition timing, compression ratio and engine speed as the variable parameters. The trends predicted were used to assess the predictive capabilities of the FFM.

Eddy break up model (EBUM) was used to compare the predictions by the FFM and these comparisons indicated that the FFM resulted in better agreement with experiments. The predicted trends of engine performance and pollutant formation with the FFM agree well with those found in the literature. This indicates the strength of the FFM as a combustion model for natural gas fuelled SI engines.

The effects of the combustion chamber geometry and exhaust gas recirculation on engine performance and pollutant formation were numerically studied and the trends obtained agree with experimental data available. The Renormalisation Group Theory (RNG) $k-\varepsilon$ turbulence model was compared with the standard $k-\varepsilon$ model and no significant effect on results was found.
Acknowledgements

I am very much grateful to my supervisors Dr. W. Malalasekera and Dr. E.H. James for the kind guidance and the assistance I received from them during my research study.

I gratefully acknowledge Dr. W. Malalasekera and Mr. H.K. Versteeg introducing the world of CFD to me and Dr. C.P. Garner and Dr. E.H. James extending my knowledge on IC engines.

My gratefulness is shown here to Dr. Sean Mendis (for experimental data), Dr. Apoorva Agarwal (for constant support and encouragement regarding the KIVA-II code), Dr. Xiaowei Zhao (for discussions on the Fractal Flame Model), Prof. Chris Sheppard (for experimental data), Prof. W.K. Cheng (for kind advice and assistance with the Coherent Flame-sheets model), Dr. K.E.D. Sumanasiri (for encouragement and for the first CFD book), Prof. J.J. McGuirk (for additional financial support and for kindness) and to Dr. H.G. Weller (for useful discussions).

The financial support and the assistance I received from the Association of Commonwealth Universities and the British Council through a Commonwealth scholarship is acknowledged here.

I would like to acknowledge University of Peradeniya, Sri Lanka for granting me study leave in order to pursue this research study. The kindness of Dr. K.E.D. Sumanasiri and Dr. M.B. Kahawatte shown by being my guarantors is gratefully reminded.

My colleagues John Jones, Mamdud Hossain, Ricardo Carroni, Jon Henson, Sudhakar Das, Mohammed Selim, Rui Chen, John Jenkins, Rohitha Weerasinghe, John Ranasinghe and Paul Birkby are thanked for the support and help I received from them in various forms.

I sincerely thank all those people, who helped my wife, Gayani not feel bored while I was engaged in the studies and made our life in the UK pleasant. John Chris Jones, Hazel and Richard Meredith and Carole Burton deserve special thanking for being more than friends to us.

Finally I thank my family (wife Gayani and son Lahiru), who kept me going, our parents and siblings, who missed our company and duties/responsibilities for several years, and my sister-in-law Rekha, who sacrificed a complete year for us.
Contents

Abstract i

Acknowledgements ii

List of tables viii

List of figures ix

Nomenclature xv

Chapter 1.
Introduction 1

1.1. SI Engine performance 3
1.2. Emissions from SI engines 5
1.3. Numerical modelling of IC engines and CFD 9
1.4. Engine combustion modelling 13
1.5. Objective of the present study 14
1.6. Outline of the thesis 15

Chapter 2.
The CFD code KIVA-II with modifications and additions 17

2.1. The CFD code 18
2.2. Governing Equations
   2.2.1. Equation of state for ideal gases 19
   2.2.2. Conservation of mass 20
   2.2.3. Conservation of momentum 20
   2.2.4. Conservation of energy 20
   2.2.5. Turbulence 21

2.3. Solution method 22
   2.3.1. Temporal and spatial differencing 23

2.4. Combustion chemistry 26
   2.4.1. Chemical kinetic reactions 26
   2.4.2. Equilibrium chemical reactions 27

2.5. Modifications and additions made to KIVA-II during the present study 28
   2.5.1. Treatment of blow-by flow 28
   2.5.2. Numerical mesh 31
   2.5.3. RNG k-ε turbulence model as an alternative to standard k-ε model 33
   2.5.4. Spark ignition Model 34
   2.5.5. Chopper for removing cell layers 35
   2.5.6. Contour plots and output of results 35
   2.5.7. Chemical reaction rate 36

Chapter 3.
Modelling of the SI engine combustion 37

3.1. Model development 37
3.2. Specialisation of PDEs to IC engines 38
3.3. Numerical scheme 38
3.4. Classification of SI engine models 39
   3.4.1. Thermodynamic models 39
   3.4.2. Dimensional models 42
3.5. Models of flame structure and flame speed 43
   3.5.1. Flame Structure models 43
3.5.2. Flame speed models 45
3.6. Modelling of Premixed Turbulent Flames 45
   3.6.1. Regimes of Combustion 46
3.7. SI Engine combustion modelling 48
3.8. Commonly used multi-dimensional models of SI engine combustion 49
   3.8.1. Global mean reaction rate models: Single reaction model (SRM) 49
   3.8.2. Statistical and stochastic models 51
   3.8.3. Eddy break up models (EBUM) 54
   3.8.4. Characteristic time models 60
   3.8.5. Flamelet models 63
3.9. Choice of a combustion model 70

Chapter 4.
Fractal Flame model 72

4.1. Fractal geometry and turbulence 72
4.2. Fractal aspects of premixed turbulent combustion 73
4.3. The multi-dimensional fractal model of Gouldin et al. 78
4.4. The multi-dimensional fractal model of Gülder 80
4.5. The multi-dimensional fractal model of Zhao et al. 81
4.6. Improvements to the FFM by De Petris et al. 84
4.7. Improvements to the FFM during the present study 85
4.8. Validation of the improved Fractal Flame Model 92
4.9. The grid dependency test 96
4.10. RNG k-ε turbulence model as an alternative to standard k-ε model 97
4.11. The FFM compared with the KIVA-II kinetic chemistry model 101
4.12. The FFM compared with the EBU model 102

Chapter 5.
Parametric studies of a natural gas fuelled SI engine 111
5.1. Natural gas as an alternative fuel  
5.2. NG engine types and applications  
5.3. Converted engines  
5.3.1. Bi-fuel engines  
5.3.2. Dual-fuel engines  
5.3.3. Otto cycle conversion from diesel engines  
5.3.4. Dedicated, optimised, natural gas engines  
5.4. Fuel metering  
5.4.1. Fuel injection in natural gas vehicles  
5.5. Parameters affecting engine performance  
5.5.1. Compression ratio  
5.5.2. Turbocharging  
5.5.3. Ignition  
5.5.4. Turbulence, flame travel speed and distance  
5.5.5. Combustion pressure  
5.5.6. Fuel composition and mixture homogeneity  
5.6. A general comparison of NG engine with gasoline and diesel engines  
5.7. Parametric study with KIVA-II using the FFM  
5.8. Effect of exhaust gas recirculation  
5.9. Effect of the combustion chamber geometry  
5.10. Improvement of Arrhenius type SR chemistry model in KIVA-II  

Chapter 6.  
Emissions from the SI engine fuelled with natural gas  

6.1. Pollutants and their formation  
6.1.1. Nitrogen oxides  
6.1.2. Hydrocarbons  
6.1.3. Carbon monoxide  
6.1.4. Aldehydes
Chapter 7.
Summary, conclusions and suggestions for further study 227

7.1. Summary 227
7.2. Conclusions 229
7.3. Suggestions for further work 231

Appendix 1 237
Appendix 2 239
References 243
## List of tables

<table>
<thead>
<tr>
<th>Table no.</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Two equation standard $k$-$\varepsilon$ turbulence model constants and the standard values used for engine calculations</td>
<td>22</td>
</tr>
<tr>
<td>2.2</td>
<td>Values of RNG $k$-$\varepsilon$ turbulence model constants</td>
<td>34</td>
</tr>
<tr>
<td>3.1</td>
<td>Production and destruction of flame surface density in CFM models</td>
<td>68</td>
</tr>
<tr>
<td>5.1</td>
<td>Properties of UK mains natural gas</td>
<td>113</td>
</tr>
<tr>
<td>5.2</td>
<td>Characteristic fuel properties of some individual gasses found in natural gas</td>
<td>114</td>
</tr>
</tbody>
</table>
# List of figures

<table>
<thead>
<tr>
<th>Fig. No.</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Typical finite difference cell ((i,j,k)) used in KIVA-II.</td>
<td>24</td>
</tr>
<tr>
<td>2.2</td>
<td>Engine blow-by path</td>
<td>29</td>
</tr>
<tr>
<td>2.3</td>
<td>The grid generated from the new program to include the crevice cells for the 'Brunel' piston (At the IVO, 135° BTDC).</td>
<td>32</td>
</tr>
<tr>
<td>3.1</td>
<td>The logic structure of Thermodynamics based simulations of the IC engine cycle</td>
<td>40</td>
</tr>
<tr>
<td>3.2</td>
<td>Thermal boundary layer in reaction zone</td>
<td>42</td>
</tr>
<tr>
<td>3.3</td>
<td>Phase diagram of regimes in premixed turbulent combustion</td>
<td>47</td>
</tr>
<tr>
<td>4.1</td>
<td>Variation of fractal dimension with the turbulent Reynolds number</td>
<td>77</td>
</tr>
<tr>
<td>4.2</td>
<td>Variation of (\bar{c}) (new) with crank angle</td>
<td>87</td>
</tr>
<tr>
<td>4.3</td>
<td>Numerical cells considered for estimating (\bar{c}) (new)</td>
<td>87</td>
</tr>
<tr>
<td>4.4</td>
<td>Variation of (\bar{c} (1 - \bar{c})) with crank angle</td>
<td>88</td>
</tr>
<tr>
<td>4.5</td>
<td>In-cylinder temperature distribution (Soon after the spark ignition)</td>
<td>91</td>
</tr>
<tr>
<td>4.6</td>
<td>In-cylinder velocity distribution (Soon after the spark ignition)</td>
<td>91</td>
</tr>
<tr>
<td>4.7</td>
<td>Measured and predicted cylinder pressure-crank angle history</td>
<td>93</td>
</tr>
<tr>
<td>4.8</td>
<td>Burned mass fraction: measured and predicted</td>
<td>93</td>
</tr>
<tr>
<td>4.9</td>
<td>Predicted rate of mass burning</td>
<td>94</td>
</tr>
<tr>
<td>4.10</td>
<td>In-cylinder temperature distribution with FFM at 12.5° BTDC</td>
<td>94</td>
</tr>
<tr>
<td>4.11</td>
<td>In-cylinder velocity distribution with FFM at 12.5° BTDC</td>
<td>95</td>
</tr>
<tr>
<td>4.12</td>
<td>Distribution of turbulent kinetic energy. FFM at 12.5° BTDC</td>
<td>95</td>
</tr>
<tr>
<td>4.13</td>
<td>Dissipation of turbulent kinetic energy with FFM at 12.5° BTDC</td>
<td>96</td>
</tr>
<tr>
<td>4.14</td>
<td>Motored engine cylinder pressure with two grid sizes</td>
<td>98</td>
</tr>
<tr>
<td>4.15</td>
<td>Average in-cylinder temperature, motored engine</td>
<td>98</td>
</tr>
<tr>
<td>4.16</td>
<td>Cylinder pressure of the combusting engine</td>
<td>99</td>
</tr>
<tr>
<td>4.17</td>
<td>In-cylinder average temperature, combusting engine</td>
<td>99</td>
</tr>
<tr>
<td>4.18</td>
<td>Burned mass fraction, combusting engine</td>
<td>100</td>
</tr>
<tr>
<td>4.19</td>
<td>Comparison of two turbulence models with FFM</td>
<td>100</td>
</tr>
<tr>
<td>4.20</td>
<td>Effect of blowby calculation on predicted cylinder pressure history</td>
<td>101</td>
</tr>
<tr>
<td>4.21</td>
<td>Single reaction model (SRM) compared with FFM</td>
<td>103</td>
</tr>
<tr>
<td>4.22</td>
<td>Eddy break up model (EBUM) compared with FFM</td>
<td>104</td>
</tr>
<tr>
<td>4.23</td>
<td>Average in-cylinder temperature, FFM and EBUM</td>
<td>104</td>
</tr>
<tr>
<td>4.24</td>
<td>Burnt mass fraction, FFM and EBUM</td>
<td>105</td>
</tr>
<tr>
<td>4.25</td>
<td>In-cylinder temperature distribution with EBUM, at 8° BTDC</td>
<td>107</td>
</tr>
<tr>
<td>4.26</td>
<td>In-cylinder velocity distribution with EBUM, at 8° BTDC</td>
<td>107</td>
</tr>
<tr>
<td>4.27</td>
<td>Distribution of turbulent kinetic energy with EBUM at 8° BTDC</td>
<td>108</td>
</tr>
<tr>
<td>4.28</td>
<td>Dissipation of turbulent kinetic energy with EBUM at 8° BTDC</td>
<td>108</td>
</tr>
<tr>
<td>4.29</td>
<td>Comparison of flame contours predicted by the two combustion models on a disc shaped combustion chamber</td>
<td>109</td>
</tr>
<tr>
<td>4.30</td>
<td>Comparison of two turbulence models with EBUM</td>
<td>110</td>
</tr>
<tr>
<td>5.1</td>
<td>Alternative transportation fuels</td>
<td>112</td>
</tr>
<tr>
<td>5.2</td>
<td>The Nebula combustion chamber</td>
<td>122</td>
</tr>
<tr>
<td>5.3</td>
<td>Effect of relative air-fuel ratio ((\lambda)) on cylinder pressure</td>
<td>128</td>
</tr>
<tr>
<td>5.4</td>
<td>Effect of relative air-fuel ratio ((\lambda)) on burned mixture mass fraction</td>
<td>128</td>
</tr>
<tr>
<td>5.5</td>
<td>Effect of relative air-fuel ratio ((\lambda)) on burned fuel mass fraction</td>
<td>129</td>
</tr>
<tr>
<td>5.6</td>
<td>Effect of relative air-fuel ratio ((\lambda)) on average temperature</td>
<td>129</td>
</tr>
<tr>
<td>5.7</td>
<td>Variation of cylinder pressure with relative air-fuel ratio ((\lambda)): A comparison from the literature</td>
<td>130</td>
</tr>
<tr>
<td>5.8</td>
<td>Variation of mass fraction burned with equivalence ratio ((\phi)): A comparison from the literature</td>
<td>130</td>
</tr>
<tr>
<td>5.9</td>
<td>Variation of exhaust gas temperature with air-fuel ratio and spark timing: A comparison from the literature</td>
<td>131</td>
</tr>
<tr>
<td>5.10</td>
<td>Effect of engine speed on cylinder pressure</td>
<td>131</td>
</tr>
<tr>
<td>5.11</td>
<td>Effect of engine speed on burned mass fraction</td>
<td>132</td>
</tr>
<tr>
<td>5.12</td>
<td>Variation of cylinder pressure with engine speed: A comparison from the literature</td>
<td>132</td>
</tr>
</tbody>
</table>
Engine speed on peak cylinder pressure, ignition at 20° BTDC
Engine speed on peak cylinder pressure, ignition at 26° BTDC
Engine speed on peak cylinder pressure, ignition at 32° BTDC
Ignition timing on peak cylinder pressure, at 1200 rpm
Ignition timing on peak cylinder pressure, at 1500 rpm
Ignition timing on peak cylinder pressure, at 1800 rpm
Ignition timing on peak cylinder pressure, at 2000 rpm
Contours of peak cylinder pressure in a natural gas engine
Burning of 10% of mixture mass with ignition at 20° BTDC
Burning of 10% of mixture mass with ignition at 26° BTDC
Burning of 10% of mixture mass with ignition at 32° BTDC
Burning of 10% of mixture mass with 1200 rpm engine speed
Burning of 10% of mixture mass with 1500 rpm engine speed
Burning of 10% of mixture mass with 1800 rpm engine speed
Burning of 10% of mixture mass with 1200 rpm engine speed
Burning of 10 - 90% of mixture mass with ignition at 20° BTDC
Burning of 10 - 90% of mixture mass with ignition at 26° BTDC
Burning of 10 - 90% of mixture mass with ignition at 32° BTDC
Burning of 10 - 90% of mixture mass with ignition at 20° BTDC
Burning of 10 - 90% of mixture mass with ignition at 26° BTDC
Burning of 10 - 90% of mixture mass with ignition at 32° BTDC
Burning of 10 - 90% of mixture mass at 1200 rpm
Burning of 10 - 90% of mixture mass at 1500 rpm
Burning of 10 - 90% of mixture mass at 1800 rpm
Burning of 10 - 90% of mixture mass at 2000 rpm
Contours of the 0 - 10% mass fraction burn period (°CA)
Contours of the 10 - 90% mass fraction burn period (°CA)
Combustion duration for 10% and 90% mixture burning: experiment and simulation
Combustion duration for 10% and 90% mixture burning: experiment and simulation
Combustion duration for 10% and 90% mixture burning: experiment and simulation
Effect of exhaust gas recirculation on cylinder pressure
Effect of exhaust gas recirculation on average cylinder temperature
5.42 Effect of exhaust gas recirculation on burned mass fraction 149
5.43 Effect of exhaust gas recirculation on mass burning rate 150
5.44 Effect of exhaust gas recirculation on combustion duration 150
5.45 The three piston geometries used for comparison 153
5.46 Three meshes of the piston geometries used for comparison 154
5.47 Comparison of the piston geometries using the FFM 155
5.48 Comparison of the piston geometries using the EBUM 155
5.49 Comparison of in-cylinder temperature distribution at −32° ATDC 157
5.50 Comparison of in-cylinder velocity distribution at −32° ATDC 158
5.51 Comparison of turbulent kinetic energy at −32° ATDC 159
5.52 Dissipation of turbulent kinetic energy at −32° ATDC 160
5.53 Comparison of in-cylinder temperature distribution at −18° ATDC 161
5.54 Comparison of in-cylinder velocity distribution at −18° ATDC 162
5.55 Comparison of turbulent kinetic energy at −18° ATDC 163
5.56 Dissipation of turbulent kinetic energy at −18° ATDC 164
5.57 Comparison of in-cylinder temperature distribution at −8° ATDC 165
5.58 Comparison of in-cylinder velocity distribution at −8° ATDC 166
5.59 Comparison of turbulent kinetic energy distribution at −8° ATDC 167
5.60 Dissipation of turbulent kinetic energy at −8° ATDC 168
5.61 Brunel piston: Effect of engine speed 170
5.62 SWRI piston: Effect of engine speed 171
5.63 New piston geometry: Effect of engine speed 171
5.64 Performance of the three pistons compared at 1200 rpm 172
5.65 Performance of the three pistons compared at 1500 rpm 172
5.66 Performance of the three pistons compared at 1800 rpm 173
5.67 Performance of the three pistons compared at 2000 rpm 173
5.68 Brunel piston: Effect of swirl 174
5.69 SWRI piston: Effect of swirl 174
5.70 New piston geometry: Effect of swirl 175
5.71 Performance of the three pistons compared at initial swirl ratio = 1 175
5.72 Performance of the three pistons compared at initial swirl ratio = 2 176
5.73 Performance of the three pistons compared at initial swirl ratio = 3 176
5.74 Predicted cylinder pressure compared (FFM, EBUM, SRM-New) 179
5.75 Comparison of predicted burned mass fraction 180
5.76 Average in-cylinder temperature with three combustion models 180
5.77 Average temperature contours at −10.5° BTDC, new SR model 182
5.78 In-cylinder velocity distribution at −10.5° BTDC, new SR model 182
5.79 Average temperature contours at −4.5° BTDC, new SR model 183
5.80 In-cylinder velocity distribution at −4.5° BTDC, new SR model 183
6.1 Effect of heat of reaction of NOx formation on cylinder pressure 188
6.2 Effect of heat of reaction of NOx formation on average temperature 188
6.3 Effect of heat of reaction of NOx formation on burned mass fraction 189
6.4 Effect of heat of reaction of NOx formation on NOx emission 189
6.5 Average in-cylinder temperature and formation of the three main pollutants at base line case with the FFM 192
6.6 Pollutant formation at base line case when the EBUM was used 193
6.7 Variation of HC, CO and NO concentration in the exhaust of a conventional spark ignition engine with fuel:air equivalence ratio 194
6.8 Comparison of variation of NOx emissions 201
6.9 Comparison of variation of CO2 emissions 201
6.10 Comparison of variation of CO emissions 201
6.11 Effect of relative air-fuel ratio (λ) on cylinder NOx formation 202
6.12 Effect of relative air-fuel ratio (λ) on CO2 202
6.13 Effect of relative air-fuel ratio (λ) on CO 203
6.14 Effect of fuel:air equivalence ratio (φ), on pollutant emissions in exhaust gasses from a natural gas engine 204
6.15 Effect of compression ratio on formation of NOx 208
6.16 Effect of compression ratio on formation of CO2 209
6.17 Effect of compression ratio on formation of CO 209
6.18 Effect of compression ratio on NOx emissions (Experimental) 210
6.19 Effect of engine speed on NOx emission, ignition at 20° BTDC 210
6.20 Effect of engine speed on NOx emission, ignition at 26° BTDC 211
6.21 Effect of engine speed on NOx emission, ignition at 32° BTDC 211

List of figures
6.22 Effect of engine speed on CO\textsubscript{2} emission, ignition at 20° BTDC  
6.23 Effect of engine speed on CO\textsubscript{2} emission, ignition at 26° BTDC  
6.24 Effect of engine speed on CO\textsubscript{2} emission, ignition at 32° BTDC  
6.25 Effect of engine speed on CO emission, ignition at 20° BTDC  
6.26 Effect of engine speed on CO emission, ignition at 26° BTDC  
6.27 Effect of engine speed on CO emission, ignition at 32° BTDC  
6.28 Effect of ignition timing on NO\textsubscript{x} emission, 1200 rpm  
6.29 Effect of ignition timing on NO\textsubscript{x} emission, 1500 rpm  
6.30 Effect of ignition timing on NO\textsubscript{x} emission, 1800 rpm  
6.31 Effect of ignition timing on NO\textsubscript{x} emission, 2000 rpm  
6.32 Effect of ignition timing on CO\textsubscript{2} emission, 1200 rpm  
6.33 Effect of ignition timing on CO\textsubscript{2} emission, 1500 rpm  
6.34 Effect of ignition timing on CO\textsubscript{2} emission, 1800 rpm  
6.35 Effect of ignition timing on CO\textsubscript{2} emission, 2000 rpm  
6.36 Effect of ignition timing on CO emission, 1200 rpm  
6.37 Effect of ignition timing on CO emission, 1500 rpm  
6.38 Effect of ignition timing on CO emission, 1800 rpm  
6.39 Effect of ignition timing on CO emission, 2000 rpm  
6.40 Effect of ignition timing on NO\textsubscript{x} emissions  
6.41 Effect of exhaust gas recirculation on NO\textsubscript{x} formation  
6.42 Effect of exhaust gas recirculation on break specific NO\textsubscript{x} emissions from a gasoline engine  
6.43 Pollutant formation at the baseline case with SRM-new  
6.44 Formation of NO\textsubscript{x} compared with three combustion models  
6.45 CO\textsubscript{2} formation compared with three combustion models  
6.46 Formation of CO compared with three combustion models
## Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Term</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>Molar concentration of specie</td>
<td>$\text{kgmol/m}^3$</td>
</tr>
<tr>
<td>D</td>
<td>Diffusion co-efficient</td>
<td>$\text{m}^2/\text{s}$</td>
</tr>
<tr>
<td>D</td>
<td>Fractal dimension</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>Mass diffusivity</td>
<td>$\text{m}^2/\text{s}$</td>
</tr>
<tr>
<td>$D_0$</td>
<td>Binary diffusion coefficient</td>
<td>$\text{m}^2/\text{s}$</td>
</tr>
<tr>
<td>E</td>
<td>Activation energy</td>
<td>$\text{kJ/kg}$</td>
</tr>
<tr>
<td>HHV</td>
<td>Higher heating value per mass of fuel</td>
<td>$\text{kJ/kg}$</td>
</tr>
<tr>
<td>I</td>
<td>Specific internal energy</td>
<td>$\text{kJ/kg}$</td>
</tr>
<tr>
<td>K</td>
<td>Thermal conductivity of the fluid</td>
<td>$\text{W/m-K}$</td>
</tr>
<tr>
<td>K</td>
<td>Karlovitz flame stretch rate</td>
<td>$\text{s}^{-1}$</td>
</tr>
<tr>
<td>L</td>
<td>Integral length scale of turbulence</td>
<td>$\text{m}$</td>
</tr>
<tr>
<td>W</td>
<td>Molecular mass</td>
<td>$\text{kg/kgmol}$</td>
</tr>
<tr>
<td>P</td>
<td>Probability density function</td>
<td></td>
</tr>
<tr>
<td>R</td>
<td>Universal gas constant</td>
<td>$\text{kJ/kg-K}$</td>
</tr>
<tr>
<td>S</td>
<td>Burning velocity</td>
<td>$\text{m/s}$</td>
</tr>
<tr>
<td>T</td>
<td>Temperature</td>
<td>$\text{K}$</td>
</tr>
<tr>
<td>Y</td>
<td>Mass fraction</td>
<td>$\text{m/s}$</td>
</tr>
<tr>
<td>a</td>
<td>Speed of sound</td>
<td>$\text{m/s}$</td>
</tr>
<tr>
<td>h</td>
<td>Specific enthalpy</td>
<td>$\text{kJ/kg}$</td>
</tr>
<tr>
<td>k</td>
<td>Turbulent kinetic energy</td>
<td>$\text{m}^2/\text{s}^2$</td>
</tr>
<tr>
<td>m</td>
<td>Mass</td>
<td>$\text{kg}$</td>
</tr>
<tr>
<td>p</td>
<td>Fluid pressure</td>
<td>$\text{N/m}^2$</td>
</tr>
<tr>
<td>q</td>
<td>Heat transfer rate</td>
<td>$\text{W}$</td>
</tr>
<tr>
<td>t</td>
<td>Time</td>
<td>$\text{s}$</td>
</tr>
<tr>
<td>$u$</td>
<td>Fluid velocity</td>
<td>$\text{m/s}$</td>
</tr>
<tr>
<td>$u'$</td>
<td>Turbulence intensity</td>
<td>$\text{m/s}$</td>
</tr>
</tbody>
</table>
Greek symbols

\( \Sigma \) Flame area per unit volume \( m^4 \)

\( \delta \) Laminar flame thickness \( m \)

\( \varepsilon \) Rate of dissipation of turbulent kinetic energy \( m^2/s^3 \)

\( \lambda \) Relative air:fuel ratio

\( \lambda \) Thermal conductivity \( W/m \cdot K \)

\( \eta \) Kolmogorov length scale \( m \)

\( \mu \) Absolute (dynamic) viscosity \( N \cdot s/m^2 \)

\( \rho \) Density \( kg/m^3 \)

\( \sigma \) Viscous stress tensor

\( \tau \) Characteristic time of combustion \( s \)

\( \nu \) Kinematic viscosity \( m^2/s \)

\( \phi \) Equivalence ratio

\( \omega \) Chemical reaction rate \( kgmol/m^3 \cdot s \)

\( \nabla \) Mathematical operator \( (i \frac{\partial}{\partial x} + j \frac{\partial}{\partial y} + k \frac{\partial}{\partial z}) \)

Subscripts and superscripts

F Fuel
L Laminar
O Oxidant
P Products of combustion
T Turbulent (subscript)
T Transpose (superscript)
b Burned
u Unburned
f Forward reaction
b Backward reaction
m species
### Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>ATDC</td>
<td>After top dead centre</td>
</tr>
<tr>
<td>BMF</td>
<td>Burned mass fraction</td>
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<tr>
<td>BTDC</td>
<td>Before top dead centre</td>
</tr>
<tr>
<td>°CA</td>
<td>Crank angle degrees</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational fluid dynamics</td>
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<tr>
<td>CFM</td>
<td>Coherent Flame sheet (flamelet) model</td>
</tr>
<tr>
<td>CI</td>
<td>Compression ignited</td>
</tr>
<tr>
<td>CN</td>
<td>Cetane number</td>
</tr>
<tr>
<td>CNG</td>
<td>Compressed natural gas</td>
</tr>
<tr>
<td>CR</td>
<td>Compression ratio</td>
</tr>
<tr>
<td>DISC</td>
<td>Direct injected stratified charged</td>
</tr>
<tr>
<td>DNS</td>
<td>Direct numerical simulation</td>
</tr>
<tr>
<td>EBUM</td>
<td>Eddy break up model</td>
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<tr>
<td>EDC</td>
<td>Eddy dissipation concept</td>
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<tr>
<td>EGR</td>
<td>Exhaust gas recirculation</td>
</tr>
<tr>
<td>EVC</td>
<td>Exhaust valve closing</td>
</tr>
<tr>
<td>EVO</td>
<td>Exhaust valve opening</td>
</tr>
<tr>
<td>FFM</td>
<td>Fractal flame model</td>
</tr>
<tr>
<td>HC</td>
<td>Hydrocarbons</td>
</tr>
<tr>
<td>HHV</td>
<td>Higher heating value</td>
</tr>
<tr>
<td>IC</td>
<td>Internal combustion</td>
</tr>
<tr>
<td>IVC</td>
<td>Intake valve closing</td>
</tr>
<tr>
<td>IVO</td>
<td>Intake valve opening</td>
</tr>
<tr>
<td>LDV</td>
<td>Laser doppler velocimetry</td>
</tr>
<tr>
<td>LNG</td>
<td>Liquified natural gas</td>
</tr>
<tr>
<td>MBT</td>
<td>Maximum break torque</td>
</tr>
<tr>
<td>MN</td>
<td>Methane number</td>
</tr>
<tr>
<td>MON</td>
<td>Motor octane number</td>
</tr>
<tr>
<td>NG</td>
<td>Natural gas</td>
</tr>
<tr>
<td>NGV</td>
<td>Natural gas vehicle</td>
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</table>
NMHC  Non-methane hydrocarbons
NOx  Nitric oxide, nitrous oxide and nitrogen dioxide
ODE  Ordinary differential equation
ON  Octane number
PDE  Partial differential equation
PDF  Probability density function
PGS  Pressure gradient scaling
PIV  Particle image velocimetry
QSOU  Quasi second order upwind
RNG  Renormalisation group theory
RON  Research octane number
SGS  Sub-grid scale
SI  Spark ignited
SIMPLE  Semi-implicit pressure linked equations
SOR  Successive over relaxation
SOx  Sulphur dioxide and sulphur trioxide
SRM  Single reaction model
SWRI  Southwest Research Institute
TDC  Top dead centre
UHC  Unburned hydrocarbons
WN  Wobbe number
rpm  Revolutions per minute

Indices and scales (See appendix-2 for details)

\[
Da = \frac{L / u'}{\delta / S_L} \quad \text{Damköhler number}
\]

\[
Ka = \frac{\delta / S_L}{(v / \varepsilon)^{1/2}} \quad \text{Karlovitz number}
\]
\[ \eta = \left( \frac{v_L^3}{u^3} \right)^{\frac{1}{4}} \]  
Kolmogorov length scale

\[ S_L = \left( \frac{\delta}{\eta} \right)^2 \]  
Laminar flame speed

\[ Le = \frac{\lambda}{D \rho c_p} \]  
Lewis number

\[ Pr = \frac{v \rho c_p}{\lambda} \]  
Prandtl number

\[ Re_T = \frac{u' / L}{\nu} \]  
Turbulent Reynolds number

\[ Sc = \frac{v}{D_0} \]  
Schmidt number

\[ WN = \frac{HHV}{\sqrt{\rho_f}} \]  
Wobbe number
Chapter 1.

Introduction

Internal combustion engines powered by gasoline or diesel fuels have been in use for more than a century as prime-movers for automobiles. The process of converting the fuel energy into useful work in the IC engine has been made increasingly efficient over the years through intensive research efforts. Although modern day automobile engines produce significantly lower levels of harmful pollutants as by-products of the energy conversion process than their counterparts manufactured a decade ago, ever increasing demands to further reduce or even eliminate such emissions have urged researchers to investigate the possibility of substituting cleaner burning fuels as alternatives for gasoline and diesel.

Natural Gas (NG) appears to be capable of performing a prominent role among alternative fuels for automobile engine applications. Compressed Natural Gas (CNG) offers a number of technical and economical advantages and the future of the NG engine looks promising. In fact, it costs less than other types of fuels and is very accessible in countries where there are existing distribution infrastructures. Among the attractive features of the NG engine are extremely low photochemical reactivity, elimination of cold enrichment which reduce cold start and low temperature emissions, high knock resistance and the comparability with fuel efficient lean-burn technology. The high octane number of natural gas allows a compression ratio higher than usual in spark ignited engines without risking engine knock thus improving the engine efficiency. Most importantly, it has been found that the use of CNG as a fuel
for IC engines with suitable modifications and improvements to the combustion chamber, fuel supply system and ignition system results in a reduction of emission of harmful pollutants from the engine.

The majority of the natural gas engine applications today are so far in stationary engine applications, such as co-generation plants. However, the technology to run road vehicles on natural gas is already well established. There are large fleets of NG vehicles, specially public transport systems using converted engines or dedicated engines, currently operating in many countries. Great progress has been made in developing the equipment necessary to operate existing vehicles on CNG. The cost of fuel supply is of importance and the price of CNG depends on the price of natural gas feedstock, transportation costs and the cost of compressing the gas. Cost estimates of natural gas compression depend on the type of refuelling technologies adopted, for example, fast filling vs. slow filling and public refuelling stations vs. home filling. CNG vehicles can have a higher fuel economy than gasoline vehicles due to the high octane number of CNG and the potential of using a lean burn strategy in CNG engines. It has been indicated by research studies that a potential fuel economy improvement as high as 30% for CNG vehicles, mainly from the use of a lean burn strategy. Without using lean burn strategies, the fuel economy improvement by CNG vehicles is limited. A significant number of research studies are being carried out around the world to develop a natural gas engine, which is efficient, powerful and in the same time pollutant emission levels are well within the accepted limits, for automobile engines. The day when light duty vehicles with natural gas fuelled engines outnumber traditional gasoline and diesel vehicles can not be far away.

The multi-faceted problem of using NG as a transportation fuel needs to address many aspects such as technical, economical, environmental and political. Most of the modern day NG engines used for automobiles (specially light duty vehicles) are bi-fuel engines or engines converted mainly from diesel engines by replacing the fuel injector with a spark plug and adding a gaseous fuel metering device. These engines are not optimised for the use of this gaseous fuel and therefore can not provide all the possible benefits of using natural gas as an engine fuel and the levels of emission of pollutants may need further controlling. To achieve all the benefits one can expect from using CNG in IC engine applications, one of the major requirements is the development of engines optimised to run solely on natural gas.
1.1. SI Engine performance

The thermal efficiency of the "Otto" engine cycle increases with increasing compression ratio but the compression ratio of SI engines is limited by abnormal combustion. Increasing the compression ratio increases the temperature and pressure of the unburned charge. During combustion, the unburned portion (end gas) is further compressed by the expansion of the burned products and may undergo rapid reactions causing rapid auto-ignition (knocking combustion) of the unburned volume. Engine knock causes reduced efficiency, increased heat transfer and, if severe, engine damage. The limiting compression ratio is directly related to the fuel octane number. However, there are means of controlling engine knock. Reducing the time available for the end gas reaction can be achieved by increasing the engine speed and/or by employing a suitable combustion chamber geometry and location of spark(s). Improving the combustion rate would facilitate engulfing the end gases by the flame front before the knock phenomenon initiate.

Flame speed is almost proportional to engine speed because the in-cylinder turbulence, which affects the flame speed, varies proportionally with the varying engine speed. The combustion rate does not necessarily follow the engine speed, however, because the initial period of flame growth tends to be independent of the engine speed. The burning rate for a given engine design and engine speed is primarily a function of the mixture air:fuel ratio. Although the engine mechanism repeats precisely each cycle, combustion does not. In particular, the initial flame growth period for very weak mixtures can vary considerably. Cycle-by-cycle variations in the growth rate and location of the flame kernel immediately after ignition, which are influenced by the ignition characteristics and mixture motion, represent the major causes of combustion variations in SI engines. The origin of cyclic variations in combustion is believed to be close to the ignition site where the influence of the ignition system on flame initiation is more important. The physical properties of the mixture and the local flow field (both the bulk flow and small scale turbulence) at the spark plug affect the initial flame kernel and subsequent flame development. Spark effects such as duration and shape influence the early period of combustion. Differences in flow patterns and turbulence are thought to be major contributing factors to the cyclic variations in burning rate. Residual mixing, inlet pressure
fluctuations and inhomogeneity of charge can also contribute but appear to be less important. Cyclic variability increases with decreasing load due to the increased residual gas fraction. Lean burn engines are of great interest among today's engine researchers and a major challenge imposed on them is the cyclic variation of engine performance. That is because the lean burn technology is highly associated with combustion instability resulting from reduced flame initiation and propagation rates. The practical approach to improving engine stability under lean mixture conditions is to secure the ignition and to shorten combustion duration through the optimal combination of advanced ignition systems with enhanced flow characteristics of the mixture.

Improving in-cylinder combustion has been of interest for many years of research. Improving the in-cylinder fluid dynamics as a way of enhancing combustion has been a result of these studies. Turbulence intensity of the bulk gas governs the flame travel while the turbulence near the chamber surface influences heat transfer losses and thermal efficiency. Increased tumble intensity and enhanced turbulence during combustion reduce the duration of burning. Small scale turbulence generated during intake does not survive the compression process but the larger scale motions, which are affected by the compression process and the chamber geometry, generate the turbulence important at the start of combustion. Thus, a large tumbling vortex may be generated during intake, spin up to a high rotational speed as it is compressed (conservation of angular momentum) and thus provide a growth in turbulence generation by shear. Because the turbulence generated in this way is not uniformly distributed, the flame moving through the compressed mixture may encounter large changes in turbulent intensity. Tumble motions give a high intensity of turbulence near TDC but they are quickly dissipated and do not provide a continuing source of turbulence. Swirling flows are more stable and thus provide a continuing source of turbulence. This makes an engine design, which incorporates controlled swirl and tumble desirable. The flame motion and product expansion also affect the turbulence during combustion and this makes it a very complex process.

Sleeves introduced into the intake ports deflect the inducted air over the intake valves, producing a tumbling vortex in the cylinder which is stronger than that generated by non-sleeved ports. This increased tumble strength further increases the turbulence intensity late in the compression stroke and increases the mean flow...
velocity near the spark plug at the time of spark discharge thus achieving convection of the flame away from the spark plug during flame development and faster flame propagation during the main combustion period. The rate of growth of flame is higher with sleeved ports than with non-sleeved ports. However, any modifications to the intake ports to manipulate the intake flow have the effect of reducing the volumetric efficiency of the engine, especially at high loads. Generally, two approaches are used to create swirl during the induction process. In one, the flow is discharged into the cylinder tangentially toward the cylinder wall, where it is deflected sideways and downward in a swirling motion. In the other, the swirl is largely generated within the inlet port. The flow is forced to rotate about the valve axis before it enters the cylinder. Flow rotation about the cylinder axis can also be generated by masking off or shrouding part of the peripheral inlet valve open area but this method is uncommon in commercial vehicles.

1.2. Emissions from SI engines

It was only about a century ago that the first workable four-stroke IC engine was invented in Germany by Nikolas Otto. Shortly afterwards Karl Benz and Gottlieb Daimler produced the world's first cars with IC engines. By the beginning of the 20th century, various practical car designs were appearing. Almost all of these vehicles were operated by burning fossil fuel oils. World consumption of oil fuel by road transport has been increasing since then. Globally, emissions of pollutants from vehicles have increased with growing energy consumption and the problem of air pollution by exhaust emissions has given rise to much world-wide concern, both in the fields of research and development and also in legislation.

Exhaust gases are the major source of pollutants while crank case blow-by and fuel tank/carburettor evaporation contribute to hydrocarbon emissions. If combustion and oxidation were complete in the engine, water and CO₂ would be the only products of combustion of fuel. Complete combustion in engines is impractical and CO is formed in considerable quantities. The toxic properties of CO are due to its ability to react with haemoglobin in the blood to produce carboxy-haemoglobin. Carbon monoxide has a greater affinity for haemoglobin than oxygen and is preferentially absorbed even when present in small concentrations. The degree of
absorption depends on the concentration of CO in the air, the period of exposure and the activity of the individual. Conditions in the combustion chamber favour the oxidation of nitrogen in the air so oxides of nitrogen (NO₄) are also formed. NO₂ being much more toxic than NO, can contribute to increased susceptibility to respiratory infections, increased airway resistance in asthmatics and decreased pulmonary function. Where there are high emissions of hydrocarbons and NOₓ together with long periods of sunshine, the formation of photochemical oxidants ("Photochemical smog") can occur, ozone being the strongest and highly toxic oxidant so formed. This situation can cause eye irritation, coughs, chest discomfort, headaches, respiratory illness, increased asthma attacks and reduced pulmonary function. Lead, sulphur dioxide, smoke and soot and hydrocarbons are other emissions of concern.

The delicate balance of global mean temperature by the greenhouse effect can be affected if the quantities of the gases that trap the long wave radiation within the atmosphere change significantly. There has been a substantial effect due to CO₂, with smaller contributions from O₃, NOₓ and CH₄. These are highly relevant to engine exhaust emissions. It is estimated that increased concentrations of these gases since the mid 19th century has raised the global mean temperature by about 0.5°C and the projected concentrations, unless action is taken to reduce them, could produce a further warming of about 1.5°C by year 2030. Emissions of CO may also be important for climatic modifications as increases in CO can increase the concentration of other greenhouse gases such as O₃, NOₓ and CH₄ by reacting with highly reactive hydroxyl radicals (OH). CO₂ is a product of 'good' combustion and is produced in direct proportion to the amount of fuel burned. Steps to minimise products of poor combustion must naturally tend to increase its emission. Reduction of CO₂ emission can only be achieved by reducing the amount of fossil fuel burned and this matter is of international concern now. Burning low carbon fuels such as CH₄ in place of traditional engine fuels can provide a significant contribution to the efforts of reducing CO₂ emissions as well as using lean burning engines.

The two main factors governing the formation of pollutants within SI engines are the composition of the air-fuel mixture and the timing of its ignition. If there is too little oxygen, combustion is incomplete and high levels of CO and hydrocarbons are emitted. These are much reduced at higher air:fuel ratios when there
is sufficient oxygen available for complete combustion. However, as the combustion becomes more efficient, the combustion temperature increases, resulting in increased formation of oxides of nitrogen. Increasing the level of excess air further reduces the in-cylinder temperature and the production of oxides of nitrogen falls. At very high or very low air:fuel ratios, hydrocarbon emissions increase due to the increased tendency for either total misfire or partial burning under the more adverse conditions for combustion. The ignition timing influences the formation of oxides of nitrogen and hydrocarbons by varying the cylinder temperature profiles. Retarded ignition results in lower peak temperatures and higher exhaust temperatures than advanced timing thus reducing the formation of NO\textsubscript{x} and the emission of hydrocarbons.

The optimisation of the processes of air-fuel metering, mixing and ignition is an important step in the production of low emission engines. The rapid development of engine related electronics and the microprocessor industry has made significant improvements possible. The conventional combination of carburettor and distributive ignition system can now be replaced by fuel injection and electronic ignition equipment of varying complexity to provide much more precise control of these important functions. In addition to many other functions, a microprocessor controls the engine’s fuel and ignition systems in accordance with the operation of the vehicle and a stored engine map. This map specifies optimum conditions for the full range of engine speeds and load settings.

Advances have also been made in the design of engines. The size, number and geometry of the valves, the configurations of cylinder head and piston, inlet manifold design and the location of spark plug(s) are of great importance in determining the efficiency of the air-fuel mixing and combustion. Optimising an engine is the process of choosing the best possible combination of all these aspects. The design and materials used for the cylinder head determine its thermal properties. An aluminium engine, for example, generally operates at lower combustion temperatures and produces less oxides of nitrogen whereas an engine with a ceramic coating losses less heat and operates at higher temperatures and may result in more NO\textsubscript{x}.

Exhaust gas recirculation is another common means of reducing the formation of NO\textsubscript{x}. The addition of a proportion of inert exhaust gas to the air-fuel mixture reduces the peak cylinder temperature. Hydrocarbons and CO in exhaust can
be oxidised by mixing the hot gases with additional air as they leave the engine. Catalytic converters have been in use for many years to control exhaust emissions. Three-way catalysts can oxidise CO and hydrocarbons and at the same time reduce oxides of nitrogen. Careful control of the air: fuel ratio is essential as the range of this ratio for the efficient operation of the three-way catalyst is very narrow and concentrates around the stoichiometry. This range of air:fuel ratio is narrower for CNG than that for gasoline and needs a higher degree of control if a three-way catalyst is to be used in association with a natural gas engine.

Lean burn engine technology is a fuel independent method of decreasing emissions. Lean burn engines have the advantage of reduced levels of CO and NO\textsubscript{x} but the disadvantages are the engine misfire due to operation close to lean limit of combustion and operating close to the lower limit of drivability. These drawbacks place great demands on the fuel and ignition control systems and on the design of the combustion chambers and inlet valves. These engines may be fitted with oxidation catalysts to control CO and HC emissions but because of the oxidising composition of the exhaust, catalytic reduction of NO\textsubscript{x} becomes impossible. For this reason, further developments are needed before lean burn engines can fully meet the increasingly stringent emission standards.

Lean burn natural gas engines tend to be quite sensitive to intake air humidity levels. This can impose a significant problem on controlling the engine performance and pollutant emissions, especially when combined with fuel composition variations. Increased humidity decreases dry air availability and thus reduces oxygen concentration, which in turn deprives engine performance. Similar effects can be seen when intake air pressure decreases (e.g. at high altitudes) and air temperature increases (e.g. hot climates).

The stratified charged engine is a type of lean burn engine in which the air-fuel charge is not uniformly mixed before ignition. This approach overcomes the combustion and drivability problems associated with fully lean mixture operation by ensuring that the air:fuel ratio is relatively low at the start of combustion and progressively gets higher as the stroke proceeds, and so still provides the benefits of lower fuel consumption and emissions of CO and NO\textsubscript{x}. The two main types of stratified charge engines are the open chamber type and the pre-chamber type. With the open chamber type stratified charge engine, the mixture composition is controlled
by the design of the combustion chamber and fuelling systems to provide a relatively rich mixture (near to stoichiometric) at the spark plug location that becomes progressively weaker as combustion proceeds. In pre-chamber engines, a stoichiometric air-fuel mixture is ignited in a small auxiliary combustion chamber introducing a jet of burning gases, which ignites the much weaker mixture in the main chamber, giving a much higher rate of burning than could take place by an ordinary spark igniting the lean mixture.

1.3. Numerical modelling of IC engines and CFD

The development of new engines, among the other things, involves the design of new combustion chambers including the valves and the location of spark plug(s) and consideration of improved in-cylinder fluid dynamics for improved performance and minimised levels of emissions. Obviously, this is a very complex process and demands a lot of resources. The in-cylinder contents of advanced internal combustion engines involve a number of complex, closely coupled physical and chemical processes such as transient, three dimensional turbulent mixing of multi-component gases, combustion and heat transfer. Details of turbulent fluid motion in engines are required for the determination of combustion rates, thermal efficiency, levels of emissions. This knowledge has traditionally been acquired by means of time consuming and expensive experiments on a specific engine design, which do not lead to similarity laws for predicting the characteristics of a different engine design. Traditional experimental methods used for this purpose can become extremely resource consuming if several engine designs are to be tested at various operating conditions. Numerical simulations of engines dramatically ease this problem by making the exploration of new aspects of engine design more economical and convenient. Studies of this nature can provide the essential understanding of operational trends resulting from change of engine’s operating and geometrical parameters thus paving the way towards designing dedicated engines optimised for natural gas. Due to the advent of computational tools and the fast growth in the capabilities of modern computing, the field of computer simulation of reciprocating engines is now developing rapidly, being invaluable for the development of cleaner,
quieter and more efficient engines for a variety of applications and fuels. The aims of these theoretical and computational developments have been

(i) to develop reliable engineering tools for predicting the fields of flow, temperature etc., within the engine
(ii) to reduce the cost of current experimental, trial and error methodologies used for the development of the relevant designs
(iii) to allow for a better understanding of the physio-chemical processes involved so that more efficient and safer equipment can be designed
(iv) to provide a platform for the convenient development and testing of new ideas.

Computational Fluid Dynamics (CFD) can be regarded as a sub-field combining both fluid dynamics and numerical analysis and has been increasingly accepted as an adjunct to experimentation in the understanding and the design of practical combustion systems. Typical of such work are those by Ahmedi-Berfui et al. (1981), Gosman et al. (1985) and Boudier et al. (1993). CFD studies are proving useful in analysing problems characterised by the need for detailed spatial information and the complex interaction of many phenomena such as turbulence, chemical reaction, heat transfer that occur simultaneously in an engine environment. However, it is impossible to resolve all the flow scales in these models. The instantaneous flow variables, when used in governing equations, are treated as the sum of the mean flow and the fluctuating quantities. The CFD models developed to analyse engine combustion use turbulence models that were developed for stationary, incompressible, thin shear flows. These models may not be valid for predicting unsteady, compressible, re-circulating flows. Also predictions from these models may not be easily compared with experimental results obtained from velocimetry (LDV, PIV) techniques and cycle resolved measurements due to cycle to cycle variations.

CFD models for IC engines have reached high levels of sophistication in spite of insufficient knowledge available of the boundary conditions at the inlet and exhaust valves or ports, the lack of accurate turbulence models and combustion models and the use of many simplifying assumptions. Due to ever increasing computational power, CFD models can provide a greater insight into gross flow and combustion processes in the engine, which was not possible before. Earlier studies
using multi-dimensional models (Diwakar 1984, Henriot 1989) suggested that the need for experimental work could not be completely eliminated. However, these models can be successfully used in the design and optimisation of certain engine parameters thus saving a significant amount of resources otherwise needed in experimentation.

The continuous improvements in computing power and knowledge in CFD techniques have resulted in a number of advanced commercial CFD codes. In most of the cases, the user has limited access to the source code and the possibility of modifying an existing mathematical model within these codes is seriously limited. However, there are some public domain, well developed CFD codes available and the advanced user can modify the source code by adding, removing or altering existing mathematical models. The CFD code, KIVA-II, which was used in this study, falls into this category.

Many flows of practical interest are difficult to describe mathematically, let alone solve exactly. These flows include complex processes such as turbulence, combustion, heat transfer and multiphase flow. Therefore mathematical models are used to describe these phenomena, using various approximations and simplifications, which in turn affect the degree of accuracy of solutions of these mathematical studies of the flow.

Much of the accuracy of numerical solutions is dependent on the quality of discretisation method (i.e. the method of approximating the differential equations, which describe the flow, by a system of algebraic equations for the variables at discrete locations in space and time) used. If the unsteady, three dimensional Navier-Stokes equations of the in-cylinder flow can be solved correctly (as in direct numerical simulation of turbulence), it is possible to obtain a complete set of data from which any quantity of physical significance can be derived. However, the accurate solution of the Navier-Stokes equations for most complex flows of engineering interest is extremely difficult and the numerical results are always approximate. This is mainly because of the simplifications that may contain in the differential equations used, the approximations used during the discretisation process and the use of iterative methods in solving those discretised equations. Discretisation errors can be minimised by using more accurate interpolation or approximations or by applying these approximations to smaller regions with the use of fine numerical grids.
These increase the computational time and the cost of obtaining a solution and hence a compromise is needed.

When the governing equations of the flow, which is of interest are known accurately, (e.g. the Navier-Stokes equations for incompressible Newtonian flow), solution of any desired accuracy can be obtained in principle. However, for many phenomena, the exact equations are either not available or numerical solution is not feasible. This is where the use of mathematical models becomes necessary. The levels of simplifications and approximations made in these models may depend on the available resources and these models need to be validated before accepting the results produced by them as representative of the real flow problem.

There are many approaches to discretisation of differential equations in CFD but the most widely used methods are the finite volume method (FVM), the finite difference method (FDM) and the finite element method (FEM). Other methods such as boundary element method (BEM) are used in CFD for special classes of problems. Theoretically, each method should yield the same solution if the numerical grid over which the discretisation is made is very fine. However, one method may prove to be more suitable than the others for a particular class of problems.

The FVM uses the integral form of the conservation equations as its starting point. The solution domain is sub-divided into a finite number of contiguous control volumes and the conservation equations are applied to each control volume. The surface integrals, which represent convective and diffusive fluxes and the volume integrals are approximated using suitable formulae. Variables are averaged over a numerical cell and the cell centroid stores these values. In order to obtain the variable values at control volume surfaces, these nodal values can be interpolated. The FVM can accommodate any type of numerical grid and hence suitable for flows involving complex geometries. Also, the FVM is simple to understand and program. However, it is comparatively difficult to develop solution methods of orders higher than second in three dimensional problems. This is due to the fact that the FVM needs two levels of approximation, namely integration and interpolation. The CFD code KIVA-II is based on the FVM.

The FDM is the oldest method of solving PDE's numerically and also the easiest method for flows involving simple geometries. The conservation equations in differential form are the starting point. Taylor series expansion or polynomial
fitting is used to obtain approximations to the first and second derivatives of the variables with respect to the co-ordinates. Although, in principle, the FDM can be applied to any type of numerical grid, on structured grids, the FDM becomes very simple and effective. It is especially easy to obtain higher order solution schemes on regular grids. The FEM is similar to the FVM in many ways. The solution domain consists of finite elements (a set of discrete volumes) which are usually unstructured. The flow equations are weighted by multiplying by a weighting function, before being integrated over the entire domain. An important advantage of the FEM is the ability to deal with arbitrary geometries and grids can easily be refined according to the needs. The finite element methods are relatively easy to analyse mathematically but the matrices of the linearised equations are not as well structured as those for regular grids making it more difficult to find efficient solution methods.

1.4. Engine combustion modelling

Modelling the very complex, interacting physical and chemical processes such as combustion, turbulence, work and heat transfer within the combustion chamber of an engine is not very easy due to several clear reasons.

(i) The system is an open one, operating at relatively high temperatures and pressures, which retains a memory of the previous cycle. This memory arises because the cylinder is not completely evacuated at the end of each cycle and because the end of one cycle provides initial conditions for the following cycle.
(ii) The operation has a repetition rate ranging from approximately 25 to 250 ms.
(iii) Some very complex chemistry (e.g. hydrocarbon combustion, NOx formation) is taking place and the time scale for some of the chemical reactions is comparable to the cycle repetition rate.
(iv) The system has movable boundaries and a complex geometry, which seriously complicate the fluid mechanics and heat transfer.
(v) The engine operation is not strictly repeatable because the engine undergoes random cycle-to-cycle variations.
The presence of turbulence and its interaction with combustion add further to the complexity of the process. The intake and the exhaust portions of the cycle generate highly turbulent flows within the cylinder and the ignition-combustion process is influenced by the level of turbulence. Heat transfer at the walls must be accounted for because heat losses represent approximately a third of the energy liberated by combustion. These losses strongly affect the temperature of the working fluid, which in turn has a strong effect on the rate determining processes taking place in the working fluid. Serious attempts to construct models of the internal combustion engine began about 1960, when digital computers were becoming increasingly available and capable of large calculations.

1.5. Objective of the present study

The main objective of this research work is to numerically study the effects of various engine operating parameters on the performance and the pollutant formation of a natural gas fuelled, spark ignited engine and understand the engine fluid dynamics and combustion characteristics. This objective is achieved through several intermediate stages. The first part of this work is a review of the numerical models available for premixed SI engine combustion in Computational Fluid Dynamics (CFD) applications. Selecting and improving a suitable model from these for the present study and incorporating it into a multi-dimensional CFD code in order to perform a numerical parametric study on natural gas fuelled SI engines will be the next stage. The combustion model chosen and improved will be validated against available experimental data and once this objective is achieved, the effects of equivalence ratio, spark timing, compression ratio, engine speed, exhaust gas recirculation and combustion chamber geometry on engine performance and the formation of pollutants will be numerically studied. The kinetic mechanisms for nitric oxide formation will also be studied to understand the influence of temperature and species concentrations on the rates of formation of nitric oxide. It is envisaged that the studies of this nature will be of great importance in developing new engines at reduced consumption of resources. The public domain, industrial CFD code KIVA-II will be modified and addition of new sub models will be made in order to facilitate achieving the above mentioned goals.
The outcome of this study will be an improved multi-dimensional combustion model, which can sufficiently accurately represent premixed, natural gas engine combustion in the flamelet regime. In addition, the comparison of numerical simulations with experimental data will indicate the validity of the flamelet assumption for combustion in SI engines. The results of the parametric study will provide a suitable basis for understanding the very complex nature of dedicated natural gas engine performance. These are envisaged to be of practical importance in the process of developing dedicated engines and optimising them for this alternative fuel.

1.6. Outline of the thesis

The rest of this thesis consists of six chapters. The whole work presented here deals with three distinct areas. They are

(i) computational fluid dynamics and engine combustion modelling
(ii) natural gas as an alternative fuel and performance of natural gas engines
(iii) pollutant formation from engines.

The literature review, therefore, will be divided accordingly and presented in relevant chapters. This approach is expected to enhance the smooth flow of the thesis contents and to relate various aspects of the present work to those found in the literature in a clear and concise manner.

Chapter 2 describes the use of Computational Fluid Dynamics in automotive industry with the emphasis given to engine modelling. A brief description of the CFD code KIVA-II with the governing equations solved and the solution method will also be given there. Modifications and additions made to this code within the framework of this study will also be described.

Chapter 3 is dedicated to a review of CFD modelling of SI engine combustion in detail. Various mathematical models commonly used for multi-dimensional CFD simulations of premixed combustion in spark ignition engines will be discussed. A choice of a model will be made from these after analysing the strengths, inherent problems and weaknesses of these models, in order to meet the objectives of the present study. As many variations of these models have been
introduced over the time, it is impossible to analyse all such models available for SI engine combustion in CFD. However, care has been taken to study the most common and recent versions of the models.

In chapter 4, the chosen combustion model and its development will be described in detail with the improvements to this model suggested during the context of the present study. The improved combustion model will be validated against suitable experimental data before performing the proposed parametric study.

There will be a review of the literature on using natural gas as an alternative fuel for automotive engines and natural gas engines in general, in chapter 5. In the same chapter, a description of the conducted parametric study of natural gas engine performance and the computational results from this study will be presented. The trends of engine performance obtained with varying several engine operational variables will be compared with some experimental trends found in the literature.

Pollutant formation and emission of these pollutants from natural gas engines will be discussed in chapter 6. The computational results of a numerical parametric study on such emissions will also be presented there. The trends of variations obtained will be compared with those available in the literature.

Chapter 7 will summarise the present research study and highlight the conclusions drawn from the work. Suggestions for further research based on the current work will also be made there.
Chapter 2.

The CFD code KIVA-II with modifications and additions

There are many aspects of automobile operation where fluid flow plays a major role. In the past, design and analysis of the components participating in such fluid flow situations were done using suitably performed experiments alone. As the capabilities and the range of applications of computational fluid dynamics got wider, many of these experiments were partially or fully replaced by CFD for improved flexibility and convenience in designing, analysis and improvement of these components. It is not only the components that handle fluid flows, but also the fluid flow within them has become the subject for analysis using CFD. This analytical tool, provides new avenues for understanding what exactly happens in those numerous fluid flow situations found in automotive applications. Uses of CFD in automotive industry include car ventilation, engine combustion and related flow, external aerodynamics, air flow through radiators, coolant flow through the engine block, catalytic converters, windscreen defrosting, turbo-charging etc.,. The development of CFD methods coupled with the recent advances in computer technology has allowed the development of very sophisticated software (in the form of packages or source codes) intended for this specific use. Most of the commercial software available today are capable of meeting of the requirements of fluid dynamic analysis in the automotive industry to sufficient levels. When coupled with advanced solid/surface modelling, mesh generating and visual analysis software, these commercial CFD
packages and many other CFD codes provide extreme flexibility and can be applied to a wide range of problems. KIVA-II is such a code that has been developed over many years and extensively used by researchers and engine developers around the world for studying engine related flow and other events such as combustion, heat transfer and pollutant formation.

2.1. The CFD code

KIVA-II was developed at the Los Alamos national Laboratories, USA and is the second release in the series of KIVA multi-dimensional codes written in FORTRAN 77. It is specifically aimed at engine based studies and applicable to a wide variety of multi-dimensional problems in fluid dynamics with or without chemical reactions or sprays. Cold flow analysis in complicated geometries, continuous spray combustors, reactive jets, non-reacting sprays, fires and Bunsen burner flames are some examples where KIVA-II can be used. Codes in the KIVA family have the ability to calculate very complex flows in engine cylinders with arbitrarily shaped piston geometries, including the effects of turbulence and wall heat transfer. It solves three dimensional, unsteady equations of motion of turbulent, chemically reactive mixtures of ideal gases (Amsden et al. 1989).

This computer program is controlled by a short main program and consists of a number of subroutines to perform various numerical calculations associated with specific processes such as the generation of the computational grid, the calculation of the mesh and cell variables, the injection and evaporation of fuel droplets, the use of kinetic chemistry and chemical equilibrium. Unlike many commercial CFD codes, KIVA-II is not a ‘black box’ production code. Instead, KIVA-II is an advanced experimental computer program and its use requires a reasonable knowledge of and experience with computational fluid dynamics, modelling of combustion chemistry and other relevant engine processes.

The modular structure of the program makes it possible to incorporate new and improved subroutines to define a physical process in more detail. The user can easily discard some subroutines if these are not required for a particular application thus improving the computational speed of the code. The existing subroutines can also be modified to suit the user’s requirements, most of the time,
without much difficulty. There are some other facilities such as the dump and restart options which make the KIVA-II computer program attractive so that one can stop the program at any time during execution for the analysis of results and if required, it can be restarted from the same point without loosing accuracy. Data can also be dumped for post processing using an existing facility in the program. A feature of engine modelling calculations with KIVA-II is the use of an expanding and contracting grid. The piston crown and cylinder head are represented using a fixed portion of the grid thus geometrical features do not change and the grid within the cylinder can be compressed to follow the piston motion.

2.2. Governing Equations

The physical laws governing the fluid flow, chemically reactive processes and heat transfer in an engine cycle when expressed in mathematical form, give the governing equations. These include the equation of state, the equations for the conservation of mass, momentum and energy for unsteady chemically reactive flows and equations describing turbulent flow characteristics including generation and destruction of turbulence within the flow. Each of these equations has a certain physical quantity as its dependent variable. The flow field is generally specified by the velocity vector \( \mathbf{u} \) with the three orthogonal components \( u, v, w \), pressure \( p \), density \( \rho \), and temperature \( T \), all of which are functions of the spatial co-ordinates \( x, y, z \) and time \( t \).

2.2.1. Equation of state for ideal gases

The ideal gas equation of state is given by

\[
p = R_0 T \sum_m \left( \frac{\rho_m}{W_m} \right)
\]  

(2.1)

where \( p \) is pressure, \( R_0 \) is universal gas constant, \( T \) is temperature, \( \rho_m \) is the mass density and \( W_m \) is the molecular weight of species \( m \).
2.2.2. Conservation of mass

For the species $m$, the conservation of mass can be written as

$$
\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \mathbf{u}) = \nabla \left[ \rho D \nabla \left( \frac{\rho_m}{\rho} \right) \right] + \rho_c^m
$$

(2.2)

where $\rho_c^m$ is the source term due to chemical reactions. If there is a fuel spray, an extra source term is added to this equation. Here, $\rho$ is the fluid density and $D$ is the diffusion coefficient.

2.2.3. Conservation of momentum

The momentum equation for the fluid is given by

$$
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u \mathbf{u}) = -\frac{1}{\alpha^2} \nabla \cdot p + A_0 \nabla \cdot \left( \frac{2}{3} \rho k \right) + \nabla \cdot \sigma + \rho g
$$

(2.3)

The dimensionless quantity $\alpha$ is used in conjunction with the pressure gradient scaling (PGS) method which is used in KIVA-II. The quantity, $A_0$ is zero in laminar flow calculations and unity when a turbulence model is used. $\sigma$ is the viscous stress tensor.

2.2.4. Conservation of energy

The energy equation is given by

$$
\frac{\partial (\rho l)}{\partial t} + \nabla \cdot (\rho l \mathbf{u}) = -\rho \nabla \cdot \mathbf{u} + (1-A_0) \sigma \nabla \cdot \mathbf{u} - \nabla \cdot \mathbf{J} + A_0 \rho \epsilon + \dot{Q}_c
$$

(2.4)

where $\dot{Q}_c$ is the source term due to chemical heat release, $l$ is the specific internal energy of the fluid exclusive of chemical energy, $A_0$ is zero in laminar flow
calculations and unity when a turbulence model is used and $J$ is the enthalpy diffusion flux which is given by

$$J = -K \nabla T + \rho D \sum_m h_m \nabla \left( \frac{\rho_m}{\rho} \right)$$  \hspace{1cm} (2.5)

where $h_m$ is the specific enthalpy of species $m$ at a given absolute temperature, $T$ of the fluid and $K$ is the thermal conductivity of the fluid. Further source terms are added if there is a fuel spray.

2.2.5. Turbulence

Two models are available in the KIVA-II code to represent the effects of turbulence. The commonly used model is the standard $k-\varepsilon$ turbulence model (Launder et al. 1972) modified to include volumetric expansion effects (Reynolds, 1981). If there is fuel injection, further source terms are added to represent the flow interaction with the spray. Alternatively, a modified version of the sub-grid scale (SGS) turbulence model (Amsden, 1985) is available. KIVA-II does not model the effects of turbulence on the mean reaction rates but the user can modify the code to include a chemistry model in which these effects are catered for.

In the two equation standard $k-\varepsilon$ turbulence model both the velocity and the length scales follow from the transport equations for $k$ and a length scale related parameter, $k^{3/2}l$. There are, however, some terms included in the equations to account for length scale changes due to velocity dilatation. The equations for the transport of turbulent kinetic energy, $k$, and the turbulent dissipation rate, $\varepsilon$, are given by eqns. (2.6) and (2.7). The source term, $(c_{\varepsilon_3} - \frac{2}{3} c_{\varepsilon_1}) \nabla \cdot u$ in the $\varepsilon$ - equation [eqn. (2.7)] accounts for length scale changes when there is velocity dilatation. Table (2.1) provides the standard values often used in engine calculations for the model constants (Amsden, 1989).

$$\frac{\partial (\rho k)}{\partial t} + \nabla \cdot (\rho u k) = -\frac{2}{3} \rho k \nabla \cdot u + \rho \nabla \cdot u + \nabla \left[ \left( \frac{\mu}{P_r k} \right) \nabla k \right] - \rho \varepsilon$$ \hspace{1cm} (2.6)
\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \nabla \cdot (\rho u \varepsilon) = -\left(\frac{2}{3} \varepsilon_1 - \varepsilon_3 \right) \rho \varepsilon \nabla u + \nabla \left[ \left( \frac{\mu}{\Pr_e} \right) \nabla \varepsilon \right] + \frac{\varepsilon}{k} \left[ \varepsilon_1 \sigma \nabla u - \varepsilon_2 \rho \varepsilon \right]
\] (2.7)

In the SGS model the turbulent dissipation rate, \( \varepsilon \) is constrained to satisfy the inequality condition

\[
\varepsilon \geq \left[ \frac{C_\mu}{\Pr_e (c_{\varepsilon_2} - c_{\varepsilon_1})} \right]^{\frac{1}{2}} k^{\frac{3}{2}} L_{SGS}
\] (2.8)

where \( C_\mu = 0.09 \) is a constant and \( L_{SGS} \) is an input SGS length scale with the typical value assigned for it is four times the cell dimension. Eqn. (2.8) is a constraint that the turbulent length scale to be less than or equal \( L_{SGS} \) as \( k^{3/2} \varepsilon \) is proportional to the \( k-\varepsilon \) length scale. The SGS turbulence model reduces to the \( k-\varepsilon \) model near the walls where all turbulence length scales are too small to be resolved by the computational mesh.

Table (2.1). Two equation standard \( k-\varepsilon \) turbulence model constants and the standard values used for engine calculations

<table>
<thead>
<tr>
<th>( c_{\varepsilon_1} )</th>
<th>( c_{\varepsilon_2} )</th>
<th>( c_{\varepsilon_3} )</th>
<th>( Pr_k )</th>
<th>( Pr_\varepsilon )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.44</td>
<td>1.92</td>
<td>-1.0</td>
<td>1.0</td>
<td>1.3</td>
</tr>
</tbody>
</table>

2.3. Solution method

The gas phase equations are solved by using the finite volume approximations based on an arbitrary Lagrangian Eulerian method (Hirt et al. 1974) on a finite difference mesh composed of cells, which are arbitrary hexahedrons. This mesh, which need not be orthogonal can conform to curved boundaries and can be
specified as a function of time allowing it to move and follow changes in the combustion chamber geometry (system boundary) with time. The transient solution is calculated in a sequence of finite time increments.

KIVA-II can solve the continuity equation for an arbitrary number of species undergoing an arbitrary number of chemical reactions, restricted only by computational storage and time requirements. Chemical reactions are distinguished as the fast reactions, which are assumed to be in equilibrium and the kinetically proceeding slow reactions. Two implicit equation solvers are available to compute chemical equilibria for hydrocarbon-air combustion. The first of these is a fast algebraic solver incorporating an algorithm devised by Meintjes and Morgan (1987) for the solution of the simultaneous equilibria of the six reactions important in hydrocarbon oxidation. The simultaneous cubic equations are solved by Newton-Raphson iteration, using the scaled concentrations from the previous cycle as an initial estimate. Since the formulation does not include the effects of heat release from the equilibrium reactions on the equilibrium constants, small cycle to cycle oscillations in temperature and species concentrations can occur in some applications. The second procedure uses an iterative solver and is suitable for general circumstances and this iteration scheme consists of the following elements (Ramshaw et al. 1985).

(i) preconditioning of the equilibrium constraint conditions described in eqn. (2.8) to make them more linear in the progress variables,
(ii) application of a one-step successive over-relaxation (SOR) - Newton iteration to the preconditioned system,
(iii) switching to a full Newton-Raphson iteration if the simpler SOR-Newton iteration fails to converge in a specified number of steps.

2.3.1. Temporal and spatial differencing

The temporal differencing in KIVA II is largely implicit and therefore the time steps are calculated based on accuracy, not on stability criteria and result in a considerable saving in computational time. This is performed with respect to a sequence of discrete times \( t^n \), where \( n = 0, 1, 2, \ldots \) is the cycle number. The time interval \( \Delta t^n = t^{n+1} - t^n \) is the computational time step. If \( Q^n \) denotes the difference
approximation to the quantity \( Q \) at time \( t^f \), the difference approximation to the derivative \( \partial Q / \partial t \) is represented by the first order expression \( (Q^{n+1} - Q^n) / \Delta t \). Here \( Q = p, \rho, T, I \) or \( \rho_m \) as well as \( k \) and \( \varepsilon \).

The spatial differencing in KIVA-II is based on the arbitrary Lagrangian Eulerian (ALE) method in which the computational domain is subdivided into a number of arbitrary hexahedral cells. These cells are arranged in such a way that the faces and vertices of the cells are shared by neighbouring cells. The cells constitute the mesh with respect to which spatial difference approximations are constructed.

Figure (2.1). Typical finite difference cell \((i,j,k)\) used in KIVA-II. The three faces of the momentum cell \((i,j,k)\), lying within this regular cell are shaded.

Except in the cells near the walls, each cell vertex has six neighbours with which it shares an edge of a cell. The vertices may be stationary or may move in an arbitrarily prescribed manner facilitating Lagrangian and Eulerian descriptions. The vertices are conventionally numbered as in figure (2.1). The cells are logically indexed by integers \((i, j, k)\) with a convention that the vertex \((i, j, k)\) is the vertex 4 for the cell...
(i, j, k). The Cartesian co-ordinates of vertex (i, j, k) are \((x_{ijk}, y_{ijk}, z_{ijk})\) and are functions of time. All the fluid properties except velocity are uniform in a cell. The mass of fluid in each cell is divided among the vertices of the cell and the velocity of the fluid is the velocity of the vertex to which it is assigned. Momentum cells are used in differencing the momentum equations. A momentum cell \((i, j, k)\) is an auxiliary cell centred about the vertex \((i, j, k)\) of the regular cell. In contrast to regular cells, which have six faces, momentum cells have twenty four faces each of which is comparable in size to one fourth of a regular cell face. Three of these twenty four faces lie within each of the eight regular cells which share common volume with the momentum cells. The volume of any momentum control volume may be calculated once the volumes of the regular cells are known.

In the finite difference approximations of the momentum equation, vector quantities (velocities) are fundamentally located at the vertices of regular cells so that

\[
u_{ijk} = \mathbf{u}(x_{ijk}, y_{ijk}, z_{ijk})
\]

and scalar (thermodynamic and other physical properties) quantities are located at cell centres so that

\[
Q_{ijk} = Q\left(x_{ijk}^c, y_{ijk}^c, z_{ijk}^c\right)
\]

A computational cycle in KIVA-II is performed in three phases named A, B and C. The phases A and B together constitute a Lagrangian calculation in which the computational cells move with the fluid velocity and there is no convection across cell boundaries. The phase A calculates mass and energy source terms due to chemistry. If there were fuel injection, the spray droplet collision and oscillation / break-up terms and the relevant source terms are also calculated. The phase B calculates, in a coupled implicit fashion, the pressure gradient in the mass and energy conservation equations, the spray momentum source if applicable and the terms due to diffusion of mass, momentum and energy. This phase calculates the remaining source terms in the turbulence equations as well. The phase C is the rezone phase. The flow
field is frozen and rezoned or re-mapped onto a new computational mesh by moving the vertices to the new positions, leading to an Eulerian calculation. This re-mapping is accomplished by convecting material across the boundaries of the computational cells, which are regarded as moving relative to the flow field. Lagrangian cell methods are not adequate for describing flows undergoing large distortions. Phase C calculations eliminate these effects by moving cell vertices with respect to the fluid maintaining a reasonable mesh structure (Amsden, 1989).

In the Lagrangian phase, implicit differencing is used for all the diffusion terms. The coupled implicit equations are solved by a method similar to the SIMPLE (Patankar, 1980) algorithm with the individual equality being solved by the conjugate residual method (O'Rourke et al., 1986). Explicit methods are used to calculate convection in the rezone phase. The convection time step is a sub-multiple of the main computational time step and satisfies the Courant stability criteria.

2.4. Combustion chemistry

2.4.1. Chemical kinetic reactions

Chemical rate expressions for the kinetic reactions in KIVA-II are Arrhenius in form and the chemical reactions occurring in the system are symbolised by

\[ \sum_{m} a_{m} x_{m} \leftrightarrow \sum_{m} b_{m} x_{m} \]  \hspace{1cm} (2.11)

where \( x_{m} \) represents one mole of species \( m \) and \( a_{m} \) and \( b_{m} \) are integral stoichiometric coefficients of the reaction. These stoichiometric coefficients must satisfy mass conservation in chemical reactions through

\[ \sum_{m} (a_{m} - b_{m}) = 0 \]  \hspace{1cm} (2.12)

The forward and backward rate coefficients, \( k_f \) and \( k_b \), are assumed to be of a generalised Arrhenius form and given by
The temperature exponents, $\zeta_f$ and $\zeta_b$, are normally taken to be zero while $A$ and $E$ are given empirical values according to the fuel being used (Westbrook et al. 1984).

There is no direct chemical coupling between different numerical cells in KIVA-II. The kinetic reactions are computed under the assumption that the participating species in a reaction is either inert, i.e. $a_m = b_m$, or appears only in one side (either forward or backward) of the reaction, i.e. $a_m b_m = 0$. A reference species, which is in greatest danger of being driven negative for the reaction, is identified and used to compute $\dot{\omega}$, the rate at which the kinetic reaction proceeds. More details of how exactly KIVA-II defines this reaction rate using the above given expressions and calculate it are given in appendix 1.

It was observed that the chemical reaction rates calculated by the existing chemistry model [eqn. (2.12)] resulted in unrealistic rates of pressure rise in SI engine simulations due to faster or irregular mixture burning rates. This kinetic chemistry model will be discussed further in section (3.8.4). In engine combustion, both the chemical reaction rate and the turbulent mixing rate are important parameters. Therefore, as a part of the present study, several turbulent combustion models that can be used in the CFD context for engine modelling were studied to choose a suitable replacement for this existing kinetic chemistry model in KIVA-II. This replacement is needed in order to include the effects of turbulent mixing on combustion. The chosen model will be validated and used as the combustion model in the present study.

### 2.4.2. Equilibrium chemical reactions

For simplicity, it is assumed that the fuel specie does not participate in any of the equilibrium reactions. The rates for these reactions are implicitly determined by the constraint conditions
\[
\prod_{m} (\rho_{m}/W_{m})^{b_{m}} = K_{c}^{'}(T)
\]  

(2.15)

where \( K_{c}^{'}(T) \) is assumed to be of the form

\[
K_{c}^{'} = \exp\left\{ A_{r} \ln T_{A} + B_{r} / T_{A} + C_{r} + D_{r} T_{A} + E_{r} T_{A}^{2} \right\}
\]  

(2.16)

where \( T_{A} = T/1000 \text{ K} \). Simultaneous equilibria of six reactions important in hydrocarbon oxidation are considered here. They are given by

\[
\begin{align*}
N_{2} & \iff 2N \\
O_{2} & \iff 2O \\
2\text{CO}_{2} & \iff 2\text{CO} + O_{2} \\
H_{2} & \iff 2H \\
2\text{OH} & \iff \text{O}_{2} + H_{2} \\
2\text{H}_{2}O & \iff 2\text{H}_{2} + \text{O}_{2}
\end{align*}
\]  

(2.17)

and solved together with four more equations which are the element conservation relations for carbon, hydrogen, oxygen and nitrogen.

2.5. Modifications and additions made to KIVA-II during the present study

2.5.1. Treatment of blow-by flow

In order to deal with experimental data obtained from high blow-by research engines, consideration of blow-by flow from the combustion chamber was needed in the calculations. Blow-by can be treated as an orifice flow situation from and to several reservoirs [figure (2.2)]. A phenomenological crevice flow model developed over the recent years by various researchers (Kuo et al. 1989, 1994 and 1995) was incorporated into the code. The version of this blow-by model by De Petris et al. (1995) avoids the use of the discharge coefficient of flow through orifices making the use of this model relatively convenient and is explained below.
This crevice flow model assumes (Kuo et al. 1989, De Petris et al. 1995)

(i) each crevice region has a uniform pressure
(ii) the temperatures of regions 0, 1, 2 and 3 do not change with time and are equal to the average of cylinder liner and piston temperature
(iii) the pressure in region 3 is atmospheric and does not change during the calculation
(iv) the chemical composition of the gas in each region is uniform but changes during the calculation according to the mass flow to and from each region
(v) the flow to and from each region is isentropic and laminar
(vi) the cylinder bore and the piston are round and the piston is always centred in the bore
(vii) the piston rings do not tilt.
With the assumption of perfect gas behaviour, the controlling equation for the regions 1 and 2 in figure (2.2) is

\[
\frac{V_1}{RT_c} \frac{dp_1}{dt} = \dot{m}_{01} - \dot{m}_{12} \tag{2.18}
\]

and for the regions 2 and 3,

\[
\frac{V_2}{RT_c} \frac{dp_2}{dt} = \dot{m}_{12} - \dot{m}_{23} \tag{2.19}
\]

where \( V_1 \) and \( V_2 \) are crevice volumes, \( T_c \) is the crevice temperature and \( R \) is the gas constant. The mean molecular weight of the mixture is assumed constant and equal to the molecular weight at the beginning of the calculation. The mass flow terms, \( \dot{m}_{ij} \) were calculated using the isentropic orifice flow equation which can be written for flow from region \( i \) to region \( j \) (i.e. \( p_i/p_j > 1 \)) as

\[
\dot{m}_{ij} = A \rho_i a_i \phi_{ij} \tag{2.20}
\]

where \( A \) is the orifice area, \( \rho \) is the gas density and \( a \) is the speed of sound. Both \( \rho \) and \( a \) are evaluated in the region, \( i \). The orifice area is given by the sum of gap area and the minimum ring contact clearance (De Petris et al. 1994). The expression for \( \phi_{ij} \) depends on the \( p_i/p_j \) ratio.

If \( \left( \frac{p_j}{p_i} \right) > \left( \frac{2}{\gamma + 1} \right)^{\frac{1}{\gamma - 1}} \) then the flow is subsonic and

\[
\phi_{ij} = \left( \frac{p_j}{p_i} \right)^{\frac{1}{\gamma}} \sqrt{\frac{2}{\gamma - 1}} \left[ 1 - \left( \frac{p_j}{p_i} \right)^{\frac{\gamma - 1}{\gamma}} \right] \tag{2.21}
\]
whereas if \( \left( \frac{p_i}{p_t} \right) \leq \left( \frac{2}{\gamma + 1} \right)^{\frac{\gamma}{\gamma - 1}} \) then the flow is supersonic and

\[
\phi_{ij} = \left( \frac{2}{\gamma + 1} \right)^{\frac{\gamma + 1}{\gamma - 1}}
\] (2.22)

In most of the blow-by models available in the literature, it had been assumed that the pressure in the top-land crevice [figure (2.2), region 0] is the same as the main chamber pressure. This may not always be the case and providing separate numerical cells representing this crevice region, as done in this study, is a more realistic approach as the pressure in these cells can be calculated without making the above assumption.

The calculated mass losses from the crevice cells due to top ring blow-by were deducted from the species mass conservation equations for each calculation cycle at each crevice cell. The specific energy lost with the mass lost was then deducted from the energy conservation equation. This treatment is essential in order to accomplish the conservation of mass and energy.

2.5.2. Numerical mesh

KIVA-II requires a structured grid representing the geometry for calculations. The existing grid generator within KIVA-II has its inherent limitations and was modified in order to facilitate the inclusion of the top ring crevice cells in the mesh for blow-by flow calculations. However, this modification to the general purpose grid generator required further modifications to several other subroutines as well. To ease the procedure, a separate structured grid generator was written using FORTRAN 77, externally to the KIVA-II main code enabling required numerical grids are generated to include crevice cells and imported into the code. This simple program could easily be added to the main code as a subroutine replacing the existing grid generation facility. The computational mesh generated is shown in figure (2.3). It should be noted the need to have at least two numerical cells between the walls in the crevice region for the law-of-the wall calculations to be meaningful.
Figure (2.3). The grid generated from the new program to include the crevice cells for the ‘Brunel’ piston (At the inlet valve closure, 135° BTDC).
2.5.3. RNG k-\(\varepsilon\) turbulence model as an alternative to standard k-\(\varepsilon\) model

Turbulence modelling is obviously a critical component of CFD studies of turbulent flows and in most engineering applications, the accuracy and reliability of the turbulence model is an important factor determining the reliability of the simulation results. KIVA-II incorporates the two equation k-\(\varepsilon\) turbulence model and an optional SGS model [described in section (2.3.5)]. The necessity to have a reliable turbulence model for engine calculations was realised when using combustion models where the effect of turbulence in the reactive medium on chemical reaction rates is included in the calculations. The two equation k-\(\varepsilon\) turbulence model has well been established as the standard turbulence model in many CFD applications and reasonable level of accuracy have been obtained. However, Han and Reitz (1995) obtained very good agreement between experiments and predictions from their engine simulations using the renormalisation group theory (RNG) based k-\(\varepsilon\) turbulence model. Encouraged by this result, the RNG k-\(\varepsilon\) turbulence model was added as an alternative option in the code and an input switch allows the user to choose the k-\(\varepsilon\) or the RNG turbulence models as required. The effect of using this alternative turbulence model on the natural gas fuelled SI engine performance will be discussed in section (4.11) of this thesis.

The RNG k-\(\varepsilon\) turbulence model was originally proposed by Yakhot and co-workers (1986, 1992-a, 1992-b) and first used for engine simulations in a CFD code of the KIVA family by Han and Reitz (1995) and Han et al. (1996). In the RNG \(k-\varepsilon\) model, the \(k\)-equation [eqn. (2.6)] remains the same but the \(\varepsilon\)-equation [eqn. (2.7)] is modified and given by

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \nabla \cdot (\rho u \varepsilon) = - \left( \frac{2}{3} c_{\varepsilon_1} - c_{\varepsilon_3} + \frac{2}{3} c_{\mu} c_{\eta} \frac{k}{\varepsilon} \nabla \cdot u \right) \rho \varepsilon \nabla \cdot u + \nabla \left[ \left( \frac{\mu}{\rho R_{\varepsilon}} \right) \nabla \varepsilon \right]
+ \frac{\varepsilon}{k} \left( c_{\varepsilon_1} - c_{\eta} \right) \sigma \nabla \cdot u - c_{\varepsilon_2} \rho \varepsilon
\] (2.23)

In this, \(c_{\varepsilon_3}\) accounts for the compressibility (non-zero velocity dilatation) and is given by
\[ c_{e_3} = \frac{1}{3} \left\{ -4 + 2 c_{e_1} + 3 (v_0 \nabla \cdot u)^{-1} \left( \frac{d v_0}{d t} \right) + (-1)^{\delta} \sqrt{6} c_{\mu} c_\eta \eta \right\} \]  

(2.24)

where \( v_0 \) is molecular viscosity, \( \delta = 1 \) if \( \nabla u < 0 \) and \( \delta = 0 \) if \( \nabla u \geq 0 \). The model constants have been derived from theoretical considerations and are given in table (2.2) while \( c_\eta \) is calculated by

\[ c_\eta = \frac{\eta \left( 1 - \frac{\eta}{\eta_0} \right)}{1 + \beta \eta^3} \]  

(2.25)

where \( \eta_0 (= 4.38) \) and \( \beta (= 0.012) \) are model constants and \( \eta (= \tau / \tau_3) \) is the ratio of the turbulent time scale, \( \tau (= k/\epsilon) \) to mean strain time scale, \( \tau_3 (= S^{-1/2}) \) where

\[ S = \frac{1}{2} \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right)^2 \]  

(2.26)

Table (2.2). Values of RNG k-\( \varepsilon \) turbulence model constants

<table>
<thead>
<tr>
<th>( c_{e_1} )</th>
<th>( c_{e_2} )</th>
<th>( c_{\mu} )</th>
<th>( Pr_k )</th>
<th>( Pr_\varepsilon )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.42</td>
<td>1.68</td>
<td>0.0837</td>
<td>0.7194</td>
<td>0.7194</td>
</tr>
</tbody>
</table>

2.5.4. Spark ignition Model

Simply defined, ignition is a process that starts with reactants and evolves towards a steadily burning flame. More formally, ignition can be defined as a transition from a non-reactive state to a reactive state in which external stimuli lead to a thermo-chemical runaway followed by a rapid transition to self sustained combustion (Kuo, 1986). The ignition process is usually very complex and involves many intricate physical and chemical activities. KIVA-II code uses a simpler approach to simulate spark ignition by adding spark energy (approximately about 1% of total
charge internal energy) into several numerical cells representing the spark plug gap region, over a period of about 3-6 crank angle degrees. This appears inappropriate because in reality, a spark releases energy in a period of a few nano-seconds (i.e. a small fraction of a crank angle degree) and a flame kernel of about 3 mm diameter having a temperature 2000K-3000K occurs after about 50 micro-seconds (Shen et al., 1994). At the same time, natural gas (methane) needs more ignition energy than gasoline due to its high activation energy and all these facts raise the need for a suitable model for spark ignition. However, spark ignition models are not simple to implement as ignition system electrical characteristics, effects of heat losses to electrodes, convection velocity of the mean flow near the spark plug gap, spark plug geometry etc. have to be mathematically considered. Variations in the flow conditions from cycle to cycle near the spark plug affect ignition quality. KIVA-II does not treat cyclic variations and average ignition conditions have to be considered if the spark is to be described. An attempt was made to represent the spark by introducing an area (a few numerical cells) of sufficiently high temperature, in this case 2500K, representing the flame kernel and the nearby hot area for a very short period of time (50 micro seconds), instead of adding energy to these cells. This was not successful and numerical stability problems resulted due to high temperature gradients, indicating that further improvements are required. However, implementation of an advanced spark ignition model is out of the scope of the present study and the available method of representing spark ignition was used for the rest of the study.

2.5.5. Chopper for removing cell layers

There exists a facility for chopping off horizontal layers of computational cells from the numerical mesh in order to maintain a reasonable cell aspect ratio during the compression stroke. This chopper had been unnecessarily removing several layers too early when there is a piston bowl (or crevice cells which was treated as a bowl by the code). This flaw was corrected and further developments were made so that the chopping off and the re-insertion of a respective layer of cells are performed almost at the same piston position respectively during the compression and the expansion strokes of the engine.
2.5.6. Contour plots and output of results

The contour plots generated by the original code were limited. This limit was extended and contour the plots of $\varepsilon$ (turbulent energy dissipation) and $k/\varepsilon$ (turbulent time scale) were added. Also, in the equivalence ratio contour plots, the spacing between the contours was reduced in order to clearly see the areas where the cell equivalence ratio changes rapidly (e.g. around the flame front).

2.5.7. Chemical reaction rate

As one of the main objectives of the study, the existing subroutine for calculating chemical reaction rates will be replaced with a suitable combustion model. In chapter 3, presently available combustion models of SI engine combustion commonly used in CFD environments will be reviewed and the model chosen from this review will be used in place of the original KIVA II chemistry model for the rest of this study.
3.1. Model development

A given level of model complexity may require more information than what is available in a particular engine situation. Under such circumstances, it is an advantage to have simpler models, which need less information to define the calculation required. Increasing the complexity of the model does not necessarily increase the validity or accuracy of the results though it certainly has the potential for doing so. Thus it seems reasonable to construct a hierarchy of models differing in complexity. Another advantage of such a hierarchy is the possibility of comparing results among the hierarchy and thus judging the significance of simplifying assumptions.

A computer program for engine modelling is composed of two essential but independent parts; (i) the set of equations used to model the physical system and (ii) the database of physical and chemical properties used in the implementation of those equations. They, in co-operation with numerical methods determine the results of model calculations. Since meaningful modelling of the internal combustion engine can not ignore the chemistry involved, a very large system of partial differential equations (PDEs) is required. Solving of these equations numerically is done on a space and time grid, which is adequate for resolving the spatial and temporal gradients, for a number of consecutive cycles. As typical engines
lack any spatial symmetry in their configurations, partial differential equations are needed in three spatial co-ordinates. Some initial and boundary conditions for these computations need to be assumed, as there are no adequate experimental data on every aspect of these very complex processes.

For simple models, PDEs are replaced by ordinary differential equations (ODEs). These equations are conventionally obtained from the corresponding PDEs by imposing simplifying assumptions and neglecting dissipative and transport phenomena. An obvious advantage of a simpler model is that it requires less information to characterise it completely than is necessary for a more detailed model. This permits calculations even in those situations where our knowledge is inadequate to characterise a more sophisticated model. The steady state equations are obtained by neglecting the temporal derivatives. The choice of modelling functions makes the equations specific for a particular physical system.

3.2. Specification of PDEs to IC engines

The Otto cycle can be decomposed into two distinctly different phases of operation as (i) the combustion phase, characterised by the presence of a propagating flame front and (ii) the non-combustion phase, identified by the absence of a flame front. The combustion phase begins with the ignition of the combustible working fluid by the spark plug and terminates when the flame has completely engulfed the combustible working fluid. The completion of the combustion phase does not signal an end to chemical reactions as these continue during the following non-combustion phase. Flow in the intake or the exhaust systems can alter the amount of working fluid during either phase of the cycle (Zeleznik et al. 1985).

3.3. Numerical scheme

The integration of the differential equations must be accomplished numerically and this then raises the problem of selecting a suitable integration scheme. A good numerical integration scheme must have two characteristics. First, it must be capable of producing an adequate approximation to the true solution. Second, it must generate the solution economically. The question of economy is a matter of
concern when the system of equations is large. It is especially significant when some of the equations arise from chemical kinetic considerations. The differential equations associated with chemical kinetics sometimes exhibit a property called stiffness, which can reveal itself in the behaviour of an integration scheme. This requires excessively small time steps, out of proportion to the rate of change of the dependent variables. Finally, solution algorithms are employed to obtain the flow parameters from the algebraic equations provided by discretisation practises of the mathematical model differential equations (Zeleznik et al. 1985).

3.4. Classification of SI engine models

Mathematical models of SI engine combustion can be divided into two main groups as thermodynamic models and dimensional models. Thermodynamic models are further classified into two groups namely single zone models and multi zone models. In a similar manner, dimensional models too are classified as one-, multi- and quasi-dimensional models. Thermodynamic models do not account for spatial flow variations and cannot provide information about, for example, the local velocity and the temperature fields. Dimensional models consider the spatial and temporal variations of the velocity, temperature and pressure fields in one-, two- or three- dimensions. Thermodynamic, energy conservation based models can be extended to produce phenomenological models and quasi-dimensional models. In phenomenological models, additional details beyond the energy conservation equation are added for each phenomenon in turn. In quasi-dimensional models, specific geometric features such as the spark ignition engine flame, the diesel fuel spray shapes are added to the basic thermodynamic approach (Heywood 1988, Ramos 1989-a & 1989-b).

3.4.1. Thermodynamic models

The logic structure of Thermodynamics based models [fig. (3.1)] shows the engine's intake, combustion, expansion and exhaust processes where conservation laws are applied to follow the changing thermodynamic and chemical state of the working fluid in the cylinder (Heywood 1980, 1994).
3.4.1.1. Single zone models

Single zone models, also called zero-dimensional models, are based around the first law of Thermodynamics, mass conservation and gas property relationships. These models account for the combustion chamber geometry in a global manner and ignore flame propagation phenomena. The cylinder charge is assumed to be homogenous in both temperature and composition and the first law of thermodynamics is used to calculate the pressure or the heat release rate (or mass burning rate). In these models, the state of the cylinder charge is defined in terms of average properties and there is no distinction between burned and unburned gases.

Because of their simplicity, single zone models can account for mass flows into and out of crevices and leakage. These models can be used as diagnostic (heat release analysis) or predictive tools and are primarily of value in analysing the energy conversion aspects of IC engines. In heat release analyses, experimentally determined pressure diagrams are used as an input to predict the heat release rate or
the mass burning rate. As the mass burning rate depends on the combustion duration, engine geometry, equivalence ratio, residual mass etc., single zone models may require tuning to predict the pressure diagrams in different engines or in the same engine operating under different conditions, when mass burning rate is specified as an input.

3.4.1.2. Multi-zone models

These models resolve the combustion phenomena in a more physical manner than single zone models do. The combustion chamber is generally divided into burned and unburned gas regions. Sometimes thermal boundary layers in the burned and unburned gases are also considered. Figure (3.2) indicates the burned and unburned gas zones separated by the flame and the thermal boundary layer considered within the engine combustion chamber. The cylinder charge is often assumed to be composed of ideal gases, which are frozen in the unburned gas region and in chemical equilibrium in the burned gas region. The first law of Thermodynamics, the equation of state and the conservation of mass and volume are applied to the burned and unburned gases. The pressure is assumed to be uniform throughout the cylinder charge and the two zones are assumed to be uniform in both temperature and composition.

The burning rate or the turbulent flame speed need to be calculated or specified as a function of, for example, the laminar flame speed, engine speed. The turbulent flame speed does not determine the mass burning rate unless the flame front surface area is specified. The flame is frequently assumed to propagate spherically throughout the combustion chamber.

Multi-zone thermodynamic models assume that the compression stroke is characterised by uniform levels of turbulence throughout the combustion chamber and neglect the mean flow field. However, as the experimental data and multidimensional calculations have shown that the large scale eddies generated during the intake stroke may persist up to top dead centre of the compression stroke and during this period, multi-zone models of engine turbulence are not accurate. These models neglect the flame structure and consider an infinitesimally thin flame and must be supplied with heat transfer correlation unless an integral method is used (Ramos 1989-a & 1989-b).
3.4.2. Dimensional models

One-dimensional models are based on the time averaged conservation equations of mass, momentum, species and energy which are averaged across the combustion chamber assuming planar, cylindrical or spherical flame propagation. In planar flame propagation models, the distance between the piston and the cylinder head must be much larger than the cylinder bore and are clearly unrealistic in conventional reciprocating engines. Cylindrical flame propagation models can simulate combustion phenomena in a more realistic way, particularly after the flame reaches the piston. However they are not accurate for predicting the initial stages of combustion. Generally the flame is treated as a thin uniform reaction sheet but in actual practice, the flame is highly wrinkled due to the effects of turbulence in the cylinder. In the absence of strong swirl, the propagation of the surface of the mean flame front can be assumed to be spherical.

Thermodynamic models and one-dimensional models cannot account for the multi-dimensionality of the flow field, fuel-air mixing, spray penetration, vaporisation and combustion etc. and multi-dimensional models (commonly referred
to as CFD models) are used in these situations. These models are based on the numerical solution of the time averaged conservation equations of mass, momentum, energy and species in spatial dimensions and time for the evolution of in-cylinder flows, heat and mass transfer and combustion. Extensive amounts of computer time and storage are required for the use of multi-dimensional models and mainly two- and three-dimensional models are used (Shih 1986, Ramos 1987, Steinthorsson 1988, Ramos 1989-a & -b, Heywood 1994).

Quasi-dimensional models are used to bridge the gap between zero and multi dimensional models. They induce a spatial dependence into processes such as combustion and heat transfer in an explicit phenomenological manner rather than deriving the spatial dependence from the solution of the full set of conservation equations. Quasi-dimensional models are useful as they do relate the model outputs to the combustion chamber geometry and aggregate flow field parameters and the computer running times are modest (Heywood 1994).

3.5. Models of flame structure and flame speed

Engine combustion models may have two distinct parts; (i) a flame structure model and (ii) a flame speed model. The flame structure models are approximations to the schematic of the turbulent wrinkled reaction sheet flame. The flame structure model then requires values for the flame speed; both laminar and turbulent and the transition between these. The flame speed model provides these values (Heywood 1994).

3.5.1. Flame Structure models

3.5.1.1. Mean flame front models

This is the simplest flame structure model and the turbulent flame is represented by its mean location obtained by averaging the turbulent fluctuations. In quasi-dimensional engine cycle simulations, this approach to flame structure also requires a flame geometry model. Often an expanding spherical mean flame surface is assumed with the flame centre at the location of the spark plug electrode gap
(Heywood 1994). This ignores the fact that flame kernel convection by the local bulk flow can be significant while the flame is small (Pischinger et al. 1990).

3.5.1.2. Entrainment and burn-up flame models

In this type of flame structure models, the mixture burning process is described as occurring in two stages. Firstly, unburned mixture is entrained into the turbulent flame brush and then burn up occurs within the flame brush at a rate governed by the amount of unburned mass within the flame divided by a characteristic burning time. A geometric model for the flame front is needed when entrainment models are used with quasi-dimensional engine simulations and often a simple spherical flame surface is assumed. These so called entrainment models have been extensively used in quasi-dimensional simulations of engine operation and have also been expanded to include more of the relevant physics (Tabaczynski et al. 1977).

3.5.1.3. Flame sheet models

In these models, the mass burning rate is given by an expression based on the surface area of the wrinkled thin reaction sheet flame. This surface area needs to be estimated and the two common approaches used for this are

(i) the fractal geometric flame model which describes the wrinkled flame surface by assuming self similarity between scales of different size resulting in a power-law scaling between the measured size and the measurement scale and

(ii) the coherent flame sheet model (CFM) which calculates the flame sheet area per unit volume, making a fundamental assumption that the reaction sheet thickness is small compared to the energy containing turbulent eddies in the turbulent flame (Heywood 1994).

There can be variants from these and the turbulent combustion models, such as the ones, which use PDFs to describe the distribution of the burned and the unburned gas within the flame, have been developed for multi-dimensional codes. Work by Borghi et al. (1987) is an example.
3.5.2. Flame speed models

Flame speed models are often correlations of experimental flame speed data for laminar and turbulent flame speeds, with physically based dimensionless scaling relationships.

3.5.2.1. Laminar flame speed models

Various relationships for the adiabatic laminar flame speed derived from experiments are used in the laminar flame speed models and they depend on the temperature gradient across the flame. Thus, non-adiabatic laminar flame speed models must incorporate either the actual burned gas temperature directly or the energy transfers (spark energy and heat loss) that make the flame non-adiabatic. An important factor in the laminar flame speed correlations is the burned gas fraction (residual and recycled) in the unburned mixture (Heywood 1994). The correlations for laminar burning velocity under different conditions have been presented by several researchers such as Rhodes et al. (1982) - the presence of exhaust gases in the mixture, Markstein (1964) - flame curvature and flame stretch, Boulouchos et al. (1994) - adiabatic and non-adiabatic conditions.

3.5.2.2. Turbulent flame speed models

Relationships between laminar and turbulent burning velocities based on experimental data are used in turbulent flame speed models. The work by Bradley (1992) and Merdjani et al. (1993) are good examples in this regard.

3.6. Modelling of Premixed Turbulent Flames

Damköhler's classical theoretical and experimental studies performed in the 1940's are generally recognised as the first scientific investigation of turbulent premixed flames. Of most importance is the idea he put forward that sufficiently large scale turbulence merely wrinkles a premixed laminar flame without significantly modifying its internal structure, while sufficiently small scale turbulence primarily
affects the transport processes inside the flame. Limiting combustion regimes are thus identified in which the microscale of the turbulence is either very large or very small in comparison with the thickness of a laminar flame. Significant research has been done on premixed turbulent flames in the past 50 years since Damköhler's pioneering work on this subject. One major achievement is the generation of the combustion diagram, which classifies the premixed turbulent flames into several different regimes.

3.6.1. Regimes of Combustion

In order to understand and quantify the complex interactions between turbulence and chemistry, it is important to identify the length and time scales encountered in SI engine combustion. A fully developed turbulent flow can be characterised by a continuous range of length and time scales. This range, which is called the inertial range, extends from the large energy containing eddies characterised by the integral length scale \( L \) at which the turbulent kinetic energy is fed into the system, down to the smallest eddies characterised by the Kolmogorov length scale \( \eta \) where the energy is dissipated. Associated with the length scales are the particular time scale; a turn over time and a particular turn-over velocity for the large scale energy containing eddies and the small scale Kolmogorov eddies. Chemical reactions impose their own length and velocity scales in the form of flame thickness and flame velocity, respectively. These scales interact with the scales of the inertial range leading to different regimes in premixed turbulent combustion.

A number of researchers (Bray 1980, Borghi 1984, Abdel-Gayed et al. 1985, Abraham et al. 1985-b, Peters 1986, Gokalp 1987, Williams 1988, Abdel-Gayed 1989, Poinset et al. 1991) have presented phase diagrams to illustrate these different regimes in premixed turbulent combustion in terms of length and velocity scale ratios. These regimes can be identified depending on the value of three main parameters, namely, the turbulent Reynolds number, \( Re_t \), the Damköhler number, \( Da \) and the Karlovitz number, \( Ka \). (See Appendix 2 for the definitions of these indices). Pope (1987) gives a phase diagram on a Damköhler number - laminar Reynolds number plane. Borghi (1988) gives this information on a turbulent Reynolds number - Damköhler number plane with logarithmic scales. Figure (3.3) is a modified version of Borghi’s diagram by Bray and Peters (1994) and in this diagram, \( Re_t = 1, \ Da = 1 \)
and $Ka = 1$ define the boundaries between different regimes of premixed turbulent combustion. When the integral length scale and turbulent kinetic energy are known, the diagram indicates whether the flow contains flamelets, pockets or a distributed reaction zone. This information is important, as the modelling approach is different within different regimes of combustion.

![Phase diagram of regimes in premixed turbulent combustion](image)

**Figure (3.3).** Phase diagram of regimes in premixed turbulent combustion

In the corrugated laminar flamelets regime and in the distributed reaction zone there is a close interaction between turbulence and combustion because neither of them is completely dominating. Work by Roberts et al. (1993) has shown that the division between laminar flamelets and distributed reactions extends to much higher values of $u'/S_L$ implying that most practical turbulent combustion systems including the SI engine fall within the flamelet regime. This indicates that the combustion process within SI engines almost always falls within the flamelet regime, though the traditional belief was that SI engine combustion ranged to both the flamelet and the distributed reaction zones, as seen in fig. (3.3).
3.7. SI Engine combustion modelling

Turbulent combustion poses many different problems that are still not completely solved. Statistical techniques, flamelet concepts and eddy break up concepts are the major approaches we have towards solving these problems. A variety of physical models of turbulent flames is now available and has been successfully used in simple and/or more complex configurations in determining the local average reaction rates. The classical approach based on statistical techniques and stochastic concepts involves a probability density function (PDF) and this PDF is often presumed or determined from the solution of an evolution equation. With the flamelet concept, the reactive flow field is viewed as a collection of flame elements embedded in the turbulent stream. The structure of these flamelets is identified and analysed separately. An important advantage with the flamelet concept is that it decouples complex chemistry and molecular transport problems from the modelling of the turbulent flow field. Eddy break up concepts relate turbulent mixing rates within the flow field to chemical reaction rates and provide a simpler approach to handle the complex problem of turbulent combustion.

As exact mathematical representation of all the processes involved in the turbulent combustion is impracticable, varying levels of simplifying assumptions are used in different models. Among the factors determining the choice of a combustion model are the expected accuracy of the numerical solution, availability of computing resources, computational costs and generality (or the global nature of applicability) of the model. Because of physical uncertainties, in particular of the nature of combustion and turbulence within the cylinder, the mathematical model cannot yet tell the whole story. Nevertheless, it provides the researcher and the designer with information, which could not otherwise be obtained. As different assumptions can be tested in a model and compared with data, an insight into some detailed fluid and combustion interactions can be gained. Due to the practical importance of turbulent combustion in engines and its effect on pollutant formation, the modelling of turbulence-combustion interaction has been the focus of intensive research work over the years. An excellent theoretical discussion on the interaction between turbulence and chemistry is given by Kollmann and Chen (1992).
3.8. Commonly used multi-dimensional models of SI engine combustion:
A review

Ramos (1989 a, b) classified the combustion models of SI engines into three different groups, namely mean reaction rate models, eddy break up or mixing controlled models and hybrid models. However, It is not difficult to find in the literature that the most commonly used CFD models fall into five distinctive categories. They are

(i) Arrhenius expressions (Mean reaction rate models),
(ii) statistical and stochastic models,
(iii) eddy break up models,
(iv) characteristic time of reaction models,
(v) flamelet models.

3.8.1. Global mean reaction rate models: Single reaction model (SRM)

For hydrocarbon fuels, the elementary reaction schemes are so complex that it is usually not feasible to consider all the chemically reacting species and their reaction rates when analysing practical combustion systems. In order to simplify this problem, an overall or a global reaction scheme, may be a set of a few reactions, can be used. However the use of such global schemes should be limited to the regimes (the ranges of equivalence ratio, pressure and temperature etc.) for which they have been tested. Even simplified schemes such as a four-reaction scheme are too complicated for practical use in present numerical codes. Thus, single-step global rate equations such as

\[ \text{Fuel} + \alpha \text{O}_2 \rightarrow \beta \text{CO}_2 + \gamma \text{H}_2\text{O} \]  \hspace{1cm} (3.1)

where \( \alpha, \beta \) and \( \gamma \) are stoichiometric coefficients, have received renewed interest in recent years. The associated global rate expression can then be written as of Arrhenius type,
\[
\dot{\omega}_{fuel} = \frac{d[fuel]}{dt} = A T^n p^m [fuel]^a [oxygen]^b \exp\left(\frac{E}{RT}\right)
\] (3.2)

where

- \(\dot{\omega}_{fuel}\) Global reaction rate
- \(A\) Arrhenius pre-exponential factor
- \(E\) Activation energy

with \(n(=0)\) and \(m(=0)\) are constants and \(a\) and \(b\) are the global constants whose values should be chosen according to the fuel in question (Borman and Ragland 1998).

In turbulent combustion, mean reaction rates like this, based on the usual Arrhenius type function of the local average properties, can result in significant errors and great exaggeration of the importance of the chemical kinetics. Modelling the effect of turbulent fluctuations on the chemical reaction rate poses an important problem due to the non-linearity of the source terms. As a consequence, the mean reaction rate may not be appropriately described in terms of the mean variables appearing in the Arrhenius expression. In this model, the contributions of the fluctuating temperature and species mass fractions to the time averaged reaction rate are neglected. This may result in a substantial under-estimation of premixed, turbulent chemically reacting flows where the temperature fluctuations may be of the same order of magnitude as the mean temperature. It is implicitly assumed that the chemical kinetics time, \(t_c\) is much larger than the mixing time, \(t_m\) and that the reaction is controlled by chemical kinetics (Carpenter and Ramos 1985). Diwakar (1984) showed that when using a mean reaction rate model, if the volumetric efficiency or the equivalence ratio were varied, case by case tuning of the model constants in the reaction rate expression is needed in order to obtain good agreement with experimental data.

Calculations in terms of the mean values of temperature, pressure, and mixture strength with the Arrhenius type relations will lead to significant errors and will exhibit a strong dependence on the temperature, pressure and mixture strength. In contrast, experimental results indicate that premixed turbulent flames are only weakly dependent on these mean quantities (Jones and Whitelaw 1982, Bray 1979).
3.8.2. Statistical and stochastic models

Mean reaction rates cannot be regarded as functions of the mean state variables alone. Fluctuations in the scalar variables that specify the instantaneous thermodynamic state of the mixture result in extra terms for the mean reaction rates in the averaged governing equations. The most convenient description of the fluctuating thermodynamic state is through a probability density function (PDF). In general, a joint PDF for all the state variables is required. The average reaction rate may be expressed in terms of this joint PDF. This approach is conceptually attractive because it is based on a framework of stochastic principles but it is not very practical especially if complex chemistry is to be considered. Furthermore, the calculation of the PDF is never carried with an exact evolution and a set of closure assumptions is required. One drawback of PDF models is that they do not distinguish the fluctuations existing in a turbulent flow in terms of their scale. The eddies of large scale, intermediate scale or small scale are thus treated indifferently while their effects on the flame are certainly not comparable.

The probability approach has the advantage of overcoming difficulties associated with non-linearities at the price of increasing the dimensionality of the problem by the number of independent variables involved (Pope 1977). The closure problem associated with non-linearities in the equations governing a turbulent flow is avoided by considering the joint PDF of the flow variables. The joint PDF of velocity, $p(v; x, t)$ provides a complete statistical description of the turbulent velocity fluctuations and in reacting flows, a complete statistical description of the chemical and thermodynamic properties is provided by their joint PDF, $p(\psi; x, t)$.

The attraction of the PDF approach appears to diminish when solving the transport equations. Analytical solutions have been obtained for PDFs in a few simple cases but in general, numerical methods are required. Such methods have to cope with the integro-differential nature of the equations and with the large dimensionality of $p(v; x, t)$ and $p(\psi; x, t)$. For example, in a steady, 2-dimensional flow, the joint PDF of velocity, $p(v_1, v_2, v_3; x_1, x_2)$, is a five-dimensional quantity. Reactive flows of practical interest usually involve many species. Consequently, the dimensionality of the PDF $p(\psi_1, \psi_2, \ldots, \psi_n; x, t)$ becomes large because $n$ is large. It has been shown that the finite difference solution of the PDF transport equation is

Chapter 3 51
almost impracticable for \( n \) greater than 3 (Pope 1981). Pope (1985), Borghi (1988) and Jones and Khaki (1996) have presented very good reviews of PDF methods for reactive flows. However, only a few cases of application of PDF methods for modelling combustion in premixed, SI engines is found in literature.

There are two alternative approaches to the solution of this PDF. The first is to use a presumed PDF for the calculations. The other approach is to calculate the PDF from its own balance equation by the Monte Carlo method.

### 3.8.2.1. Presumed PDF method

This method tries to combine the advantages of PDF method, which are able to take into account the influence of fluctuations on the mean reaction rates and the advantages of the moment method which do not require the computation of the full PDF equation. The basic principle of the presumed PDF method is to use an approximate shape for the PDF. As the shape of the PDF has to be different for different types of flames and eventually for different locations for the same flame, it is necessary to adopt a shape depending upon a few parameters and to compute these at every location based on the balance equations of the first moments. It is more difficult to find realistic shapes of the PDF for a function of two or more variables than for a function of a single variable. The idea that the PDF is supported by a peculiar domain clearly restricts statistical independence assumptions to the case where only small fluctuations are present. For that reason, the presumed PDF method is well suited only for perfectly premixed flames where the PDF can be assumed to be one dimensional (Borghi 1988). Double delta function used by Khaki et al. (1975), clipped Gaussian shape used by Lockwood and Naguib (1975) and the \( \beta \)-function used by Peters (1982) are common shapes assumed for the PDFs.

### 3.8.2.2. The Monte-Carlo methods

For problems with a large number of independent variables, the Monte-Carlo method usually provides an alternative means of obtaining numerical solutions (Dahlquist and Björck 1974). With the Monte-Carlo method, for a PDF of the type \( p(\psi_1, \psi_2, \ldots, \psi_n; x, t) \), the computational expense rises only linearly with \( n \) which is the
best that can be achieved by any algorithm. Consequently, the solution of the PDF transport equation by the Monte-Carlo method can be envisaged for turbulent flows involving many reactive species. In general, for simple problems, the Monte-Carlo method is inefficient compared with the standard numerical techniques but for multidimensional problems, the Monte-Carlo method remains practicable while other methods demand prohibitive amounts of computational capabilities. Finite difference solutions of the equations are impracticable mainly because of the large dimensionality of the PDFs. The ability of the Monte-Carlo method to handle joint PDFs of large dimensionality has allowed combining the velocity and composition PDFs (Pope 1985). Pope and Anand (1984) solved this joint PDF for a premixed flame. Tatschl et al. (1994) used a Monte Carlo PDF approach for simulation of an SI engine considering a PDF of a reaction progress variable as the mixture fraction \( f \) is a constant for a homogeneous premixed charged combustion. The transport equation for the reaction progress variable continuous PDF is given by

\[
\frac{\partial}{\partial t} \{\bar{p}\bar{p}(c)\} + \frac{\partial}{\partial x_j} \left\{ \bar{p} U_j \bar{p}(c) - \Gamma_c \frac{\partial \bar{p}(c)}{\partial x_j} \right\} = \\
\frac{\partial}{\partial c} \left\{ \bar{p} \bar{p}(c)s(c) \right\} + \bar{p} \frac{2C_m}{\tau} \int_0^c \bar{p}(c-c') \cdot \bar{p}(c+c') \cdot dc' - \bar{p}(c) \tag{3.3}
\]

where \( \rho \) is the mixture density, \( U_j \) are velocity vector components, \( \Gamma_c \) is mass diffusion coefficient, \( C_m \) a model constant with \( p(c) \) being the probability that at location \( x \) and time \( t \) the quantity \( c \) is within the range \( c - dc < c < c + dc \). The mean density is given by

\[
\rho = \left\{ \int_0^c \bar{p}(c) \, dc \right\}^{-1} \tag{3.4}
\]

It is claimed that the PDF approach can overcome the major closure problems in modelling turbulent combustion and have been shown to be tractable for complex flows with realistic finite rate kinetics. However, there are different opinions about the PDF method. Peters (1986) argues that the support for modelling reacting
flows using the PDF approach has always been based on the fact that the highly non-linear chemical source term does not need to be modelled. However, if reaction occurs in thin layers only, as in the flamelet regime, reaction and molecular diffusion are closely coupled and the difficulty with the chemical source term is shifted towards modelling of the molecular diffusion. Pope (1990) also recognises the problem and states that “the flamelet combustion regime is inherently difficult to treat in PDF methods, because the small scale structure of the composition field is dominated by reaction (strongly coupled with diffusion) rather than being determined by the large scales via a cascade process. Instead, a flamelet model that explicitly represents the flame sheet structure offers a more natural approach”.

3.8.3. Eddy break up models (EBUM)

As a consequence of the interaction between turbulence and chemical reactions, mixture structure becomes very inhomogeneous. Eddy break up type combustion models give a more physically based representation of combustion because they take into account the effects of turbulence on the mean chemical reaction rates and also because the closure problems of this method occur at a more fundamental level. These models account for the intermittent appearance of reactants at a given point in the flow and assume that the large scale eddies are responsible for stretching and bringing the fuel and oxidiser (or the unburned mixture and the hot products in the case of premixed combustion) into contact with each other. In these mixing controlled reactions the characteristic time scale of the large eddies or mixing time is considered larger than the chemical conversion time; the well known fast chemistry assumption. Mixing is expected to occur in small scales (Spalding 1977).

Spalding (1971) first developed the eddy break up model to predict the spread of a premixed turbulent flame behind a baffle in a plane-walled duct. He used two distinct models in the calculation of mean reaction rates. In the first model, the mean reaction rate was related to the time mean concentrations and temperature at the point in question by a bi-molecular Arrhenius expression, that is

\[
\bar{\omega}_{\text{kinetic}} = A p^2 \bar{Y}_f \bar{Y}_o \exp \left( - \frac{E}{R T} \right) \tag{3.5}
\]
where

\[ \bar{\varrho}_{\text{kinetic}} \text{ mean volumetric rate of consumption of fuel} \]

\[ A \text{ pre-exponential factor} \]

\[ p \text{ local pressure} \]

\[ \bar{Y}_f \text{ local time mean mass fraction of the fuel} \]

\[ \bar{Y}_o \text{ local time mean mass fraction of the oxidant} \]

This first combustion model was unsuccessful in following the trends of experimental data qualitatively or quantitatively for any value of the empirical constants in the Arrhenius expression. As this model predicted concentration profiles, which were steeper than experimental value, it was realised that the chemical reaction was too concentrated in the high temperature region of the flame. Spalding (1971) then indicated the need to formulate this reaction rate in a way which enlarges the influence of local turbulence level and diminishes that of the chemical kinetic constants.

Spalding identified that the reaction rate in a premixed flame is only weakly dependent on temperature, pressure and mixture strength. Instead the reaction process is controlled by turbulent mixing. He proposed another model for the reaction rate, which does not account explicitly for the effect of chemical kinetics and presumes that the combustion rate is entirely turbulent mixing controlled. Even though the assumption that the eddy break up rate controls the combustion rate is not completely correct for premixed turbulent combustion, it does demonstrate the important role of turbulence in modelling turbulent combustion. According to this model, the mean reaction rate is proportional to the rate at which the largest eddies are broken into the smallest dissipative eddies by the action of turbulence. The time required to break up a turbulent eddy was taken as the characteristic mixing time scale, which is proportional to the ratio of turbulent kinetic energy over its dissipation rate, \( k/\varepsilon \). The EBU expression was then given by

\[
\bar{\varrho}_{\text{EBU}} = C_{\text{EBU}} \frac{\varepsilon}{k} \left( \frac{\bar{Y}_f^2}{\bar{Y}_o^2} \right)^{1/2} \tag{3.6}
\]
where $Y_f'$ is the fluctuation in fuel mass fraction.

The second model was formulated such that the effect of turbulence level was enlarged and that of the chemical kinetics was diminished and this model was formulated as

$$\bar{\omega}_{\text{fuel}} = \left[ (\tau \cdot \bar{\omega}_{\text{kinetic}})^{-1} + (1 - \tau) \cdot \bar{\omega}_{\text{EBU}} \right]^{-1}$$  \hspace{1cm} (3.7)

where

- $\bar{\omega}_{\text{kinetic}}$ mean reaction rate calculated from the first model [eqn. (3.5)]
- $\bar{\omega}_{\text{EBU}}$ eddy break up rate which is proportional to the mean strain rate
- $\tau$ reactedness defined as

$$\tau = \left( \frac{Y_f - Y_{fu}}{Y_{fb} - Y_{fu}} \right)$$  \hspace{1cm} (3.8)

where

- $Y_f$ mean mass fraction of the fuel
- $Y_{fu}$ mean mass fraction of the fuel in the unburned gas
- $Y_{fb}$ mean mass fraction of the fuel in the fully burned gas

Eqn. (3.7) is a simple combination of the effects of turbulence and chemistry on the mean reaction rate. As expected, better agreement with experiment was achieved by Spalding, with this improved model.

The EBU model of Spalding is applicable only for single step, fast reaction cases and would give good predictions of time mean flow and composition (Khalil et al. 1975). It can not be generally applicable to both premixed and diffusion flames. Modifications to the EBU model and models of similar type have since been proposed by a number of authors to include other important parameters such as the Kolmogorov length scale, the laminar burning velocity and the effects of flame stretching etc. Mason and Spalding (1973) improved the model by replacing the
dissipation rate of turbulent kinetic energy with viscous dissipation, $\overline{\chi}$. Modifications proposed by Said and Borghi (1988) and Mantel and Borghi (1991) included the laminar burning velocity as an important parameter in determining the rate of reaction. The most popular of these is the model proposed by Magnussen and Hjertager (1976). This differs from the original EBU model in relating the dissipation of eddies to the mean concentration of the intermittent quantity instead of the concentration fluctuation. This is an advantage, especially when taking into consideration the lack of certainty in determining the concentration fluctuations of the reacting species and the model is also applicable to diffusion flames. Since there is a correlation between the fluctuations in the concentrations of fuel and oxygen and their respective mean values, the rate of dissipation can be expressed by the mean concentrations of the reacting species. Accordingly, depending on whether the flame is locally fuel-starving or oxygen-starving, the rate of combustion of fuel (kg/m$^3$s) can be expressed as

\[
\overline{\omega}_f = A \overline{C_f} \frac{\varepsilon}{k} \quad \text{(Fuel starving)} \tag{3.9}
\]

\[
\overline{\omega}_f = A \overline{C_{O_2}} \frac{\varepsilon}{r} \frac{1}{k} \quad \text{(Oxygen starving)} \tag{3.10}
\]

where $\overline{C_f}$ and $\overline{C_{O_2}}$ are the local mean concentrations of fuel and oxygen, $r$ is the stoichiometric oxygen/fuel mass ratio and $A$ is a model constant. For premixed flames, fuel and oxygen occur in the same eddies. These eddies are separated by eddies containing hot combustion products. The rate of combustion can be assumed to be determined by the rate of intermixing or dissipation of these eddies on a molecular scale. Therefore an extra expression is needed in order to account for the dissipation of hot eddies in cases where the concentrations of hot combustion products is low and

\[
\overline{\omega}_f = A \cdot B \frac{\overline{C_{prod}}}{1+r} \frac{\varepsilon}{k} \quad \text{(Premixed)} \tag{3.11}
\]

where $\overline{C_{prod}}$ is the local mean concentration of the combustion products and $B$ is a model constant. The equation that yields the minimum rate is the one that determines
the local rate of combustion and the mean reaction rate of Magnussen and Hjertager's EBU model is given by

\[ \bar{\omega}_r = A \frac{\varepsilon}{k} \min \left( \frac{\bar{C}_r}{k}, \frac{\bar{C}_a}{r} \right) \left( \frac{B \cdot \bar{C}_{pr}}{(1+r)} \right) \]  

(3.12)

The EBU reaction model obtains a linear relationship between the turbulent burning velocity and the turbulent intensity. However in many cases, experimental observation shows that turbulent burning velocity is not linearly related to the turbulence intensity. Hence considerable errors in the prediction of the turbulent burning velocity are produced by this type of models. By the nature of assumptions inherent in the EBU models, local flame extinction cannot be accounted for, as it is valid only in the limit of fast chemistry. However the usefulness of the EBUM lies in its simplicity and its ability to account for the effect of mixing on combustion.

3.8.3.1. Eddy dissipation concept (EDC Model)

The eddy dissipation concept (EDC) proposed by Magnussen and Hjertager (1976) and extended by Magnussen (1980, 1989) is a reactor concept. In the EDC model, chemical reactions are assumed to occur in the small scale structures that characterise a turbulent flow. Chemical reactions occur when reactants are mixed at molecular level at sufficiently high temperatures. The molecular mixing determines the rate of chemical reactions in turbulent flows and the microscale processes that control it are highly intermittent i.e. they are concentrated in isolated regions that occupy a very small fraction of the volume of the fluid (Bradley 1992). These regions are occupied by fine structures whose dimensions are small in one or two directions but not in the third. These fine structures are believed to be vortex tubes, sheets or slabs whose characteristic dimensions are of the same magnitude as the Kolmogorov microscale (Gran et al. 1994).

Since the fine structures are responsible for the dissipation of turbulence into heat and for characterising the molecular scale processes, it can be assumed that within these structures, fuel and air will be mixed at molecular level. For
modelling purposes, one can assume that the reactants are mixed homogeneously within the fine structures so the parameters needed to calculate reaction rates with the EDC model are the mass transfer rate between the fine structures and the surrounding fluid and the volume occupied by the small scale structures where reactions occur (Gran 1994).

The turbulent fine structures are assumed to be concentrated in fine structure regions and the mass fraction of the flow occupied by such regions is given as

\[ \gamma = \left( \frac{3C_{D2}}{4C_{D1}} \right)^{\frac{3}{4}} \left( \frac{v^*}{k^2} \right)^{\frac{1}{4}} \]  

(3.13)

where \( C_{D1} = 0.134 \) and \( C_{D2} = 0.5 \) are model constants. The superscript * refer to the fine structures. The mass fraction occupied by the fine structures is \( \gamma' \). The time scale for the mass transfer rate between the fine structures and the surrounding is given as

\[ \tau^* = \left( \frac{C_{D2}}{3} \right)^{\frac{3}{2}} \left( \frac{v^*}{k^*} \right)^{\frac{1}{2}} = \left( \frac{C_{D2}}{3} \right)^{\frac{3}{2}} \tau_n \]  

(3.14)

where \( \tau_n \) is the Kolmogorov time scale. Although, \( \gamma' / \tau^* \) seems to give the rate of mass exchange between the fine structures and the surrounding, Magnussen (1989) found this under-predicts the mass exchange rate. This rate, therefore, is calculated as

\[ \dot{m}^* = \frac{\gamma^2}{\tau^*} = \frac{3}{2C_{D1}} \frac{\varepsilon}{k} \]  

(3.15)

and the mean species reaction rate is given by

\[ \dot{\rho}_s = \overline{\rho} \dot{m}^* \chi (Y_s - Y_s^*) \]  

(3.16)

where the superscript \( \circ \) refer to the fluid surrounding the fine structures and \( \chi \) is the fraction of fine structures where reaction occurs.
With the EDC, calculation of the fluctuation in species mass fraction is not required as in the original EBUM of Spalding. No additional equations to be solved for concentration fluctuations as in a PDF approach. Gran (1994) has shown that finite rate kinetics should be incorporated into the EDC approach to ensure good agreement with experimental results. Chemical kinetics effect are taken into account by treating the turbulent fine structures as constant pressure homogeneous reactors.

Eddy break up models can predict, after appropriate tuning, the correct trends of the flame speed, heat release and pressure as a function of the engine speed and load. However, mixing controlled models are inadequate to study ignition, knock, pollutant formation, rich and lean misfire limits and wall quenching because these phenomena are controlled by chemical kinetics (Ahmadi-Befrui et al. 1981, Abraham et al. 1985-a). The EBU and the EDC models have no provision for initiating combustion. It is common practice to employ the chemical kinetic single reaction SR model [section (3.8.1)] of Arrhenius type with a suitable criterion to switch over to the EBU or the EDC model.

Mixing controlled turbulent models generally suffer from what is known as the cold front boundary problem in which the reaction rate may not be uniquely determined. A remedy for this problem can be obtained by modifying the EBU model so that the reaction rate near the cold front is reduced to a level at which flame quench occur.

3.8.4. Characteristic time models

These models, which are based on the eddy break up concept, were first developed for SI engines by Abraham et al. (1985-a) and was then extended to diesel combustion by Kong et al.(1992). The basic conception behind these models is that the rate of change of the density of species, $i$ due to the conversion into another chemical species is governed by a characteristic time to achieve equilibrium, $\tau_c$, which is given by

$$\frac{dY_i}{dt} = \frac{Y_i - Y_i^*}{\tau_c}$$  \hspace{1cm} (3.17)
Here $Y_i$ is the mass fraction of species $i$ and $Y_i^*$ is the local, instantaneous thermodynamic equilibrium mass fraction for species $i$. The characteristic time, $\tau_e$, is a combination of the laminar kinetics time, $\tau_l$ and the turbulent mixing time, $\tau_t$. A delay coefficient, $f$ controls the transition from kinetics to mixing controlled time scales and $\tau_e$ is then given by

$$\tau_e = \tau_l + f \cdot \tau_t$$  \hspace{1cm} (3.18)

This formulation ensures that the process with the largest characteristic time controls the combustion. The forms of $\tau_l$ and $\tau_e$ are specific to the application (i.e. whether for the SI engine or the CI engine). In the case of SI engines, after the spark, this model simulates the growth of the initial flame kernel and its development into a fully turbulent flame and the turbulent propagation. The laminar kinetic time, $\tau_l$, based on experimental laminar flame speed data is given by (Kuo and Reitz 1992)

$$\tau_l = \frac{A T P^{-(1+2\beta)} e^{\left(\frac{E \cdot g(\phi)}{T}\right)}}{C_F^2}$$  \hspace{1cm} (3.19)

where

$$\beta = -0.16 + 0.22(\phi - 1.0)$$  \hspace{1cm} (3.20)

and

$$g(\phi) = 1.0 + B(|\phi - 1.15|)$$  \hspace{1cm} (3.21)

which would account for the effects of equivalence ratio, $\phi$ (Kuo and Reitz 1989, Reitz and Kuo 1989). In order to account for the effect of residual gases on laminar kinetics time, $C_F$ is used as

$$C_F = 1.27(1.0 - 2.1r)$$  \hspace{1cm} (3.22)
where \( r \) is the local residual mass fraction. If there is no residual gases present, \( C_F \) is taken to be unity. The turbulent mixing time, \( \tau_t \) which is proportional to the eddy turnover time is given by

\[
\tau_t = \frac{C_{m2} \eta k}{\varepsilon} \tag{3.23}
\]

Here, \( \eta \) is a parameter which is based on the progress or completeness of combustion and \( \eta = 1 \) when \( h \geq 1 \) and \( \eta = 1/h \) when \( h < 1 \) and \( h \) is given by

\[
h = \frac{C_{m2}}{C_{m3}} \left( \frac{Y_P - Y_{P_s}}{Y_F - Y_F^* + Y_{O_2} - Y_{O_2}^*} \right) \tag{3.24}
\]

Here \( Y \) is the mass fraction with superscript \( * \) for equilibrium condition and subscript \( s \) for the value at the time of spark. Subscripts \( F, O_2 \) and \( P \) are for the fuel, oxygen and products respectively (Abraham and Bracco 1985-a).

The delay co-efficient, \( f \) which models the increasing effect of turbulence as the flame kernel grows to a size comparable to the turbulent eddy size, \( l \) and is given by

\[
f = 1 - e^{-\left( \frac{t - t_s}{\tau_d} \right)} \tag{3.25}
\]

where \( (t - t_s) \) is the time elapsed after spark, \( S_L \) is the laminar flame speed and

\[
\tau_d = \frac{C_m l_t}{S_L} \tag{3.26}
\]

with

\[
l_t = \frac{C_{m4}^{\frac{3}{2}} k^{\frac{3}{2}}}{\kappa \varepsilon} \tag{3.27}
\]
where $\kappa$ is wall boundary layer Prandtl number and $C_\mu = 0.09$. In above expressions, $A$, $B$, $C_{m1}$, $C_{m2}$, $C_{m3}$ are model constants and their values have to be chosen according to the specific application and the fuel being used. Kuo and Reitz (1992) and Hampson et al. (1996) give these values for several different applications. It is seen that the model constant $C_{m1}$ needs heavy tuning as engine operating conditions are changed. Also, the model constants for Natural gas (Methane) is not available and needs to be experimentally established making this model not of much use for the present study.

3.8.5. Flamelet models

Of the regimes of combustion illustrated in fig. (3.3), the flamelet concept is applicable in the wrinkled laminar flamelet and the corrugated flamelet regimes. Most practical problems of turbulent premixed combustion including SI engine combustion fall in these flamelet categories (Abraham et al. 1985-b, Bray and Peters 1994). In these cases, the chemistry is fast enough so that one can consider that the unburned gases are separated from the burned gases by thin flamelets.

Two alternative definitions of the flamelet regime of combustion are given by Poinsot et al. (1991). The first is called the laminar flamelet assumption. It is based on the following hypotheses.

(i) The reacting flow field may be viewed as consisting of two distinct fluids: the unburned and the burned gases, separated by an interface (the flame surface) where chemical reactions take place.

(ii) The local structure of the flame front behaves exactly like a laminar flame (a flamelet).

Under this flamelet assumption, gases burn before they can diffuse and mix. This is equivalent to the classical ‘fast chemistry’ assumption, which reduces the problem of turbulent combustion to the description of the flame surface. By assuming the local flamelet is planar and steady, the local burning rate is then equal to that of a steady planar laminar flame so that only the flame front area needs to be modelled.
The second definition, or the extended flamelet assumption includes the fast chemistry assumption but the flamelet, however, does not necessarily have an exact laminar structure so that the local consumption rate is not directly related to the laminar flame speed. This approach allows the use of a modified laminar flame speed in the calculation of a local burning rate. Recent direct numerical simulations show that the local consumption rate is a quantity which changes in smaller proportion than the flame surface area so that its precise determination is probably less critical than a knowledge of the flame surface area (Rutland and Trouve 1990, Haworth and Poinso 1990).

It has been shown that the flame surface may be subjected to curvature, strain or unsteady effects without invalidating the flamelet assumption, as long as these effects do not disrupt the flame front, i.e., they do not quench it. Even length scales smaller than the flame front thickness might interact with the flame if their only effect is to thicken the flame front and increase the transport coefficients inside the flame zone. When the flame front is only slightly perturbed by the turbulent eddies, the regime corresponds to “wrinkled flamelets”. In more intense turbulence, pockets of unburned gases surrounded by burned products may exist in an extended flamelet regime as long as each pocket is surrounded by an active flame front. This mode of combustion is in the “corrugated flamelet” regime. If the local stretch induced by the turbulent flow on the flame front is sufficiently large and the flame is quenched at a given location, combustion ceases in the vicinity of this point and reactants will diffuse into the products without burning. In this situation, the flamelet concept becomes less adequate. Therefore, quenching in a turbulent premixed flame determines the limit between two essentially different behaviours and is an important mechanism in the description and modelling of turbulent combustion (Poinsot et al. 1991).

The essence of the laminar flamelet models of a turbulent premixed flame is that the local time-dependent flame structure consists of an ensemble of laminar flames. These models assume that combustion and heat release in a turbulent flame can be represented through the effects of one or more moving laminar flamelets. The most fundamental property of these flamelets is that they are asymptotically thin layers having a well defined inner structure and are embedded within the turbulent flow field. In the flamelet regime, the flame thickness is small compared to the
smallest scale of turbulent flow (i.e. Kolmogorov scale) and the flamelet concept is valid only if this is true. The chemical time scale and thermal diffusivity determine the flame thickness and the flame velocity, which in turn describe characteristic length and velocity scales respectively. Overall flame thickness is governed by the Damköhler number of the rate determining reaction. For the flamelet to be thin, the Damköhler number of the second kind (ratio of thermal diffusion time scale to reaction time scale) has to be large and this is the most common situation in practical combustion systems. Combustion reactions occur only within these flamelets and therefore the reaction and the molecular diffusion is closely coupled. Thermal diffusion and heat conduction remain important within the flamelet structure while convection is a lower order term in the chemically reacting part of the flamelets as long as they are asymptotically thin.

A genuine property of premixed flamelets is their ability to propagate and to interact with eddies of a specific scale (Gibson scale). Stretch effects can be imposed on flamelets and the flame velocity is changed due to the response from the inner of the flamelet and in some cases the flame may extinguish. In premixed combustion, flamelets are not attached to the surface imposed by the mixing field but they propagate normal to themselves into the turbulent mixture. Hence the interaction between flamelets and the outer flow is much stronger and therefore the location of the flamelet depends on the flow field itself (Bray 1985, Peters 1986).

A variety of models using the flamelet concept has been devised in recent years. In certain cases a PDF is used to couple the local flamelet analysis to the flow description (Liew et al. 1981, Peters 1984). Pope and Cheng (1988) proposed a stochastic flamelet model for turbulent premixed combustion in which the flame sheet is represented statistically by infinitesimal flamelets, each characterised by its position, its unit normal vector, and its area. The evolution of the position and normal are completely determined by the fluid velocity and its spatial derivatives following the flamelet, which are modelled by stochastic processes. Some flamelet models rely on the flamelet crossing frequencies to evaluate the mean reaction rates (Bray 1986, Bray et al. 1988, Cheng et al. 1988). The most significant feature of the crossing frequency concept is that it can be measured directly in experiments using simple laser techniques. Still another approach is based on a balance equation for the available flame area and this equation describes the transport of the flame surface by the
turbulent flow field and the physical mechanisms, which produce and destroy the reactive surface. The latter approach has evolved as the coherent flamelet model and will be discussed below, with specific consideration given only to the case of premixed combustion. The other flamelet approach, which has been under development in recent years, based on the fractal or statistical geometry of flamelets, will be discussed in details in chapter 4.

However diverse these many approaches to the flamelet description are, they all share the following elements (Candel et al. 1990)

(i) a laminar flamelet sub-model(s) providing the local structure and properties of the reactive elements
(ii) a description of the turbulent flow comprising mass average equations describing the mean flow variables, the mean species mass fractions and the relevant closure equations
(iii) a set of rules which couple the flamelet sub-model(s) to the turbulent flow description and
(iv) additional sub-models accounting for chemical reactions taking place outside the flamelets.

Reviews due to Peters (1984, 1986), Bray (1987) and Candel et al. (1990) describe some of the possible ways in specifying and combining these elements. An important advantage of the flamelet concept is that it essentially decouples the complex chemistry problems from the modelling of the turbulent flow.

3.8.5.1. Coherent flame sheet model (CFM)

Coherent flame models, first introduced by Marble and Broadwell (1977) for diffusion flames, identify important physical mechanisms of turbulent combustion such as the production of flame area by stretching, destruction of flame by flame shortening and the central influence of the strain rate acting on the local flamelets. The CFM for premixed flow configurations have been introduced by Candel et al. (1982) and Veynante et al (1989) presented a new description of the CFM that can account for both premixed and non-premixed flamelets.
With the aid of spark Schlieren photographs, it has been observed that the increase in flame surface area is essentially due to the strain rates acting in the plane of the flame while its dissipation is determined by the consumption of the fresh mixture and the mutual annihilation of adjacent reactive sheets. In the same time, some of the excessively high rates of turbulent strain may be responsible for a reduction of the flame surface (Candel et al. 1982). In the CFM context, it is assumed that the flame elements are convected and destroyed by the turbulent motion but that they retain an identifiable structure.

The local strain rate acting in the plane of the flame modifies its structure and changes the local reaction rate. Therefore the local consumption rate per unit of flame area may be obtained from an analysis of strained laminar flames. The mean consumption rate of a species \( m \), per unit volume at a point of the flow, \( \omega_m \) may be determined as the product of the mean flame surface density at that point (i.e. the flame surface per unit volume), \( \Sigma_f \) and the consumption rate of laminar strained flame elements per unit of flame area, \( V_f \) obtained from the analysis of local strained laminar flamelets

\[
\omega_m = \rho_u \cdot V_f \cdot \Sigma_f
\]  

(3.28)

In its simplest form, the coherent flame description of turbulent flows combines a model for the turbulent flow, a local model for \( V_f \) and a balance equation for \( \Sigma_f \). Chemical and molecular effects are represented in \( V_f \), while turbulence effects are represented in \( \Sigma_f \). The conservation equation for \( \Sigma_f \) is

\[
\frac{\partial \Sigma_f}{\partial t} + \frac{\partial}{\partial x_i}(U_i \Sigma_f) = \frac{\partial}{\partial x_i}(D_i \frac{\partial \Sigma_f}{\partial x_i}) + S - D
\]  

(3.29)

where \( S \) is the production of flame surface by turbulent strain, \( D \) is the destruction of flame surface by mutual collision of adjacent flamelets, quenching etc. and \( D_i \) is turbulent diffusivity, which is given by

\[
D_i = C_{\mu} \frac{k^2}{\epsilon}
\]  

(3.30)
where \( C_\mu = 0.09 \).

Several variations of the CFM for SI engine combustion are available in the literature due to the improvements (usually, different aspects of turbulent combustion such as flamelet stretch effects being added to the model) made by many researchers. These differences are mainly in the expressions used for the production and the destruction terms of flame surface density (\( S \) and \( D \)) in the conservation equation [eqn. (3.29)]. Table (3.1) summarises some of the most commonly used variations for \( S \) and \( D \) terms.

Table (3.1). Production and destruction of flame surface density in the CFM models

(\( \alpha \) and \( \beta \) in these terms are the adjustable model constants)

<table>
<thead>
<tr>
<th>Model</th>
<th>( S )</th>
<th>( D )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cheng and Diringer (1991)</td>
<td>( \alpha C_e \frac{e}{k} \Sigma_f )</td>
<td>( \beta \frac{S_L}{Y_1} \Sigma_f^2 )</td>
</tr>
<tr>
<td>Boudier et al. (1992)</td>
<td>( \alpha \Gamma \frac{e}{k} \Sigma_f )</td>
<td>( \beta \frac{S_L + C_D}{Y_1} \Sigma_f^2 )</td>
</tr>
<tr>
<td>Zhao et al. (1994)</td>
<td>( \alpha \Gamma \frac{C_e}{k} \left( \frac{15}{L} \right) \Sigma_f )</td>
<td>( \beta \frac{S_L}{Y_1} \Sigma_f^2 )</td>
</tr>
<tr>
<td>Choi and Huh, CFM-1, (1998)</td>
<td>( \alpha \left( \frac{e}{15v} \right)^{\frac{1}{2}} \Sigma_f )</td>
<td>( \beta \frac{S_L}{Y_1 (1 - Y_1)} \Sigma_f^2 )</td>
</tr>
<tr>
<td>Choi and Huh, CFM-2, (1998)</td>
<td>( \alpha \frac{u^*}{l_{fc}} \Sigma_f )</td>
<td>( \beta \frac{S_L}{Y_1 (1 - Y_1)} \Sigma_f^2 )</td>
</tr>
</tbody>
</table>

In those models, \( \alpha \) and \( \beta \) are the adjustable model constants, \( S_L \) is the unstrained laminar burning velocity and \( Y_1 \) is the unburned mixture mass fraction. In Cheng and Diringer's CFM (1991), \( C_e (= 5.0) \) is a constant. In the CFM version by Boudier et al. (1992), \( C_D (= 0.1) \) is a constant and
\[ \Gamma_k = \Gamma_k - \frac{3}{2} \left( \frac{L}{\delta_L} \right) \left( \frac{u'}{S_L} \right) \ln \left( \frac{1}{1 - p_q} \right) \]  

(3.31)

where \( \Gamma_k \) is the total flame stretch normalised by the mean strain rate, \( L \) is the integral length scale, \( \delta_L \) is the laminar flame thickness, \( u' \) is the turbulence intensity and \( p_q \) is the total fraction of flame surface undergoing quenching. Relationships for \( \Gamma_k \) and \( p_q \) are due to Meneveau and Poinsot (1991). In the CFM version by Zhao et al. (1994), \( Re_T \) is the turbulent Reynolds number and \( \gamma (= 0.7) \) is a constant. \( \Gamma_k \) and \( C_x \) are as explained before. In Choi and Huh versions (1998), \( \nu \) is kinematic viscosity and \( l_{tc} \) is an arbitrary length scale introduced for dimensional consistency and could be combined with the model constant \( \alpha \) as a single arbitrary tuning constant for the production term, \( S \).

In order to implement this model in the CFD code, KIVA-II, the quantity \( \rho \Sigma_f \) is treated as a pseudo-species partial density so that no extra coding of the left hand side terms of the conservation equation for \( \Sigma_f \) is necessary. This benefit is obtainable due to the way KIVA-II has been coded. However, \( S_L \) has to be calculated considering the dependence of temperature, pressure, fuel type used, equivalence ratio and residual gas fraction.

3.8.5.2. Fractal flame model (FFM)

Gouldin (1987) was the first to apply the concept of fractals to the modelling of premixed turbulent flames, claiming that the importance of the multi-scaled nature of flame surface wrinkling was not accounted for in earlier flamelet models. This model takes the fractal nature of the turbulent flame front into consideration with the laminar flamelet assumptions. Unlike the CFM, the use of fractal geometry explicitly accounts for the entire distribution of flame wrinkling scales. Also, the FFM incorporates only one model constant and does not require solution of an additional differential equation for flame surface density. An improved version of the FFM was incorporated as the combustion model in KIVA-II for the present study and is described in detail in Chapter 4.
3.9. Choice of a combustion model

It is not easy to make a choice of a combustion model for a particular application. New promising methods are frequently developed and old techniques are often improved. However, the making of a certain choice is a matter of necessity, otherwise the search for the final ideal model may last forever. Level of accuracy expected in calculations, computational resources available and computational time affordable for certain applications etc. may be decisive factors in choosing a suitable combustion model.

During the discussion above, it was possible to gather the inherent strengths and weaknesses of commonly used CFD models for premixed combustion in SI engines. The SRM did not have the most important aspect of fluid flow within the cylinder, the effects of turbulence on combustion included in it. The EBUM is simple to handle but did not have the effects of chemical kinetics included in the model and usually the model constants need adjusting, or tuning for a particular engine geometry etc. It was found that determining the two constants in the EBU model for a particular engine application using trial and error is a tedious task. The flamelet combustion regime where SI engine combustion falls in is inherently difficult to treat with PDF methods, as discussed above. Characteristic time model, being an extension of the EBU type models, needs experimentally establishing the model constants and other related empirical constants for natural gas combustion in SI engines before using for the present study. It also has model constants of less global nature and needs re-adjusting as conditions change. Flamelet models, therefore, proved to be the best choice. When compared with the CFM, the FFM does not require solving an extra equation and had only a single adjustable constant and computationally, this provides a significant saving of resources. Working with a single model constant makes life much easier when establishing the constant for a particular engine application by trial and error method while minimising the errors possible when handling several model constants in the same manner. Most importantly, Zhao et al. (1994) showed that the FFM has a better predictive capability compared to the CFM for a propane fuelled SI engine. Further, De Petris et al. (1995) established the strength of the FFM as a combustion model for an iso-octane fuelled SI engine. Also considering the work by Mantzaras et al. (1989) and Hall et al. (1992), which strengthened the idea of fractal
nature of flames in SI engines, the FFM was chosen as the combustion model to be implemented in the CFD code KIVA-II for the present study.
After analysing several commonly used SI engine multi-dimensional combustion models in chapter 3, the Fractal Flame Model (FFM) was chosen to be used in the present study. This model uses the concepts of fractal geometry to account for the effects of turbulence on flame wrinkling and is described here with the implementation of the model in KIVA-II code and the validation of the model. Further, the FFM will be compared with two other commonly used combustion models, namely the Arrhenius type single reaction model (SRM) and the eddy break-up (EBU) model.

4.1. Fractal geometry and turbulence

Mandelbrot (1982) suggested that several facets of fully developed turbulent flows are fractals, which by definition are objects that display self-similarity over a wide range of scales. Analogous to the Euclidean dimensions of classical (ordinary) objects, each fractal object is characterised by a fractal dimension, which is a measure of its fragmentation or degree of wrinkling. For a turbulent flame the fractal dimension is a quantitative measure of the distribution of the flame wrinkling scales.
Sreenivasan and Meneveau (1986) studied the fractal dimensions of many types of surfaces found in turbulent flows. Their studies showed that some of these surfaces are fractal-like and experimental measurements were made to obtain the corresponding fractal dimensions.

4.2. Fractal aspects of premixed turbulent combustion

Flame visualisation studies have shown that flame surfaces in a turbulent combustion process can be extremely rough and therefore it can be very difficult to characterise the flame surface area. Flame images have shown that the flames in SI engines are fractal surfaces (Mantzaras et al. 1989, Dai et al. 1991, Hall et al. 1992). Gouldin (1987) was the first to apply fractal geometry to the study of turbulent flames. He pointed out that the earlier models of wrinkled laminar flames attempted to predict flamelet area and combustion rates in terms of turbulent properties either in the reactant or product flows and these attempts were not successful in part due to the fact that only one scale of surface wrinkling was considered. Using fractal geometry and assuming homogeneous and isotropic turbulence, Gouldin showed that the actual area of the flame front, $A_f$ in the flamelet regimes can be calculated by

$$A_f = A_i = A_o \left( \frac{\varepsilon_i}{\varepsilon_o} \right)^{2-D}$$  (4.1)

where

- $\varepsilon_i$ inner cut-off length scale (the minimum flame wrinkling scale)
- $\varepsilon_o$ outer cut-off length scale (the maximum flame wrinkling scale)
- $A_i$ measured flame surface area using length scale $\varepsilon_i$
- $A_o$ measured flame surface area using length scale $\varepsilon_o$
- $D$ fractal dimension of the flame surface

The flame wrinkles are caused by the interaction between the flame and the turbulent eddies. Thus, the inner cut-off results from the smallest turbulent
eddies - those of the size of the Kolmogorov length scale, $\eta$. However, the local laminar flame propagation process tends to smooth out these small scale wrinkles and it is known that the minimum flame wrinkling scale is somewhat larger than the Kolmogorov scale. It has been shown that the minimum flame wrinkling scale is 1.3 to 5.8 times larger than the Kolmogorov scale for V-shaped and grid stabilised flames (Gouldin et al. 1988, Murayama and Takeno 1988). The minimum flame wrinkling scale has not been measured in an engine as both the Kolmogorov scale and the minimum flame wrinkling scale, under engine conditions, are smaller than the thickness of the laser sheet that is used to obtain the images for such analyses. The outer cut-off or maximum flame wrinkling scale is caused by the interactions between the flame and the largest turbulent eddies - those of the size of the integral length scale, $L$. However, these large wrinkles can grow due to the flame propagation process. The maximum flame wrinkling scale has been shown to be larger than the integral length scale for laboratory burner flames (Gouldin et al. 1988). Mantzaras and co-workers (1988, 1989) claim to have resolved the maximum flame wrinkling scale in an engine as twice the integral length scale. A theoretical basis for predicting the outer cut-off has not yet been developed. However, it is obvious that the maximum scale of flame wrinkling cannot be larger than the flame dimension. During early flame growth, the flame dimension is smaller than the integral scale and increases as the flame propagates.

Matthews (1991-a, -b) and co-workers (Chin et al. 1992, Wu et al. 1993) were the first to apply the concepts of fractal geometry to predict the combustion process in SI engines, in their case via a quasi-dimensional code, UTFES. In their earlier work (Matthews 1991-a), they assumed that the ratio of the maximum-to-minimum scales of flame wrinkling was equal to the ratio of the maximum-to-minimum scales of turbulence. That is, during fully developed turbulent combustion,

$$\frac{\varepsilon_0}{\varepsilon_i} = \frac{L}{\eta} \quad (4.2)$$

Similarly, since the maximum flame wrinkling scale cannot be larger than the flame dimension, during early flame growth the ratio of the flame wrinkling scales was assumed to be
where \( r_f \) is the flame radius. Matthews and co-workers found that these assumptions gave accurate results over a range of equivalence ratios and loads for the engine they studied. A study by Wu et al. (1993) showed that the same assumptions provide excellent predictions for the two engines studied over a range of engine speeds.

Measurements by Mantzaras et al. (1988, 1989) showed that the fractal dimension of the flame surface increased with increasing \( u'/S_L \). Over the range of conditions they studied, the maximum fractal dimension they found was \( \sim 2.37 \). North and Santavicca (1990) conducted an experimental study on a freely propagating premixed turbulent flame over a range of turbulent Reynolds numbers from 52 to 1431 and Damköhler numbers from 10 to 889. They confirmed that the fractal dimension of the flame increased with \( u'/S_L \) and a heuristic relationship was developed as

\[
D = D_L \frac{S_L}{u' + S_L} + D_T \frac{u'}{u' + S_L}
\]  

where

- \( D_L \) fractal dimension for a smooth flame surface
- \( D_T \) maximum possible fractal dimension for a turbulent passive scalar in a high Reynolds number flow
- \( u' \) turbulence intensity
- \( S_L \) unstretched laminar flame speed

Santavicca and co-workers (North and Santavicca 1990, Liou et al. 1990) suggested values of 2.0 and 2.35 for \( D_L \) and \( D_T \), respectively, based upon their experimental results. The value for \( D_L \) is obviously correct, as the fractal dimension of a smooth flame surface should equal its topological dimension. However, several theories exist for the value of \( D_T \). Kerstein (1988) analysed the fractal dimension of turbulent premixed flames based on the Kolmogorov cascade picture of fully developed turbulence. He suggested that the flame front was not effectively a passive
interface in the fractal range of length scales as previously assumed by other researchers and he predicted a fractal dimension of \( D = 7/3 \) (\( \equiv 2.33 \)). Liou et al. (1990) used different techniques to derive the same result of \( D_T = 2.33 \) while theories predicting \( D_T \) as high as 2.41 have also been proposed (Francke and Peters 1990). In fact, 2.33 seems too low for \( D_T \) since Santavicca and co-workers measured maximum fractal dimensions of 2.35 in a turbulent flow reactor while Mantzaras et al. (1988, 1989) measured a maximum value of 2.37 in an engine. For the present study, the value \( D_T = 2.35 \) was chosen because of the previous excellent results that had been obtained with eqn. (4.4) by Zhao et al. (1994).

Wu et al. (1993) noted that the heuristic model developed for laboratory flames [eqn. (4.4)] can be extrapolated to flames in engines on the evidence of the universal nature of fully developed turbulent flames. The physical argument for eqn. (4.3) is that the turbulence, which is characterised by \( u' \), wrinkles the flame while the small scale wrinkles are smoothened by the local laminar flame propagation process characterised by \( S_L \). However, during early flame growth, the flame radius is smaller than many of the scales of turbulence. Thus, Zhu et al. (1992, 1993) argued that the appropriate eddy velocity used in calculating the fractal dimension during early flame growth cannot be \( u' \) since the flame cannot be wrinkled by integral size eddies, rather the eddy velocity that corresponds to the largest eddies that can wrinkle the young flame kernel, \( u_{\text{max}} \), resulting in

\[
D = 2.0 \frac{S_L}{u_{\text{max}} + S_L} + 2.35 \frac{u_{\text{max}}}{u_{\text{max}} + S_L} \tag{4.5}
\]

These researchers then noted that, since the largest eddies should be of the scale of the flame radius, the corresponding eddy velocity can be determined from eddy cascade arguments

\[
\epsilon = \frac{u'^3}{L} = \frac{u_{\text{max}}^3}{r_f} \tag{4.6}
\]

where \( r_f \) is the flame radius. However, in their quasi-dimensional engine simulations, Wu et al. (1993) tested the use of eqn. (4.5) against the use of eqn. (4.4) during early
flame growth and found that this choice made essentially no difference in the resulting predictions of burning rate or cylinder pressure history.

A different correlation for calculating the fractal dimension had been obtained by Zhao et al. (1994) by curve-fitting North and Santavicca's (1990) measurements of fractal dimension using the turbulent Reynolds number $Re_T$ as shown in fig. (4.1). This new correlation was used in the present study in calculating the fractal dimension of the wrinkled turbulent flame surface and given as

$$D = 2.0 \frac{200}{Re_T + 200} + 2.35 \frac{Re_T}{Re_T + 200} \quad (4.7)$$

![Figure (4.1). Variation of the fractal dimension with the turbulent Reynolds number](image)

Several theories have been proposed for using the fractal geometry for the evaluation of both the global turbulent flame speed (Gouldin 1987, Gülder 1990-b) and the local mean reaction rate (Gouldin et al. 1989). The FFM used in the present study for multi-dimensional modelling calculations is based on the original formulation developed by Gouldin et al. (1989) and will be discussed in the following
section. The modifications that have been made to the original formulation in order to
develop the FFM will be discussed afterwards.

4.3. The multi-dimensional fractal model of Gouldin et al.

Gouldin et al. (1989) proposed a fractal model for turbulent premixed combustion, specifically developed for use in multi-dimensional calculations. They assumed combustion to occur in homogeneous and isotropic turbulence and that the flame surface can be represented as a fractal surface. A relationship for calculating the mean flame surface area in the cell volume \( L_c^3 \) was formulated as

\[
A_f = A_i = A_0 \left( \frac{\varepsilon_i}{\varepsilon_o} \right)^2 - D P_c
\]  

(4.8)

where

- \( \varepsilon_i \) inner cut-off length scale (the minimum flame wrinkling scale)
- \( \varepsilon_o \) outer cut-off length scale (the maximum flame wrinkling scale)
- \( A_i \) measured flame surface area using length scale \( \varepsilon_i \)
- \( A_o \) measured flame surface area using length scale \( \varepsilon_o \)

Compared to eqn.(4.1), eqn.(4.8) consists of an additional parameter \( P_c \), which Gouldin et al. (1989) proposed to account for the probability that a flamelet lies in the volume \( L_c^3 \). This quantity is necessary for multi-dimensional simulations in which local burning rates, instead of the global burning rate, are calculated. A formulation was proposed by Gouldin et al. (1989) for this probability function as

\[
P_c \approx \bar{c} (1 - \bar{c}) \frac{L_c}{L_F}
\]  

(4.9)

where

- \( L_c \) the cell dimension
- \( L_F \) flame brush thickness
and the degree of reaction, $c$ is defined as

$$c = \frac{Y_{fu} - Y_f}{Y_{fu} - Y_{fb}}$$

(4.10)

where

- $Y_f$ mass fraction of fuel in the mixture
- $Y_{fu}$ mass fraction of fuel in the unburned region
- $Y_{fb}$ mass fraction of fuel in the burned region

Gouldin et al. then argued that the value of $L_c$ should be comparable to the integral length scale $L$. If $L_c$ was too small, the flame surface in $L_c$ would not be representative of all scales of wrinkling. On the other hand, if $L_c$ were too large, the distribution of flame surface in $L_c^2$ would not be homogeneous and isotropic. Gouldin et al. therefore assumed that $L_c = L = \varepsilon_0$ in their burning model. For the inner cut-off wrinkling scale, they proposed that $\varepsilon_i = \eta / f$ where $\eta$ is the Kolmogorov microscale, which represents the minimum possible scale of surface wrinkling and $f (<1)$ is a monotonically increasing function of $u'/S_L$ ratio and turbulent Reynolds number and accounts for smoothing at the smallest scales of wrinkling due to flamelet propagating relative to the reactant flow. Also, $A_o$ in eqn. (4.8) has been estimated as proportional to $L_c^2$. The burning model originally proposed by Gouldin et al. can then be expressed as

$$\bar{\omega} = C_{RI} \rho_u S_L (\Delta Y_f) \left( \frac{\eta}{L \cdot f} \right)^{2-D} \frac{c(1-c)}{L_f}$$

(4.11)

where $\bar{\omega}$ is the average mass burning rate, $\Delta Y_f$ is the change of fuel mass fraction across the flamelet, $L$ is integral length scale and $C_{RI}$ is a model constant. Gouldin et al. suggested that the flame brush thickness $L_f$ in eqn. (4.11) can be calculated as the distance between $c = 0.1$ and $c = 0.9$ but in multi-dimensional simulations this is difficult to accomplish, especially when the flame surface is distorted by the flow.
Numerical studies by Zhao (1994) showed that this fractal model by Gouldin et al. under-predicts the turbulent flame speed and the burning rates were not scaled correctly with the turbulent Reynolds number (or turbulence intensity) as the model does not have a strong enough dependency on the turbulence intensity.

4.4. The multi-dimensional fractal model of Gülder

Gülder (1990-b) revised the formulation by Gouldin et al. (1989) for calculating the ratio of wrinkling scales and proposed a different relationship for the inner cut-off wrinkling scale, \( \varepsilon_i \), which is given by

\[
\varepsilon_i = 10 \left( \frac{u'}{S_L} \right)^{-3/2} \eta
\]  

(4.12)

and used the integral length scale as the outer cut-off length scale, or \( \varepsilon_o = L \). Assuming the fractal dimension \( D = 7/3 \), a formulation for the turbulent flame speed was then given by

\[
\frac{S_T}{S_L} \propto \left( \frac{u'}{S_L} \right)^{1/2} \frac{1}{Re_T^{1/4}}
\] 

(4.13)

By substituting \( \frac{u'}{S_L} = Re_T \frac{8}{L} \), this becomes

\[
S_T = C_{R2} S_L \left( \frac{8}{L} \right)^{1/2} Re_T^{3/4}
\] 

(4.14)

where \( C_{R2} \) is a constant of proportionality. Gülder (1990-b), using this expression, achieved good agreement between predictions and a variety of experimental data for the turbulent flame speed, including results for several different fuels and oxidants. However, one problem with Gülder’s formulation for the inner cut-off [eqn. (4.12)] is that in order to satisfy the condition \( \varepsilon_i \geq \eta \),
has to be true (or \( u' / S_L \leq 4.642 \)). Therefore, to follow Gülder's model completely when using his formulation for the turbulent flame speed, one has to add the restriction, \( u' / S_L < 4.642 \) to eqn. (4.13). Unfortunately, this restriction means that Gülder's model is only applicable to low \( u' / S_L \) region. However, it is obvious that a large \( u' / S_L \) must have been assumed when Gülder derived the model because a fractal dimension \( D = 7/3 \) which is only true at large \( u' / S_L \) has been used. Despite this incompatibility, eqn. (4.14) appears to give very good predictions of turbulent flame speed for a variety of conditions.

4.5. The multi-dimensional fractal model of Zhao et al.

Based on Gülder's model and using the assumption

\[
\frac{\varepsilon_0}{\varepsilon_1} = \frac{L}{\eta} \quad (4.2)
\]

which gave excellent results when used in the quasi-dimensional Fractal Engine Simulation, UTFES by Wu et al. (1993), Zhao (1994) proposed a new fractal model given by

\[
S_T = C_{R3} \rho_o S_L \left( \frac{\varepsilon_1}{\varepsilon_0} \right)^{2-D} \quad (4.15)
\]

Substituting from eqn. (4.2) and assuming \( C_{R3} \propto \left( \frac{u'}{S_L} \right)^{\frac{\gamma}{2}} \)

\[
S_T = C_{R3} \rho_o S_L \left( \frac{u'}{S_L} \right)^{\frac{\gamma}{2}} \left( \frac{\eta}{L} \right)^{2-D} \quad (4.16)
\]
where $C_F$ is a new constant of proportionality. Substituting for $u'/S_L$ and $\eta$ yields

$$S_T = C_F \rho_\infty S_L \left( \frac{\delta_L}{L} \right)^{\frac{3}{2}} (Re_T)^{3/4}$$  \hspace{1cm} (4.17)$$

At high Reynolds numbers, taking $D = 7/3$ yields

$$S_T = C_F \rho_\infty S_L \left( \frac{\delta_L}{L} \right)^{\frac{3}{2}} (Re_T)^{3/4}$$  \hspace{1cm} (4.18)$$

or

$$S_T \propto S_L \left( \frac{\delta_L}{L} \right)^{\frac{3}{2}} (Re_T)^{3/4}$$  \hspace{1cm} (4.19)$$

which is the same as Gülder's result [eqn. (4.14)] but without the restriction $u'/S_L < 4.642$. Thus, this fractal model could be expected to provide the same excellent comparisons of numerical predictions with the data, as obtained by Gülder but without the logical difficulties or restrictions. However this model does not include the effect of flame stretch, which has the highest significance at high turbulent Reynolds numbers, and therefore poor predictions were obtained by Zhao (1994) at high turbulent Reynolds numbers.

In a turbulent reacting flow, flame stretch is caused by the motion of turbulent eddies and each different size of eddy will contribute to the total stretch of the flame surface. A general definition of flame stretch is given as the time derivative of the logarithm of the flame surface area. A mathematical derivation of the relation for flame stretch was obtained by Candel et al. (1990) using a general transport theorem as

$$K = \frac{1}{A_f} \frac{\partial (A_f)}{\partial t} = - (v_i v_j + \eta_i \eta_j) \left\{ \frac{\partial u_i}{\partial x_j} + S_L \frac{\partial \eta_i}{\partial x_j} \right\}$$  \hspace{1cm} (4.20)$$

where

$K$ Karlovitz flame stretch rate
According to this, flame stretch consists of two parts $K = K_S + K_C$, where $K_S$ is due to the strain in the tangential plane (first term on the RHS in eqn. (4.20)) and $K_C$ is the flame stretch associated with flame curvature (second term on the RHS). However, according to the experimental study by Lee et al. (1992), it is possible to neglect the flame stretch due to curvature and therefore $K = K_S$.

Zhao et al. (1994) used the model developed by Chung and Law (1988) to predict the effect of stretch on the laminar flame speed, $S_L$. For flames with a Lewis number of 1, the stretched laminar flame speed, $S_{L,S}$ was calculated as

$$S_{L,S} = S_L \left( 1 - \frac{v}{S_L^2} K \right) \quad (4.21)$$

where $v$ is the laminar kinematic viscosity of the unburned mixture and $K$ is the Karlovitz flame stretch rate. Several models for calculating the flame strain due to turbulent eddy motion have been proposed (Abdel-Gayed et al. 1987, Meneveau and Poinsot 1991, Chin et al. 1992, Wu et al. 1993) and suitably, Zhao et al. assumed

$$K_S = A \sqrt{\frac{\varepsilon}{\nu}} \quad (4.22)$$

which can be rewritten by noting that $\varepsilon = u'^3/L$ as

$$K = A \frac{u'}{L} Re_T^{1/2} \quad (4.23)$$

where $A (= 0.1)$ is a model constant after Wu et al. (1993). Substituting eqn. (4.23) into eqn. (4.21) with $\nu = S_L \delta_L$ and $u'/S_L = Re_T \delta_L/L$ yields
\[ S_{L,S} = S_L \left( 1 - A \left( \frac{\delta_f}{L} \right)^2 (Re_T)^{3/2} \right) \]  

(4.24)

Incorporating this into eqn. (4.18) yields

\[ S_T = C_F S_L \left( \frac{\delta_f}{L} \right)^{1/2} (Re_T)^{(3D-4)/2} \left( 1 - A \left( \frac{\delta_f}{L} \right)^2 (Re_T)^{3/2} \right) \]  

(4.25)

and this is the flame speed model with flame stretch effects included. A very good agreement has been obtained between the measurements and the predictions using eqn. (4.25) by Zhao \textit{et al.} (1994) for propane-air mixtures. Adopting the probability function relationship used by Gouldin \textit{et al.} (1989) for multi-dimensional simulations, the new fractal model was given as

\[ \bar{\omega} = C_F' \rho_u S_L \left( \frac{\delta_f}{L} \right)^{1/2} \left( 1 - A \left( \frac{\delta_f}{L} \right)^2 (Re_T)^{3/2} \right) \left( \frac{Re_T^{(3D-4)/4}}{L_F} \right) \bar{c} (1 - \bar{c}) \]  

(4.26)

where \( C_F' \) is a model constant and the degree of reaction, \( \bar{c} \) defined as

\[ \bar{c} = \frac{\bar{Y}_{fu} - \bar{Y}_f}{\bar{Y}_{fu} - \bar{Y}_{fb}} \]  

(4.10)

The fractal dimension can be calculated using eqn. (4.7). The flame brush thickness, \( L_F \) was taken as proportional to the integral length scale, \( L \) and Zhao named this model the Fractal Flame Model (FFM).

4.6. Improvements to the FFM by De Petris \textit{et al.}

De Petris \textit{et al.} (1995) used the FFM expression [eqn. (4.26)] with the single model constant, \( C_F' \) expanded allowing the consideration of the fuel properties. This expanded model constant is given as
\[
C_F' = \frac{C_F''}{(b_1 - b_2)(\alpha_s - 1)MW_F}
\]

where \(b_1, b_2\) are the stoichiometric coefficients of the fuel species, \(\alpha_s\) is the stoichiometric air/fuel ratio, \(MW_F\) is the molecular weight of the fuel and \(C_F''\) is a new constant. They used this extended constant in their numerical simulations of iso-octane combustion in an SI engine and obtained very good agreement with experiments.

4.7. Improvements to the FFM during the present study

Zhao (1994) assumed the following for the model development.

1. The gases in the combustion chamber are divided into two species; burned and unburned.
2. The composition of the burned gas is that resulting from complete combustion.
3. The dominant effect of turbulence on the flame is to wrinkle the flame surface while the inner structure of the flame is not significantly altered by the turbulent flow field.

It is argued here that the first of these assumptions is not suitably applicable in the case of a multi dimensional CFD study in which the combustion chamber (numerical domain) is divided into many numerical cells. Unlike the way two-dimensional combustion calculations consider two or three generalised zones within the combustion chamber, CFD multi-dimensional calculations individually consider chemical reactions that take place in each numerical cell, i.e. in many smaller zones. This approach permits the idea of unequal reaction rates at different locations within the combustion chamber and considering the reactions taking place behind the flame front. In such a situation, the definition of a distinct flame front dividing the gases in the combustion chamber as unburned and burned is not possible in the context of CFD calculations, especially when using orthogonal structured grid methods. To get closer to a spherical flame front with fractal nature dominating, an extremely fine grid needs to be used.
Suitably, the idea of treating the unburned mixture as an individual species was discarded in the present calculations and the constituent species (Fuel, O₂ and N₂) were considered individually. Similarly, the constituent species of the burned mixture (CO₂, H₂O and N₂) are considered as individual species, not as the single species called the burned mixture. The second assumption of Zhao was unnecessary as equilibrium chemistry was incorporated in the present study, enabling the calculation of CO emissions and OH concentrations [eqn. (2.17)]. To be compatible with these improvements, the degree of reaction at each numerical cell, which was given by eqn. (4.10) is re-defined as

\[
\varepsilon = \frac{\text{Mass of reactants in the cell}}{\text{Total cell mass}}, \quad (0 \leq \varepsilon \leq 1) \tag{4.28}
\]

Initially, once the fresh charge is sealed in the cylinder by closed valves and if no residual gases from the previous cycle are present, there will only be reactants in the combustion chamber giving the situation where \( \varepsilon = 1 \). At the end of combustion, provided that complete combustion has converted all the reactants into combustion products, the situation where \( \varepsilon = 0 \) arises. In all other situations including when there is recirculated exhaust gases present in the initial unburned charge and during combustion while still a portion of initial reactants are waiting to be converted to combustion products, \( 0 < \varepsilon < 1 \) situation will prevail. As seen in eqn. (4.26), the value of \( \varepsilon \) plays an important role in calculating the reaction rate in a numerical cell and therefore the proper definition \( \varepsilon \) is of great importance.

Figure (4.2) shows the variation of this re-defined \( \varepsilon \) with crank angle during a combusting cycle, at four different numerical cells in the combustion chamber. The locations of these four computational cells considered for assessing \( \varepsilon \) are given in fig. (4.3) and these sites were chosen to suitably represent different zones within the combustion chamber. Cell-A is in the piston bowl and cell-B is in the crevice region. Cell-C is in the main part of the chamber but closer to piston wall, where the flame reaches relatively late. Cell-D is in the spark ignition site and experiences completion of combustion before other cells in the domain. Figure (4.4) shows the variation of \( \varepsilon (1 - \varepsilon) \), which appears in the combustion model expression [eqn. (4.26)], with crank angle.
Figure (4.2). Variation of $\bar{c}$ (new) with crank angle

Figure (4.3). Numerical cells considered for estimating $\bar{c}$ (new) shown in fig. (4.2)
The rate and the nature of the variation of the term $\bar{c}(1 - \bar{c})$ are not uniform at different numerical cells, according to fig. (4.4). The value of $\bar{c}(1 - \bar{c})$ always increases to a peak, which cannot be more than 0.25 and this peak occurs at different crank angles and may take different duration to drop back. This indicates the nature of the influence by the term $\bar{c}(1 - \bar{c})$ on calculating the reaction rate at different cells.

The FFM is considered valid only for the fully developed turbulent combustion phase. The flame kernel formation and the early flame growth (the laminar combustion phase) have to be calculated using another suitable model. In order to calculate the mass burning rate during this laminar phase of combustion, Zhao (1994) used an expression for flame surface area, which incorporated the fractal dimension, instantaneous flame radius, Kolmogorov length scale and the volume of the computational cell containing the ignition site. De Petris et al. (1995) used a different formulation independent of the fractal dimension, for the same purpose. However, Ahmadi-Befrui et al. (1981) and Abraham et al. (1985-a) showed the
importance of chemical kinetics during the laminar combustion phase, especially
during ignition. Following them, in the present study, the Arrhenius expression (the
single reaction model described in section (3.8.1) was used for calculating the reaction
rate during the laminar combustion phase. This also allows the fuel properties to be
considered in the calculations. The single reaction model is already available in the
CFD code KIVA-II and this is another reason for using this approach. Spark ignition
was represented by the addition of spark energy into the numerical cells representing
the spark site. Approximately 1% of the total energy of the charge was added this way
as the spark energy. The exact amount of ignition energy added was decided by the
computer program by checking if the total energy added is equal or just exceeded the
1% of the total charge energy and stopping the energy addition. The Unstrained
laminar burning velocity, $S_L$ of natural gas was calculated using an empirical
expression by Iijima and Takeno (1986) and given by

$$S_L = S_{L,S} \left[ 1 + \beta \log \left( \frac{p}{p_s} \right) \left( \frac{T_u}{T_{u,S}} \right)^\alpha \right]$$  (4.29)

where $p_s$ (= 1 atm) and $T_{u,S}$ (= 298 K) are the reference pressure and temperature
respectively, $T_u$ is the unburned mixture temperature and $S_{L,S}$ is the burning velocity at
the reference pressure and temperature. $S_{L,S}$, $\alpha$, and $\beta$ are all functions of the
equivalence ratio, $\phi$ and given by

$$S_{L,S} = 36.9 - 210(\phi - 1.12)^2 - 335(\phi - 1.12)^3$$  (4.30)

$$\alpha = 1.60 + 0.22(\phi - 1)$$  (4.31)

$$\beta = -0.42 - 0.31(\phi - 1)$$  (4.32)

The numerical transition from the laminar combustion phase to the
turbulent combustion phase is important and there have been several transition criteria
used by various researchers and found in the literature. These are in order to signal the
computer code to switch the combustion calculations from the laminar phase to the
turbulent phase. Some such criteria used by the CFD engine combustion modellers are the time elapsed after the spark ignition, flame radius reaching a pre-determined value (usually the integral length scale), temperature of computational cells reaching a pre-determined threshold value or a specific amount of the intake mixture being burned. In the present work, the transition from the laminar to the turbulent phase was assumed after the flame radius has reached the integral length scale of turbulence. The flame radius was calculated using the following expression from Zhao (1994).

\[
R_f = \left[ R_f^0(3-D) + (3-D) S_k \left( \frac{T_b}{T_u} \right) \right]^{\frac{1}{3-D}}
\]

(4.33)

where

- \( R_f \) Flame radius
- \( R_f^0 \) Spark kernel radius (=1 mm)
- \( T_b \) Burned gas temperature
- \( T_u \) Unburned gas temperature
- \( t \) Time from start of calculation
- \( t_{ign} \) Time at ignition

Figures (4.5) and (4.6) show the spherical flame (in terms of temperature contours and velocity vectors) soon after ignition, as predicted by the single reaction model (Arrhenius expression), which was used during the laminar combustion phase.

A separate subroutine, FRACTAL, was written incorporating the FFM into the KIVA-II code for the calculation of the turbulent combustion phase. This subroutine is called by the main program, only for the calculations of a combusting cycle and once the transition from laminar phase to turbulent phase of combustion is signalled by the code. Unlike De Petris et al. (1995), a single, unexpanded model constant was used in the present study following Zhao (1994). This was due to the fact that the effect of having several constants in order to include fuel properties in the model can be achieved by having a single adjustable constant, which makes tuning the constant for a particular situation considerably convenient.
Figure (4.5). In-cylinder temperature distribution, soon after the spark ignition

Figure (4.6). In-cylinder velocity distribution, soon after the spark ignition
4.8. Validation of the improved Fractal Flame Model

Experimental data by Mendis (1997) was used to validate the improved Fractal Flame Model used in the present study. The data for natural gas combustion in an SI engine consisted of the pressure-crank angle history recorded for 360 consecutive cycles of the combusting engine. This information was available for a variety of operating conditions of the engine. These data were statistically averaged in order to obtain the mean pressure-crank angle data for each experimental condition. The engine operating condition of 1500 rpm engine speed, 13.1:1 compression ratio, 32° BTDC spark ignition with stoichiometric air-fuel ratio was considered to be the base line case. The averaged pressure-crank angle data for this base line case was compared with the numerically predicted pressure-crank angle information for the same operating conditions in order to validate the combustion model. For enhanced reliability of the model validation, in-cylinder mixture burning rates were also compared. The numerical grid of the combustion chamber, which included the top-land crevice region and used for the present calculations was explained before and shown by fig. (2.3). It was assumed that the flame does not reach the crevice region.

Figures (4.7) and (4.8) show the results of the numerical simulation of the base line case using the improved FFM, in terms of cylinder pressure – crank angle history and the burned mass fraction. Although the experimental results were available only in the form of cylinder pressure – crank angle data, the respective burned mass fraction data were derived using a computer program (Jenkins, 1997) which uses the Rassweiler and Withrow method (1938). It is clearly seen that the simulation results for the base line case very closely agree with the experiment, quantitatively and qualitatively. This is a very encouraging result as it strongly supports the concept of the fractal nature of the flame front used in the development of the FFM and proves the validity of using the Fractal Flame Model in simulating combustion in natural gas fuelled spark ignition engines. It also proves the suitability of flamelet models, in general, for this specific purpose. Examining the temperature contours [fig. (4.10)] and the velocity vectors [fig. (4.11)] at a randomly chosen intermediate stage of combustion, it is also possible to strengthen the general assumption of the spherical nature of the flame front in an average SI engine.
Figure (4.7). Measured and predicted cylinder pressure-crank angle history

Figure (4.8). Burned mass fraction: measured and predicted
Figure (4.9). Predicted rate of mass burning

Figure (4.10). In-cylinder temperature distribution with the FFM at 12.5° BTDC
Figure (4.11). In-cylinder velocity distribution at the same stage. FFM at 12.5° BTDC

Figure (4.12). In-cylinder distribution of turbulent kinetic energy. FFM at 12.5° BTDC
Figure (4.13). Dissipation of turbulent kinetic energy with the FFM at 12.5° BTDC

4.9. The grid dependency test

The mesh size, in terms of number of cells, used here was chosen after assessing similar studies done by other researchers and the quality of results they obtained with the mesh sizes they had used. However, it is of importance to establish the validity of the mesh density by performing a grid dependency test. The present mesh is of 15x15x15 cells in axial, azimuthal and radial directions respectively and was tested against a mesh of 35x15x30 cells in the same respective directions. The results of this test are given by figs. (4.14) - (4.18). There is no noteworthy difference in the predicted cylinder pressure and average cylinder temperature from using this finer mesh for the motored, non-combusting operation of the engine. However, with a combust ing engine, a drop in peak pressure resulted when the finer mesh was used. This can be easily attributed to the reduction in cell size in the ignition site due to a finer mesh. In KIVA-II, spark is simulated by defining a spark site of predetermined number of cells into which ignition energy is added [Section (2.6.4)]. With a smaller cell size, the area this energy added will be made smaller. In order to rectify this, a
larger ignition site was defined with this finer mesh in order to achieve a size of the site as close as possible to the one available with the coarse mesh.

The results obtained with the finer mesh, with an ignition site of almost the same size as that with the coarse mesh show no significant difference. The test indicated that a mesh size of $15 \times 15 \times 15$ is adequate for the present study. Taking the advantage of axial symmetry available due to the central spark plug location, a slice of $15 \times 1 \times 15$ cells was used for all the calculations thus significantly reducing the use of computational resources.

4.10. RNG $k$-$\varepsilon$ turbulence model as an alternative to standard $k$-$\varepsilon$ model

The choice of the turbulence model for engine simulations has a significant impact on the simulation results. Han and Reitz (1995) showed that the use of renormalisation group theory (RNG) based turbulence model improved the results of simulations of a compression ignition engine compared to when the standard $k$-$\varepsilon$ turbulence model was used. Following those researchers, the RNG $k$-$\varepsilon$ model was included in present calculations and the model was explained in section (2.5.3). Simulations using the RNG turbulence model indicated [fig. (4.19)] that in terms of predicted cylinder pressure, there was no significant improvement of the results of the present calculations of natural gas combustion in an SI engine compared to those obtained with the standard $k$-$\varepsilon$ turbulence model. This may be due to the fact that no fuel sprays in the form of jets interacting with the bulk of the fluid flow in the chamber are considered in this study. Therefore, the standard $k$-$\varepsilon$ turbulence model was used throughout this study. The use of the standard $k$-$\varepsilon$ model for modelling the premixed combustion of the SI engine is well established.

Further, the effect of loss of charge mass through the piston ring crevices due to engine blow-by flow was studied [section (2.6.1)] and the results given in fig. (4.20) indicate that blow-by flow does not significantly affect the results of the present simulations. Therefore, no calculations of blow-by flow were made throughout the rest of the study in order to increase the speed of performance of the calculation procedure. As there was no information about the level of blow-by experienced with the experimental engine, which produced the data for comparison in this study, it appears reasonable not to consider the blow-by effects in calculations.
Figure (4.14). Motored engine cylinder pressure with two grid sizes

Figure (4.15). Average in-cylinder temperature, motored engine
Figure (4.16). Cylinder pressure of the combusting engine

Figure (4.17). In-cylinder average temperature, combusting engine
Figure (4.18). Burned mass fraction, combusting engine

Figure (4.19). Comparison of two turbulence models with the FFM
Figure (4.20). Effect of blow-by calculation on predicted cylinder pressure history

4.11. The FFM compared with the KIVA-II kinetic chemistry model

The Arrhenius type model, which is originally available in KIVA-II was discussed in section (2.4.1) [and in section (3.8.1)] and the forward reaction alone (the Single Reaction Model - SRM), was used to compare the FFM for the baseline case, assuming no backward reaction following Westbrook and Dryer (1981). Spark ignition was introduced by depositing spark energy in several cells representing the ignition site, as in the case of the FFM. A temperature threshold value of 800 K was used to signal the code when to start the chemical reactions in any numerical cell. Using the forward reaction Arrhenius type SRM originally available in KIVA-II for the complete calculation of in-cylinder combustion of natural gas in the SI engine was not a success. The value of the constant $A_f$ in eqn. (2.13) was found to be extremely sensitive and too high a value resulted in an excessive level of heat release and an abrupt rise in pressure. A too low value did not sustain sufficient combustion or no combustion resulted at all. A similar observation has been made by Henson (1998).
The initial stage of combustion, where chemical kinetics are dominant, has been well represented while the later stages of combustion have not been captured correctly. In the present study, it was almost impossible to obtain stable and reasonable combustion with the form of single reaction rate model (Arrhenius rate) originally available in KIVA-II. The comparison [fig. (4.21)] indicates that the FFM is far stronger as a combustion model for simulating the natural gas combustion in an SI engine for the baseline case considered.

4.12. The FFM compared with the EBU model

Being an algebraic formulation for the mean reaction rates, the Eddy Break-up model (EBUM) is relatively simple to program. The EBUM formulation by Magnussen and Hjertager [eqn. (3.12)] was implemented in KIVA-II and a new subroutine, named EBU, was written to calculate the fuel consumption rate at each numerical time step for each computational cell. This subroutine was called by the main program in place of FRACTAL subroutine once the transition from laminar to turbulent phase of combustion was signalled by the code. The laminar phase was calculated using the Arrhenius type SRM as with the FFM and other conditions were kept the same. The reaction between natural gas (assumed to be pure methane) and oxygen was assumed to occur through a single step reaction [eqn. (4.34)] and the combustion products were assumed to consist only of carbon dioxide and water.

\[
\text{CH}_4 + 2\text{O}_2 \Rightarrow \text{CO}_2 + 2\text{H}_2\text{O} \quad \text{(4.34)}
\]

Knowing the rate of consumption of the fuel, \( \bar{\omega}_{\text{CH}_4} \), the rate of change of other species involved in the reaction (oxygen, carbon dioxide and water) can be found from the stoichiometry of the reaction.

\[
\bar{\omega}_{\text{O}_2} = 2\bar{\omega}_{\text{CH}_4} \frac{W(\text{O}_2)}{W(\text{CH}_4)} \quad \text{(4.35)}
\]

\[
\bar{\omega}_{\text{CO}_2} = -\bar{\omega}_{\text{CH}_4} \frac{W(\text{CO}_2)}{W(\text{CH}_4)} \quad \text{(4.36)}
\]
\[
\bar{\omega}_{\text{H}_2\text{O}} = -2 \bar{\omega}_{\text{CH}_4} \frac{W(\text{H}_2\text{O})}{W(\text{CH}_4)}
\]  

(4.37)

Here, \(W(X)\) is the molecular weight of species \(X\). Once the rates of formation (or destruction) of each species are known, the heat release rate due to the chemical reactions can be calculated.

The values used for the EBU model constants by other researchers at various engine operating conditions with different fuels and engine geometries were found not effective for this particular calculation. For the present study, these constants were established by the best possible matching of predicted pressure-crank angle data with the experimental results for the baseline case. This is a rather tedious trial and error work compared to the establishment of the single model constant used with the FFM. The simulation results of the base line case with these two combustion models are compared in figures (4.22) – (4.24).

Figure (4.21). Single reaction model (SRM) compared with the FFM
Figure (4.22). Eddy break up model (EBUM) compared with the FFM

Figure (4.23). Average in-cylinder temperature, the FFM and the EBUM
The results of this comparison between the FFM and the EBUM for the same engine operating conditions show some clear and important differences in the behaviour of these two models. It can be noted that during the compression stroke, while the FFM follows the experiment sufficiently closely, the EBUM deviates from the experiment. It does not follow the same pattern of pressure rise and produces a sharper pressure gradient after a slow initial rate. This behaviour of the EBUM can clearly be seen in fig. (4.24), which shows that the EBUM takes longer to get sufficient initial combustion established. Once this stage has passed, the model then results a faster rate of mass burning, obviously accounting for a faster rise in cylinder pressure. Towards the end, by the time the experiment and the FFM show ~99% of mass burned, the EBUM has yet resulted only about 96% of mass burning. These differences have a direct influence on the predicted in-cylinder temperature and the formation of pollutants. These differences are further investigated below using the figs. (4.25) – (4.28). It was not possible to qualitatively compare them at the same crank angle simply due to the reason that by the time the crank angle position used to
produce the FFM figures is reached, the EBUM had not produced a similar level of combustion comparable to the FFM as explained above. The crank angle at which the figs. (4.10) – (4.13) resulted from the FFM are produced (i.e. 12.5° BTDC) was arbitrarily chosen in order to suitably present the in-cylinder distribution of the temperature and show that the FFM predicts a flame contour more closely following a real flame in a typical SI engine, depicting the generally spherical nature of the flame front. The crank angle at which the EBUM figures [figs. (4.25) – (4.28)] are produced was then chosen using fig. (4.24) so that the same fraction of mass is burned as with the FFM at 12.5° BTDC.

With the FFM, the temperature contours showing a spherical nature of the flame are seen in fig. (4.10) and the centre of this flame hemisphere is reasonably located around the spark plug site. Colder zones of the mixture are at the far ends of the combustion chamber where the flame has yet to reach. This is the usual picture one would expect in an average engine combustion situation with a centrally located spark plug. However, this is not the same one could see in fig. (4.25), which is obtained using the EBUM. Although it is still possible to see the spherical nature in the flame there, some high temperature zones have appeared outside the hot flame hemisphere, in the far ends of the combustion chamber, especially near the chamber walls. This explains the faster rate of mass burning predicted by the EBUM once the initial stage of combustion is established. The coldest region calculated has actually appeared in an unlikely location. The whole idea of this comparison is to identify qualitative differences between the behaviour of these two models and a quantitative comparison between the temperatures in the colder zones predicted by the FFM and the EBUM will not be made. The distributions of turbulent kinetic energy within the chamber as predicted by both models are reasonably similar. Although there is some similarity between the predicted distribution of dissipation of turbulent kinetic energy by the two combustion models, especially near the combustion chamber walls, it is not the case with the predicted distributions of in-cylinder temperature. The high temperature areas outside the flame sphere, resulted by the EBUM have occurred more or less where the high dissipation of turbulent kinetic energy occurs in the chamber, that is near the far walls. The FFM temperature distribution, on the other hand, does not follow the distribution of dissipation of turbulent kinetic energy. This is a very interesting situation where further attention is required.
Figure (4.25). In-cylinder temperature distribution with the EBUM, at 8° BTDC

Figure (4.26). In-cylinder velocity distribution with the EBUM, at 8° BTDC
Figure (4.27). Distribution of turbulent kinetic energy with the EBUM at 8° BTDC

Figure (4.28). Dissipation of turbulent kinetic energy with the EBUM at 8° BTDC
The comparison of the significant difference seen in the in-cylinder temperature distribution by the two combustion models would be convenient if a simple disc shaped combustion chamber is used. The engine combustion chamber with the experimental conditions used by the researchers at Leeds University (Sheppard and Buran, 1997) was therefore used for this comparative simulation and the same model constants validated earlier were used. It should be noted that these simulations with the disc shaped chamber is made only for the purpose of highlighting some important differences identified between these two combustion models. Figure (4.29) shows the comparison of the FFM and the EBUM in terms of predicted temperature variation within the disc shaped combustion chamber with a centrally located spark plug.

![Flame contours comparison](image)

**Figure (4.29).** Comparison of flame contours predicted by the two combustion models on a disc shaped combustion chamber
Again, the FFM has produced a realistic shape for the flame front, as one would expect whereas the EBUM has predicted a flame front with abnormal features. There, the flame has bent outwards in the direction of the propagation with the flame being thick. This is a direct consequence of the turbulent time scale, \( \tau_t = \frac{k}{\varepsilon} \), which appears in the EBUM reaction rate expression [eqn. (3.12)] being extremely low near a wall. The obvious result of this lowered \( \tau_t \) is a higher rate of reaction near walls hence increased temperatures.

After learning the strength of the effect of turbulence on the EBUM, the use of RNG \( k-\varepsilon \) turbulence model is again compared with the standard \( k-\varepsilon \) model for the base line case, using the EBUM as the combustion model [fig. (4.30)]. However, as resulted with the FFM [fig. (4.19)], there is no significant difference in predicted cylinder pressure with the EBUM and these two turbulence models. It can therefore be concluded that the use of RNG \( k-\varepsilon \) turbulence model has not significantly affected the performance of the EBUM for simulating natural gas combustion in an SI engine studied.

![Figure (4.30). Comparison of two turbulence models with the EBUM](image-url)
Chapter 5.

Parametric studies of a natural gas fuelled SI engine

5.1. Natural gas as an alternative fuel

The complete dependency on petroleum products as vehicular fuels is not very sensible due to several primary reasons such as insecure petroleum supplies, high indirect economic costs (e.g. international trade deficits), increased global warming and urban air pollution. These problems were also the reasons to initiate a serious interest of transition to alternative transportation fuels (Nakamura et al. 1991).

Alternative fuels can be divided into two distinct groups as those, which could completely replace gasoline and/or diesel and those, which can be low level additives to gasoline/diesel. Many of the near-term interests, particularly in urban areas with very high levels of carbon monoxide pollution, are in gasoline additives such as ethanol, methanol and methyl tertiary butyl ether (MBTE) which can be added to the present day gasoline and provide immediate carbon monoxide reduction (Alson et al. 1988).

There are some alternative fuels such as methanol, hydrogen, compressed natural gas (CNG), ethanol etc. that are believed to have the potential in the near or medium term to completely replace petroleum derived fuels. These alternative fuels are generally known as ‘clean’ fuels compared to gasoline and diesel fuels because of the low levels of combustion emissions associated with them. There
are, of course, other fuel sources such as electricity and the fuel-cell that could provide very significant reductions in urban pollution due to combustion related emissions but there appears to be little likelihood that these sources will be feasible in a large scale in the near term. Figure (5.1) shows the general relationship among these alternative fuels (Alwin and William 1990).

![Diagram of alternative transportation fuels](image)

Figure (5.1). Alternative transportation fuels (Alwin and William 1990)

Natural gas deposits exist either as free gas or in association with crude oil. Useful quantities are also derived from the degassing of coal mines. Natural gas does not require innovative technology and time to process like other alternative fuels. The resources are vast and the supply is in a relatively high state of purity. In addition to the conventional world wide supplies, natural gas is renewable and can be obtained from a wide variety of unconventional sources such as sewage and biomass, landfills, tight sands, shale oil, coal seam methane and other renewable resources and new technologies. Substitute natural gas from oil and light petroleum distillate is also available (Hay and McArdle 1988).

The low cost of natural gas makes it a suitable fuel for transportation and the relative cleanliness of natural gas has enhanced its value as a premium fuel.
Relatively clean, high octane combustion is its most attractive fuel characteristics. Excellent cold startability, being safer than other usual fuels, availability of larger reserves, readily availability etc. are other benefits offered by this fuel (Alson et al. 1988, DeLuchi 1988).

Natural gas mainly consists of methane but having evolved from organic deposits, invariably contains some higher hydrocarbons together with traces of inert nitrogen-carbon dioxides and/or hydrogen sulphide depending on the geological location and history. Ethane and heavier hydrocarbons such as propane and butane appear as major species next to methane, the dominant species in NG. Other compounds present in NG include nitrogen as N₂, sulphur as H₂S, and odorants such as ethyl mercaptan (C₂H₅SH), carbon dioxide and water. Natural gas from various parts of the world can be substantially different in composition and such differences can markedly affect their combustion characteristics. Table (5.1) shows the typical volumetric and gravimetric composition of natural gas (Carlton et al. 1990). Table (5.2) gives the fuel properties of some hydrocarbon gases commonly found in natural gas (Naber et al. 1994).


<table>
<thead>
<tr>
<th>Component</th>
<th>Volume (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>94.4</td>
</tr>
<tr>
<td>Ethane</td>
<td>3.5</td>
</tr>
<tr>
<td>Propane</td>
<td>0.4</td>
</tr>
<tr>
<td>Butanes (iso-, n-)</td>
<td>0.1</td>
</tr>
<tr>
<td>Pentanes</td>
<td>0.03</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>0.37</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>1.17</td>
</tr>
<tr>
<td>Water and other</td>
<td>0.03</td>
</tr>
<tr>
<td>Total</td>
<td>100.0</td>
</tr>
</tbody>
</table>
Table (5.2). Characteristic fuel properties of some individual gases found in natural gas (Naber et al. 1994)

<table>
<thead>
<tr>
<th>Gaseous fuel</th>
<th>Molecular weight (g/mol)</th>
<th>Specific heat ratio, $\gamma$</th>
<th>Lower calorific value (MJ/kg)</th>
<th>Laminar flame speed (cm/s)</th>
<th>Density at STP (kg/m$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>16.04</td>
<td>1.23</td>
<td>50.00</td>
<td>38.3</td>
<td>0.7168</td>
</tr>
<tr>
<td>Ethane</td>
<td>30.07</td>
<td>1.13</td>
<td>47.48</td>
<td>40.6</td>
<td>1.3566</td>
</tr>
<tr>
<td>Propane</td>
<td>44.09</td>
<td>1.09</td>
<td>46.35</td>
<td>42.3</td>
<td>2.0096</td>
</tr>
<tr>
<td>Butane</td>
<td>58.12</td>
<td>1.06</td>
<td>45.72</td>
<td>42.6</td>
<td>2.7320</td>
</tr>
</tbody>
</table>

More than 40 years of natural gas vehicle use have shown the safety of CNG as a vehicle fuel. In general, NG is considerably more benign than gasoline. NG is not toxic, carcinogenic or caustic though it can be an asphyxiant. Very few hazards of NG usage have been identified. Contact with liquid natural gas (LNG) may result in severe frostbite. Also, the sudden cooling effect that result in when highly compressed NG expands to normal atmospheric pressure can cause frostbite. LNG is virtually never considered as a transportation fuel, primarily because it is thought to be too dangerous and costly (California energy comm. 1987).

The ability of a fuel to resist knock is usually indicated by its octane number being high. The current published value of methane’s octane numbers are 120 (RON 130) or greater while iso-octane has the octane number rating of 100. The fuel composition variations directly affect its actual octane number. Although the main constituent of NG, methane has a high knock resistance, increasing amounts of heavier hydrocarbons (e.g. ethane, propane) in the NG mixture result in lower knock resistance. The presence of these minor constituents in NG can have a profound effect on its combustion properties (Adams 1985, Kubesh and King 1992). Studies (Bull et al. 1979, Roydon et al. 1991) have shown that the addition of very small quantities of ethane can sharply reduce the ignition delay times with respect to methane - air mixtures. Similar results have been observed when the minor component is propane or butane (Eubank et al. 1981). In comparison with methane itself, the presence of the additional components gives natural gas about an 8% increase in density, a 4% reduction in specific energy and a 4% increase in energy density. Because of its high
activation energy, the laminar flame speed of natural gas is lower than that of other hydrocarbon fuels (Kubesh and King 1992). To burn or detonate, NG needs a higher concentration in air. All these flammability criteria make \( \text{CH}_4 \) (NG) less hazardous than gasoline. Its relatively high diffusivity, which is three times that of gasoline vapour and relatively low density are important properties. Leaked \( \text{CH}_4 \) (NG), if unconfined, will disperse to a density below its lower flammability limit quickly (DeLuchi et al. 1988).

5.2. NG engine types and applications

Stationary engines and automotive engines are the usual engine applications of NG though it has a potential for being used as a gas turbine fuel as in aviation applications. Existing natural gas vehicles (NGVs) are mainly heavy duty applications such as buses and trucks due to the economical reasons in engine conversions and used in fleets for ease of refuelling and maintenance. Light duty automotive applications such as passenger cars are fast emerging and have a promising future in front of the stringent emission regulations.

Most of the present day NGVs use converted SI or CI engines as NG requires no major changes in the current engine design and can be adopted to the existing fuelling system. These conversions retain the option to run the vehicle on its original fuel. It is also possible to convert diesel engines to run as spark ignition units. Such conversions are relatively costly and do not provide all the benefits realisable from an optimised, dedicated natural gas engine. Converting engines optimised for liquid fuels to use NG detract from the performance achievable from NG, particularly in the areas of thermal efficiency, power output, emissions and engine durability. The low flame speed of NG is most significant under lean conditions as this results in a longer duration of combustion, impairing efficiency unless the spark timing is advanced to compensate for it. The need for advanced timing can be offset to a considerable degree by high compression ratios and compact turbulent combustion chambers. These increase flame speed and decrease the distance the flame must travel (Fricker et al. 1991, Al-Himyary and Karim 1987)
5.3. Converted engines

Since only few NG engines are available from manufacturers at present, it is often necessary to convert existing diesel or petrol engines to run on NG. There are three commonly used types of engine conversions, namely bi-fuel engine conversions, dual fuel engine conversions and Otto cycle conversion from diesel engines (Ekelund 1988)

5.3.1. Bi-fuel engines

When a petrol engine is converted for alternative but not simultaneous operation with petrol or NG, it is a bi-fuel engine. It runs on Otto cycle and is spark ignited. NG or gasoline can be alternatively selected by a switch. The most obvious problem in this conversion strategy is the variation in air/fuel ratio when the inlet fuel is selected between two fuels. In the NG mode, restriction by the fuel mixer reduces the mixture mass entering the engine causing a power loss. In the gasoline mode, this mixer restricts air flow causing a rich mixture as it does not restrict the liquid fuel. With a well designed bi-fuel engine, the operation should not be affected when the fuels are switched (Fricker et al. 1991, Kimbara 1986).

5.3.2. Dual-fuel engines

Diesel engines running on a NG/diesel mixture when necessary or on diesel only at other times are called dual-fuel engines. The proportion of gas into the combustion chamber depends on the conversion type. In pilot fuel injection dual-fuel engines, charge is mainly a lean mixture of air/NG and maximises the use of the gaseous fuel. A very small quantity of diesel fuel (pilot fuel) is injected to assist the ignition of the mixture. About 80-95% of the diesel fuel can be substituted with NG. On the other hand, in fumigation dual-fuel engines, gaseous fuel is added to a fully operational diesel engine to provide extra fuel loading hence additional power. Supplementary gaseous fuel is added only after a pre-specified load level and usually not added at light load. Some 20-50% of the diesel fuel is substituted by NG in this method (Ekelund, 1988).
5.3.3. Otto cycle conversion from diesel engines

Diesel engines are converted to run on NG with spark assisted ignition and are widely used for heavy duty engines. Controlling the thermal loading of these high rated engines and exhaust emissions, particularly NO\textsubscript{x}, are two major difficulties with this conversion method. These converted engines can be stoichiometric, lean burning or variable mixture engines.

5.3.4. Dedicated, optimised, natural gas engines

As the bi-fuel and dual-fuel engines are not optimised for NG use, the maximum benefits expected from an NGV can not be achieved. The dedicated NG engine running solely on NG is the solution as it can be optimised for using NG. Reducing heat losses, increasing the compression ratio and improving combustion are among ways of improving efficiency. The higher RON of NG compared to gasoline and the gaseous state of NG will work to increase thermal efficiency with reduced levels of pollutants. As it is a gas, unlike liquid gasoline, NG thoroughly mixes with air at any ambient temperature giving better mixture conditions, which is especially important at cold start. The higher octane number of NG allows the engine to have a higher compression ratio. Heat losses can be reduced by an optimised combustion chamber with reduced surface area. Although lower flame speeds tend to reduce efficiency, advancing the spark timing can compensate for this at the expense of increased NO\textsubscript{x} and HC emissions. It has been suggested that optimised NGVs should be about 20% more efficient than gasoline vehicles. In practice, the actual efficiency gain in a dedicated NG engine depends on the air/fuel ratio, how well the engine is optimised for NG combustion, whether CNG or LNG is used, the fuel injection scheme and other factors (The Aerospace Corp. 1982, Hyun et al. 1993).

5.4. Fuel metering

The task of the engine induction and fuel system is to prepare an air-fuel mixture that satisfies the requirements of the engine over its entire operating regime. There are three distinct and different technologies of fuel control and
induction to be identified on natural gas engines. The first of these is carburetion where the pressure drop created by an air flow across a restriction draws a proportional volume of fuel into the air stream. The second is the upstream fuel injection where fuel is introduced into the air stream prior to admission into the cylinder and can either be metered as choked (sonic) or unchoked flow. The third type is direct fuel injection into the cylinder. Different combustion control techniques demand different metering methods.

Modern stoichiometric and lean burn techniques used to achieve stringent emission regulation demand maintaining the air/fuel ratio in a very narrow range (Klimstra 1989, Kekedjian and Krepec 1994). Although the air/fuel ratio is often used to describe the mixture, it is not precise with natural gas as the stoichiometric air/fuel ratio of natural gas varies with the fuel composition. From a control system's standpoint, natural gas must be considered as a flexible fuel with varying fuel properties. Since the gas composition affects the physical properties of the fuel, the quantity of fuel metered will also be affected. This changes the equivalence ratio to the engine and due to this, it is impractical to assign a standard value for the stoichiometric, mass based air/fuel ratio for natural gas. The variability in air requirement offers a challenge for control on natural gas engines (Liss and Thrasher 1991). The Wobbe number (WN), which is defined as the gross calorific value of the gas divided by the square root of its specific gravity with respect to air (Weaver 1951), is used as the single parameter concerning the natural gas with varying composition. For a given air velocity, the chemically stored energy supply to the engine remains constant if the Wobbe number remains constant. It can be shown that the air/fuel ratio will vary proportionally to the WN and the WN represents the energy flow rate resulting from a certain pressure drop (King 1992, Unich 1993). The WN increases when the content of non-methane hydrocarbons (NMHCs) increases as the NMHCs have higher densities. The WN decreases when the inert gas concentration rises (Weaver 1989, Klimstra 1992).

The temperature of gasoline as it is metered through the carburettor in a gasoline engine has a negligible effect on the accuracy of fuel metering since the density changes are small. With natural gas, the situation is different when operating a carburetted natural gas engine with varying ambient conditions. If the provided air and fuel temperatures are equal, the temperature can be varied with no apparent effect on
the equivalence ratio. However, significant variations can occur if the fuel and air temperatures are allowed to deviate from one another. Equivalence ratio variations of more than 10% are possible with fuel temperature swings of 100°F (38°C). Electronic controllers are needed to compensate for temperature and pressure variations to eliminate metering inaccuracies resulting from variations in air and fuel supply conditions. In practice, fuel temperature is related to a variety of factors including ambient temperature, engine compartment temperature, fuel flow rate, heat transfer rate in the gas regulator and pressure in the downstream piping and upstream regulator. Clearly, the fuel temperature of a natural gas vehicle can be considerably different from the ambient temperature and should be monitored directly and as close to its metering point as possible (Liss and Thrasher 1991).

5.4.1. Fuel injection in natural gas vehicles

Injected fuel is metered based on predetermined engine operating conditions such as engine speed, intake manifold pressure and throttle position and can be controlled mechanically or electronically. The fuel flow, therefore, is dependent on known conditions of the engine and is independent of air flow. As the volumetric efficiency of an engine is constant for a fixed speed and load, the total volume flow of the air-fuel mixture must remain constant though the air/fuel ratio can vary. Two basic fuel injection systems are found; namely central (throttle body) injection systems with one or two centrally located injectors and port fuel injection systems with one fuel injector at the inlet manifold of each cylinder. The injectors are essentially on-off switches, opening and closing completely and very rapidly. One of the most difficult challenges is improving the injector durability because CNG does not provide any lubrication on the moving parts of injector. Since the density of gas is low, the injector (or any other metering device) has to handle correspondingly larger volumes and hence needs larger components. Achieving the required fast actuation with these substantially larger components in injectors is another challenge (Weaver 1989, Hodgins et al. 1992, Kekedjian and Krepec 1994)
5.5. Parameters affecting engine performance

5.5.1. Compression ratio

The engine thermal efficiency is a function of compression ratio (CR) and increasing the CR gives immediate benefits. The higher the Octane number of the fuel, the higher the allowable CR, and the greater the power available. Hyun et al. (1993) has shown that increasing the CR from 10 to 13.6 in a natural gas engine gives about 2% increase in wide open throttle (WOT) power. The knock rating of gasoline engines limits the CR to approximately 10:1 whilst diesel engine must operate close to 20:1 in order to achieve sufficient levels of fuel ignition. Unfortunately increased internal frictional losses above ratios of 15:1 negate any gain in thermal efficiency and reduce engine efficiency. Dedicated, partially optimised engines usually operate with the CR increased to between 12:1 and 13:1 (DeLuchi 1988, Yamamoto et al. 1994).

5.5.2. Turbocharging

Turbocharging a natural gas engine can boost its power considerably beyond the gasoline baseline, albeit at extra cost. A turbocharged engine is smaller than the naturally aspirated engine that gives the same power output (with other conditions unchanged). This is because, a higher mixture mass is possible inside the cylinder prior to combustion, when turbocharged. Ignition timing may need retarding to avoid knock as increased compression increases mixture temperature thus promoting knock (Heywood 1988).

5.5.3. Ignition

Due to the high auto-ignition temperature (low Cetane number) of NG, ignition aids are needed when NG is used as the fuel in either CI or SI engines. The minimum energy required to effect a successful ignition of a air-fuel mixture within the flammability limit is relatively large for mixtures involving methane (Karim and Wierzba 1983). To ignite using a spark or with a pilot fuel, sufficient energy to heat the gas locally to a temperature well above the minimum spontaneous ignition
temperature and in excess of the adiabatic flame temperature has to be supplied. When
the mixture is lean or purposely diluted with EGR etc., the conventional ignition
system is limited in its ability to provide positive ignition by its constrained spark
location and limited energy supply. Plasma jet ignition systems and electronic gaskets
provide higher spark energies and would be more suitable. The inherent turbulence in
the plasma discharge puff can produce a more rapid flame growth and shorter overall
combustion duration. Studies have shown that the use of plasma jet igniters with
methane as the fuel enhances the burning rates in the initial stages of combustion,
especially with very lean mixtures and the lean limit of engine operation is also
extended (Karim et al. 1989). Electronic gaskets give multi-point ignition and create
more effective and complete combustion (Hong et al. 1993). Multiple spark plug
configurations give better performance as they produce greater horse power and
higher thermal efficiencies for all equivalence ratios by reducing the flame travel
distance to complete combustion and as the misfire rate is reduced (Meyer et al.
1992). As NG has a relatively high ignition temperature and a slower laminar burning
velocity, which decreases with increasing pressure, improved performance can be
expected with these methods of ignition. As NG combustion is slower (i.e. slower
flame speed than that of gasoline) and needs a longer duration to complete
combustion, the ignition timing for NG engines has to be advanced. Unlike with
gasoline engines, MBT ignition timing for NG engines rarely changes as load
variations affect little on performance compared to gasoline engine. Advanced timing
compensates for the greater volumetric displacement of the gaseous fuel (Yamamoto
et al. 1994).

5.5.4. Turbulence, flame travel speed and distance

Increased flame speed and reduced flame travel distance provide
complete combustion conditions. Increased turbulence and swirl provide increased
flame speeds. Fast burn combustion chambers with optimised shapes for NG (at no
extra cost under mass production) would therefore increase power (Seal 1983,
Fleming and O'Neal 1985). The Nebula combustion chamber (Kingston Jones and
Heaton 1989) is an example of flow enhancing bowl designs [Figure (5.2)].
In pre-chamber combustion engines, a portion of the fuel mixture at near stoichiometric conditions (then it is easy to start combustion there) is ignited by an electric spark in a separate pre-chamber. The hot combustion products rushing into the main chamber as a violent jet ignite the leaner mixture and introduce a high turbulent field in order to improve combustion conditions (Beaty et al. 1992).

5.5.5. Combustion pressure

With CNG, the combustion pressure increases more slowly (low \( dp/d\theta \)) and takes approximately 20% longer than gasoline to combust. This has to be seriously considered when designing a CNG fuelled engine. Advancing ignition and/or generating faster, improved combustion conditions are needed (Yamamoto et al. 1994).

5.5.6. Fuel composition and mixture homogeneity

Variations in NG composition are known to considerably affect engine performance and emission of pollutants through changes in fuel metering.
characteristics, energy content and knock resistance of the fuel (Kubesh and King 1992). Further research and development of improved techniques are needed to deal with this problem.

5.6. A general comparison of NG engine with gasoline and diesel engines

The lower heating values of the stoichiometric air-fuel mixtures are quite similar for NG and gasoline but NG has a lower density than gasoline vapour and this produces a negative effect on the volumetric efficiency. In fact the energy content of a certain volume of stoichiometric gas-air mixture is about 10% lower for NG compared to gasoline. The volumetric energy content of CNG at 3150 psi (≈ 220 bar) and 15°C is 8.0 MJ/l and is 75% less than gasoline and 78% less than diesel. Due to this, NGV travel range is shorter between refuelling for vehicles, in particular, where the space allowable for CNG cylinders is small. The weight of the CNG cylinders would be another problem as every 1% increase in vehicle weight will result in about 0.8% loss in efficiency (Unich et al. 1993).

As NG can be evenly and completely mixed with air upon start-up, without enrichment, smoother and cleaner cold operations are possible resulting in much lower CO emissions than from gasoline or diesel engines. CH₄ flames are colder and therefore radiate less heat and CH₄ ignites spontaneously at a higher temperature (813 K) and is therefore safer than gasoline. Relative to unleaded gasoline, CH₄ needs slightly more energy to ignite. When emission legislation becomes more stringent, NG offers advantages particularly over diesel fuel. The low levels of sulphur and the low emissions of HC and particulates associated with NGVs should extend the catalyst life and improve the performance of the catalyst. Particulate emissions from CNG combustion are negligible when running with stoichiometric or lean mixtures (Fricker et al. 1991).

The high knock resistance of natural gas indicates that it could safely be used with engine compression ratios as high as 15:1 compared to 8 - 10:1 for 91-octane gasoline. Natural gas engines using these higher compression ratios can reach significantly higher efficiencies than possible with gasoline. The optimised, single fuel NG engines, properly serviced and well maintained are expected to have lower maintenance costs and last longer than gasoline engines because methane is a single
carbon fuel containing no nitrogen or sulphur and does not mix with lubricating oil. It does not foul the combustion chamber, engine oil and spark plugs as much as gasoline does. When compared with a diesel engine, essentially no particulate materials, smoke, SOx or unregulated pollutants are formed and an NGV is noticeably quieter. No lead and much lower CO2 emissions are formed compared to petrol engines (Frank 1983, Liss and Thrasher 1991).

5.7. Parametric study with KIVA-II using the FFM

After validating the combustion model discussed in chapter 4 for calculations of natural gas engine combustion in KIVA-II computer code, a parametric study was performed. Studying the effects of engine operating parameters on engine performance and pollutant formation was the objective. Compression ratio, equivalence ratio, engine speed and ignition timing are the operating parameters varied. The test matrix consists of three compression ratios (10:1, 13.1:1, 15:1), five relative air-fuel ratios ($\lambda = 0.9, 1.0, 1.1, 1.2, 1.3$), three spark timings ($32^\circ, 26^\circ$ and $20^\circ$ crank angles BTDC) and four engine speeds (1200, 1500, 1800, 2000 rpm). The model constant validated in the base line case (1500 rpm, 13.1:1 CR, $\phi = 1.0$ and $32^\circ$ BTDC ignition) was used, unchanged, for this parametric study. It is not possible to validate the complete set of results from this parametric study as the relevant experimental data for all the engine operating conditions studied are not available for an engine with exact geometric features of the combustion chamber geometry studied. It is therefore, regarded as a parametric study with the objective of studying if the newly employed combustion model and the CFD code as a whole can successfully predict the trends of an engine’s performance. In order to examine this, the results will be compared with general experimental trends available in literature for light duty, natural gas fuelled, SI engines. This approach is to verify the ability of the improved FFM and the KIVA-II CFD code in predicting the trends of natural gas fuelled SI engine performance. It can strengthen the idea of using CFD modelling as a tool for the design of new engine combustion chambers and the optimisation of these chambers for a particular fuel and operating conditions. However, it is noteworthy that experimental results obtained with other fuels from the literature have been used in
some places here in order to compare the predicted engine operational trends when suitable work for natural gas could not be found.

As the operation of engines with a fuel rich mixture is not the usual practice and running lean is a well established way of controlling emissions of nitric oxides from an engine, in this parametric study, only one relative air-fuel ratio ($\lambda$) value (i.e. $\lambda = 0.9$ or $\phi = 1.111$) from the rich side has been considered. Due to the gaseous state of CNG, lean operation of engines is possible even at cold start and this is also a reason for concentrating more on the lean side of operation for this study.

Figures (5.3) – (5.6) show the effect of varying the relative air-fuel ratio ($\lambda$) from the base line case on cylinder pressure, burned mixture mass fraction, burned fuel mass fraction and average in-cylinder temperature. Figure (5.7) from Heel et al. (1998) shows experimentally and numerically obtained trends of the variation of cylinder pressure with $\lambda$ and those results are sufficiently comparable with the respective trends obtained in the present study and shown by fig. (5.3). The general trend predicted is a lowering of the peak cylinder pressure and a late occurrence of this peak with increasing $\lambda$ and they are agreeably seen in the work by Heel et al. as well. These results are due to the direct consequences of the lower energy content and the reduced laminar burning velocity in a leaner mixture. Another suitable result found from the literature for comparison is given by fig. (5.8), which was originally from Tabaczynski et al. (1977). This shows the mass fraction burned when the fuel-air equivalence ratio, $\phi$ ($= 1/\lambda$) varied. There is reasonable agreement between this result and the prediction from the present study, which is shown in fig. (5.4). The trend predicted in this work is that the higher the $\lambda$, (i.e. the lower the $\phi$), the slower the burning and the longer it takes to burn the mixture. Tabaczynski et al. too have obtained a similar trend except for the case, where $\phi=1$, in which the burning is faster than the $\phi=1.2$ case. This difference may have been due to the different spark timing, engine speed and, most of all, the different fuel used by Tabaczynski et al. Figure (5.6) shows an interesting result on average in-cylinder temperature with $\lambda$ from the present simulation. Here, the highest and the lowest average peak temperatures occur when $\lambda$ is at the lowest and the highest, respectively. However, at the exhaust valve opening (EVO) at 127° ATDC, the resulting temperatures in the exhaust gas are not following the same order. Firstly, the exhaust gas temperature increases as $\lambda$ increases.
and then drops with further increasing $\lambda$. A higher exhaust gas temperature can be expected with a higher $\lambda$ as more burning occurs towards the EVO due to the slower burning rate resulting from a lean mixture and this is seen in fig. (5.4). However, at higher $\lambda$ situations, total energy content in the mixture is low and hence a lowered effective temperature results. Accordingly, one can expect this rise and fall of exhaust gas temperature with increasing $\lambda$ of the mixture. Morgan and Hetrick (1976) have experimentally obtained this trend for three spark timing values and that can be seen in fig. (5.9). Here, this rise and fall of exhaust gas temperature around a certain air-fuel ratio is indicated and the variation of the spark timing has not affected this trend.

The effect of the variation of engine speed from the base line case on cylinder pressure and burned mass fraction is shown by figures (5.10) and (5.11) and a comparable work from the literature (Heel et al. 1998) is given by figure (5.12). The general trend noticeable from the results is the occurrence of a lowering of the peak pressure, as the engine speed increases. This peak occurs later in the expansion stroke as the speed increases. Also, it can be noticed that the difference between the peak pressure value and the difference between the duration it takes for this peak to occur in terms of crank angles reduce as engine speed increases. The very same trends have been obtained by Heel et al. (1998), experimentally and numerically.

Further, the effects of varying the individual operating parameter on the natural gas engine performance were studied. Trends of the variation of peak cylinder pressure with relative air-fuel ratio and engine speed at different ignition timings used are shown by figs. (5.13) - (5.15) and ignition timing varied with different engine speeds are given by figs. (5.16) - (5.19). These results indicate, for the range of the variation of parameters studied that the richer the mixture, the higher the resulting peak cylinder pressure and the lower the engine speed, the higher the peak cylinder pressure. The higher peak cylinder pressure at richer mixtures is again due to the higher energy content in the mixture and the lower peak pressure with higher speeds is due to the late occurrence (in terms of crank angles) of the main phase of combustion during the expansion stroke. Peak cylinder pressure is seen increasing as ignition timing is advanced from TDC. This is a result of more energy in the mixture being converted into heat by the time TDC is reached when an advanced ignition timing is employed compared to a spark timing closer to TDC. Figure (5.20) is an experimentally obtained result by Stone et al. (1996) describing trends of

Chapter 5
variation of peak cylinder pressure with relative air-fuel ratio and ignition timing. The trends seen here are well predicted by the present work.

In engine combustion research, 0-10% of mixture burning and 10-90% of mixture burning are important stages as they are regarded as the early burning and main burning phases. These phases were examined numerically and results for 0-10% mixture burning phase are shown by figs. (5.21) – (5.27) and for the 10-90% mixture burning phase are shown by figs. (5.28) – (5.34). These show the effect of the variation of ignition timing while keeping the engine speed constant and the effect of varying engine speed while keeping the ignition timing constant for the range of λ studied. Although fig. (5.4) showed that the burned mass fraction, as a whole, reduces when the mixture is made leaner, these figures indicate that this is a combined result of the slowed down combustion in both the early (0-10%) and the main (10-90%) phases of burning. Comparable experimental results by Stone et al. (1996) are given by figs. (5.35) and (5.36), which are in the form of contour plots. The trends obtained here numerically are sufficiently comparable with the experimental trends seen in these results. As these experiments have shown and as shown by the present study, the 0-10% mixture burning phase takes longer as the ignition timing is advanced from TDC. This is because of the lower mixture temperature at the time of ignition with an advanced ignition timing, which lowers the laminar burning velocity. Although fig. (5.36) by Stone et al. does not conclude a distinctive trend for the 10-90% mixture burning phase due to insufficient contour density in some regions, it can be still seen that the combustion duration for the 10-90% burning generally becomes shorter as ignition is advanced. A similar trend obtained experimentally, by Hires et al. (1976) and numerically, by Blumberg et al. (1979) is shown by fig. (5.37). However, present calculations have been unable to capture this trend correctly. Some more experimental results by Hires et al. and simulation results by Blumberg et al. are given by figs. (5.38) and (5.39) and they indicate that the combustion duration in both phases becomes longer as engine speed increases and as the mixture becomes leaner. These trends have been obtained reasonably correctly by the present calculations. The effects of varying these engine operating parameters on the formation of pollutants will be discussed in chapter 6.
Figure (5.3). Effect of relative air-fuel ratio ($\lambda$) on cylinder pressure

Figure (5.4). Effect of relative air-fuel ratio ($\lambda$) on burned mixture mass fraction
Figure (5.5). Effect of relative air-fuel ratio (λ) on burned fuel mass fraction

Figure (5.6). Effect of relative air-fuel ratio (λ) on average temperature
Figure (5.7). Variation of cylinder pressure with relative air-fuel ratio ($\lambda$). A comparison from the literature (Heel et al. 1998), M: Measured, C: Computed.

Figure (5.8). Variation of mass fraction burned with equivalence ratio, $\phi$. A comparison from the literature (Tabaczynski et al. 1977)
Figure (5.9). Variation of exhaust gas temperature with air/fuel ratio and spark timing. A comparison from the literature (Morgan and Hetrick 1976)

Figure (5.10). Effect of engine speed on cylinder pressure
Figure (5.11). Effect of engine speed on burned mass fraction

Figure (5.12). Variation of cylinder pressure with engine speed. A comparison from the literature (Heel et al. 1998), M-Measured, C-Computed.
Figure (5.13). Engine speed on peak cylinder pressure with ignition at 20° BTDC

Figure (5.14). Engine speed on peak cylinder pressure with ignition at 26° BTDC
Figure (5.15). Engine speed on peak cylinder pressure with ignition at 32° BTDC

Figure (5.16). Ignition timing on peak cylinder pressure with 1200 rpm engine speed
Figure (5.17). Ignition timing on peak cylinder pressure with 1500 rpm engine speed

Figure (5.18). Ignition timing on peak cylinder pressure with 1800 rpm engine speed
Figure (5.19). Ignition timing on peak cylinder pressure with 2000 rpm engine speed

Figure (5.20). Contours of peak cylinder pressure (bar) in a natural gas engine
(from Stone et al 1996)
Figure (5.21). Burning of 10% of mixture mass with ignition at 20° BTDC

Figure (5.22). Burning of 10% of mixture mass with ignition at 26° BTDC
Figure (5.23). Burning of 10% of mixture mass with ignition at 32° BTDC

Figure (5.24). Burning of 10% of mixture mass with 1200 rpm engine speed
Figure (5.25). Burning of 10% of mixture mass with 1500 rpm engine speed

Figure (5.26). Burning of 10% of mixture mass with 1800 rpm engine speed
Figure (5.27). Burning of 10% of mixture mass with 1200 rpm engine speed

Figure (5.28). Burning of 10 - 90% of mixture mass with ignition at 20° BTDC
Figure (5.29). Burning of 10 - 90% of mixture mass with ignition at 26° BTDC

Figure (5.30). Burning of 10 - 90% of mixture mass with ignition at 32° BTDC
Figure (5.31). Burning of 10 - 90% of mixture mass with 1200 rpm engine speed.

Figure (5.32). Burning of 10 - 90% of mixture mass with 1500 rpm engine speed.
Figure (5.33). Burning of 10 - 90% of mixture mass with 1800 rpm engine speed

Figure (5.34). Burning of 10 - 90% of mixture mass with 2000 rpm engine speed
Figure (5.35). Contours of the 0 – 10\% mass fraction burn period (\textdegree CA)
(from Stone et al 1996)

Figure (5.36). Contours of the 10 – 90\% mass fraction burn period (\textdegree CA)
(from Stone et al 1996)
Figure (5.37). Combustion duration for 10% and 90% mixture burning: experiment (Hires et al. 1976) and simulations (Blumberg et al. 1979)

Figure (5.38). Combustion duration for 10% and 90% mixture burning: experiment (Hires et al. 1976) and simulations (Blumberg et al. 1979)
Figure (5.39). Combustion duration for 10% and 90% mixture burning: experiment (Hires et al. 1976) and simulations (Blumberg et al. 1979)

5.8. Effect of exhaust gas recirculation

As another component of the parametric study, the effect of exhaust gas recirculation (EGR) was studied. Exhaust gas recirculation is a widely used and well established technique for controlling NOx emissions from an engine. As the formation of NOx has a strong proportionality to the in-cylinder temperature, the requirement is to bring the temperature down as a means of reducing NOx formation. One way of achieving this is by the addition of a suitable diluent to the fresh charge in the chamber. Recirculating a suitable quantity of exhaust gases from the previous cycle of the engine operation provides a convenient way of diluting the mixture. Three levels of EGR (5%, 10% and 15% of the charge mass) were studied and the results were compared with the performance when there is no EGR. The presence of EGR (or any diluent) in the combustion chamber has an effect on the in-cylinder mixture burning speed and hence on the performance. The diluents absorb heat from the mixture and bring the in-cylinder temperature down or effectively reduce the specific heat capacity of the mixture. In order to accommodate these mechanisms in the
calculations, the expression used for calculating the laminar burning velocity needs to be modified. The laminar burning velocity, \( S_L \), when no EGR is present was calculated using the expression [eqn. (4.29)] suggested by Iijima and Takeno (1986). This does not have a provision for EGR and in the absence of a suitable expression for \( S_L \) of methane under EGR conditions, an expression used for gasoline combustion under EGR conditions (Metghalchi and Keck 1982) is used here. As the main objective of this study is to understand the trends of variations in performance when EGR is present, the decision to use an expression not derived for methane can be justified. The expression used is given by

\[
S_{L,\text{EGR}} = S_L (1 - 2.1 Y_{\text{EGR}})
\]  

(5.1)

where \( S_{L,\text{EGR}} \) is the effective laminar burning velocity when EGR mass fraction \( Y_{\text{EGR}} \) is present in the initial mixture.

Figure (5.40) shows the effect of EGR on cylinder pressure. With increasing levels of EGR replacing the fresh charge of air-fuel mixture, the total chemical energy content available within the combustion chamber decreases and this results in a lowering of the peak cylinder pressure. As seen with eqn. (5.1), laminar burning velocity decreases with increasing levels of EGR, resulting in slower combustion and the peak pressure occurring late in the expansion stroke. This too reduces the peak pressure. This result indicates how important it is to choose the right levels of EGR in order to reduce \( \text{NO}_x \) emissions to desired levels while still maintaining sufficient power availability from the engine. This also indicates how useful and convenient CFD can be as a tool for optimising the levels of EGR for a particular engine and for the evolution of a good engine design.

Figure (5.41) shows the important aspect of \( \text{NO}_x \) emission control; the in-cylinder temperature. As one would expect, peak average in-cylinder temperature decreases with the increasing levels of EGR and also the peak occurs late in the expansion stroke, towards EVO. This can act in two ways for controlling \( \text{NO}_x \) emissions. As the peak temperature is lowered, proportionally, the level of \( \text{NO}_x \) formation is also reduced. Also, as \( \text{NO}_x \) formation is a function of time and having the peak temperature later in the cycle reduces the time available for \( \text{NO}_x \) formation.
before EVO. Figures (5.42) and (5.43) show the effect of EGR respectively on burned mass fraction and mass burning rate within the engine. These results indicate that it takes longer to complete the combustion of the fresh charge due to the direct result of the lowered laminar burning velocity of the mixture in the presence of EGR as a diluent. These results agree well with the trends [fig. (5.44)] obtained by Hires et al. (1976) and Blumberg et al. (1979).

Another noticeable feature gathered from these results of the EGR study is that the curves in the pressure, temperature, burned mass fraction and mass burning rate plots [figs. (5.40) – (5.43)] are more or less uniformly spaced for the uniformly spaced EGR levels studied here. This differs from fig. (5.10), in which the effect of engine speed on engine performance is given and the spacing between the curves reduces even if the engine speed is increased at uniform intervals. This uniform variation of pressure etc. with uniform variation of EGR enables the making of reasonable estimates about the engine performance at other levels of EGR by simple interpolation. Engine speed of 1500 rpm, ignition timing at 32° CA BTDC, relative air-fuel ratio, $\lambda=1$ and 13.1:1 compression ratio situation was used for this EGR study.

Figure (5.40). Effect of exhaust gas recirculation on cylinder pressure
Figure (5.41). Effect of exhaust gas recirculation on average cylinder temperature

Figure (5.42). Effect of exhaust gas recirculation on burned mass fraction
Figure (5.43). Effect of exhaust gas recirculation on mass burning rate

Figure (5.44). Effect of exhaust gas recirculation on combustion duration
(Hires et al. 1976 and Blumberg et al. 1979)
5.9. Effect of the combustion chamber geometry

As discussed in section (5.3.4), choosing a suitable combustion chamber is an important step towards optimising an engine to run solely on natural gas fuel. The combustion chamber needs to be compact in order to minimise heat losses and to compensate for the slower burning velocity of NG compared to gasoline. It should also be able to aid enhanced combustion by generating suitable levels of turbulence and swirl. Currently, there is a significant number of ongoing experimental researches aimed at studying suitable combustion chambers for this gaseous fuel. Meyers and Meyer (1994), Einewall and Johnasson (1997) and Evans (1999) are examples.

The task of experimentally testing and comparing several different combustion chamber geometries or various modifications to those designs is painstaking, time consuming and expensive. Numerical modelling can be an extremely helpful tool for this situation. The setting up of a required geometry and numerically studying it can be done relatively easily with less resources being utilised. Another very attractive advantage of using numerical modelling for the study of combustion chambers is that various geometrical features and properties can be tested by simply changing the dimensions fed into a computer code. Some such variables one can easily change and test with numerical modelling are the location of spark plug(s), piston bowl size and eccentricity, squish clearance height, stroke/bore ratio and valve lift.

In order to investigate these possibilities, three different combustion chambers were numerically tested in the current study, as a first step. The objectives were to understand the essentials of modelling different combustion chamber geometries, to study the universal nature and the behaviour of the combustion model used in the present study when geometry changed and to study the effect of combustion chamber geometry on engine performance and pollutant formation. For clarity and convenience in the generation of the geometry, the crevice cells were not considered and accordingly, the blow-by flow was not calculated.

The piston geometry used so far in this study (The ‘Brunei piston’) has a cylindrical bowl [Fig.(2.3)]. The horizontal and vertical faces of this piston provide more surface area for heat transfer and flame quenching. A dish shaped piston...
geometry, as used by researchers at Southwest Research Institute (Meyers and Meyer 1994), was also studied. This dish shape, which is identified as ‘SWRI piston’ during the present study, in a way, mimics the curved flame front propagating towards it and is expected to give less flame quenching on the piston face. Although in this dish shaped piston the level of flame quenching can be less, the generation of turbulence may be higher in the Brunel piston due to the stronger recirculation zone in the deeper bowl and squish.

In order to study the effects and interaction of these two important activities, i.e. flame quenching and turbulence generation, a new piston geometry was proposed. This new geometry, when features are compared, falls in between the SWRI and Brunel pistons. The new piston geometry has a deep bowl as in the Brunel piston but in the same time it attempts to reflect the dish shape of the SWRI piston (in order to mimic the shape of the flame front) with the bowl walls suitably inclined instead of being vertical as with the Brunel piston. These three geometries used are graphically shown in fig. (5.45) and the numerical meshes used to study them are shown in fig. (5.46). It is noteworthy that, in order to study the effect of geometry alone on engine performance, all piston bowl dimensions were carefully chosen to give the same bowl volume and the same compression ratio.

The fractal flame model (FFM) and the eddy break up model (EBUM) were used to study these three combustion chambers. This was in order to understand the performance strength of these two combustion models when the geometry is changed. A combustion model showing a consistent performance with different geometries would be the better choice during the phase of numerically optimising a combustion chamber for this gaseous fuel. However, to establish such a conclusion, reliable experimental data must be made available for these three geometries for comparison. Again, an engine speed of 1500 rpm, ignition timing at 32° CA BTDC, relative air-fuel ratio, λ=1 and 13.1:1 compression ratio situation was used for this study.

Figure (5.47) gives a comparison of engine performance, in terms of cylinder pressure, for the three pistons used in the study with the validated FFM. The same comparison is shown with the EBUM used as the combustion model is given by fig. (5.48).
Figure (5.45). The three combustion chamber geometries used for comparison.
Figure (5.46). Three meshes of the combustion chamber geometries used for comparison.
Figure (5.47). Comparison of the piston geometries using the FFM

Figure (5.48). Comparison of the piston geometries using the EBUM
Both these results given by fig.s (5.47) and (5.48) show a similar variation in cylinder pressure for the three engine geometries. The SWRI dish piston is seen to produce the highest cylinder pressure, with both combustion models and this is a good indication that the piston bowl, which mimics the flame front results in less flame quenching. The Brunel piston has produced the lowest pressure during compression stroke, compared to the two other pistons and after TDC but it has started to gain a higher pressure than the new piston geometry. Again the same trend is seen with both combustion models.

The three pistons studied are compared at three different crank angles in figs. (5.49) – (5.60). The in-cylinder distribution of temperature, which indicates the flame propagation, velocity, turbulent kinetic energy, $k$ and dissipation of $k$ are compared here. This comparison is made at three crank angles (-32°, -18° and -8° CA BTDC) and these three angles were chosen for mere convenience in comparison. The same number of numerical cells has been maintained for each mesh used but the respective cell sizes have not always been the same. As an example, the width of the cells outside the bowl towards the wall in the SWRI dish piston is relatively smaller compared to their counterparts in the two other meshes. The effect of this non-uniform distribution of cell sizes on the results is unknown and a proper investigation is needed, may be through a grid dependency test.

It can be seen that the spherical nature of the flame front has been preserved in all three geometries. The velocity distribution in the three pistons looks similar but does not match quantitatively. Areas of recirculation can be clearly seen and this information is of great importance when deciding the location of spark plug(s).

At the spark timing of -32° CA BTDC, the Brunel piston has gained the highest level of turbulent kinetic energy, $k$, in the cylinder, as seen in fig. (5.51). However, as combustion progresses through the mixture, the SWRI dish piston defeats the Brunel piston and gains the highest level of $k$, which can directly contribute to the improved mixing of burned products of combustion and unburned reactants thus improving and/or speeding up the combustion rate. The Brunel piston continues to have a high rate of dissipation of $k$. 
Figure (5.49). Comparison of in-cylinder temperature distribution at -32° CA ATDC
Figure (5.50). Comparison of in-cylinder velocity distribution at -32° CA ATDC
Figure (5.51). Comparison of turbulent kinetic energy distribution at -32° CA ATDC
Figure (5.52). Dissipation of turbulent kinetic energy at $-32^\circ$ CA ATDC
Figure (5.53). Comparison of in-cylinder temperature distribution at $-18^\circ$ CA ATDC
Figure (5.54). Comparison of in-cylinder velocity distribution at $-18^\circ$ CA ATDC
Figure (5.55). Comparison of turbulent kinetic energy distribution at $-18^\circ$ CA ATDC
Figure (5.56). Dissipation of turbulent kinetic energy at $-18^\circ$ CA ATDC
Figure (5.57). Comparison of in-cylinder temperature distribution at \(-8^\circ\) CA ATDC
Figure (5.58). Comparison of in-cylinder velocity distribution at $-8^\circ$ CA ATDC
Figure (5.59). Comparison of turbulent kinetic energy distribution at $-8^\circ$ CA ATDC
Figure (5.60). Dissipation of turbulent kinetic energy at -8° CA ATDC
The results of this study do not lead to any firm conclusions but they have presented how the early stages of designing of new engines and then optimising can be suitably done using numerical studies. At the time of spark, it is advantageous to have a high level of turbulent kinetic energy near the spark so the flame kernel can efficiently and effectively spread through to the adjacent unburned area. Also, there should be a lower mean velocity near the spark in order to avoid the flame kernel being blown out. The present results with different geometries would help suitably locating spark plug(s) in different engine geometries.

The effect of engine speed on each of the three piston geometries has been studied with the FFM and is given by figs. (5.61) – (5.63). All three pistons have behaved in a similar manner, producing a higher pressure at a lower speed and a lower pressure at a higher speed, as discussed in section (5.7). A better insight can be achieved if these three geometries are compared at each speed, separately as in figs. (5.64) – (5.67). These show an important picture that the SWRI dish piston performing with an early pressure peak compared to the other pistons at 1200 rpm and this quality of the SWRI dish piston diminishing as higher engine speeds are considered. At 1200 rpm, the Brunel piston produced the lowest peak cylinder pressure, later in the expansion stroke than the other two pistons. As engine speed is increased, the Brunel piston is seen to produce a pressure peak earlier than the others and a higher peak value than that produced by the new piston geometry. At all four speeds considered, the new piston geometry performed less favourably compared to the SWRI dish piston, in terms of peak cylinder pressure produced and the crank angle at which this peak occurs. The SWRI dish has produced the highest pressure compared to the two other pistons during the compression stroke hence requiring more work done on the engine to compress the gases. The Brunel piston requires the minimum work done on it for the compression of the charge. However, these results need proper experimental validation and further investigation before any firm conclusions can be made.

The effect of the initial level of swirl at inlet valve closure (IVC) on engine performance with the three piston geometries was evaluated. Three levels of swirl were studied here and figs. (5.68) – (5.73) show the effect of swirl on cylinder pressure. The swirl level number used (i.e. swirl = 1, 2 or 3) in these figures is the
initial swirl ratio, which is the ratio between rotational velocities of the air and the crankshaft.

Swirl assists the combustion by bringing in unburned mixture into hotter regions in the engine, resulting in faster and efficient combustion. A higher level of initial swirl would therefore obviously generate a higher peak cylinder pressure. In the swirl = 1 (low swirl) situation, the SWRI dish piston produces the highest peak pressure. The BruneI piston produces the lowest pressure during compression. As the initial swirl ratio is increased, all three pistons begin to behave in a similar manner but the BruneI piston produces a lower peak cylinder pressure. This is an indication that the effect of swirl is unable to sufficiently penetrate into the cylindrical bowl of the BruneI piston whereas the wider entrances of the bowls of the SWRI dish piston and the new piston geometry satisfactorily 'sense' the effect of swirl from the main chamber.

Figure (5.61). BruneI piston: Effect of engine speed
Figure (5.62). SWRI piston: Effect of engine speed

Figure (5.63). New piston geometry: Effect of engine speed
Figure (5.64). Performance of the three pistons compared at 1200 rpm

Figure (5.65). Performance of the three pistons compared at 1500 rpm
Figure (5.66). Performance of the three pistons compared at 1800 rpm

Figure (5.67). Performance of the three pistons compared at 2000 rpm
Figure (5.68). Brunel piston: Effect of swirl

Figure (5.69). SWRI piston: Effect of swirl
Figure (5.70). New piston geometry: Effect of swirl

Figure (5.71). Performance of the three pistons compared at initial swirl ratio = 1
Figure (5.72). Performance of the three pistons compared at initial swirl ratio = 2

Figure (5.73). Performance of the three pistons compared at initial swirl ratio = 3
5.10. An improvement made to the Arrhenius type SR chemistry model in KIVA-II in the context of SI engines fuelled with natural gas

The originally available single reaction chemistry model, SRM in KIVA-II is of the Arrhenius type rate calculation of the chemical kinetic reaction of fuel oxidation. It does not incorporate the effect of in-cylinder flow turbulence into the expression and taking this the main reason, many users of the KIVA family of codes replace this chemistry model with some other generally available combustion model. It was not possible to find in the literature the use of this originally available model for an SI engine situation, where the charge is premixed and the combustion behaviour is completely different to that of a diffusion type engine combustion with fuel injection. An attempt has been made to use the originally available KIVA-II chemistry model in the present study to calculate the reaction rates of natural gas combustion in an SI engine.

Although one of the authors of the code (Johnson 1998) claims that this model could be used for SI engine premixed combustion, the results of the present study shown by fig. (4.21) in section (4.11) indicate that the use of the KIVA-II chemistry model for natural gas combustion in an SI engine is a complete failure. The major difficulty encountered with the use of this model is choosing the model constant value of $A_f$ in eqn. (2.13), provided that the constant $E_f$ and reaction orders for each species are kept constant at the values suggested by Westbrook and Dryer (1981) for methane combustion. The constant $A_f$ is found uncontrollably sensitive and the range of values attempted for $A_f$ either resulted in an extremely fast and abrupt rise in pressure releasing excessive heat or did not sustain sufficient combustion or no combustion resulted at all. In the present study, it was almost impossible to obtain stable and acceptable combustion with the form of single reaction rate model originally available in KIVA-II.

It was found, after extensive analysis, that the quantity $\tilde{p}_k/W_k$ appearing in the KIVA-II originally available reaction rate expression [eqn. (A1.8), appendix I] caused heavy inconsistencies in the calculated reaction rates at neighbouring cells in some areas of the domain, especially behind the flame front. This may have been due to the premixed nature of the combusting mixture considered in the present study of natural gas fuelled SI engine and after an exhausting study, this
difficulty was overcome by redefining this quantity making it suitable for a premixed combustion situation. Instead of calculating this quantity for the reference species, $K$, it was calculated individually for the fuel, oxygen and the products of combustion (all other species considered in the calculations) as

$$\frac{\bar{\rho}_{\text{fuel}}}{W_{\text{fuel}}} \quad \text{for fuel},$$

$$\frac{\bar{\rho}_{O_2}}{r \cdot W_{O_2}} \quad \text{for oxygen}$$

and

$$\frac{\bar{\rho}_{\text{products}}}{(1 + r) \cdot W_{\text{products}}} \quad \text{for the products of combustion}$$

where $r$ is the oxygen:fuel stoichiometric mass ratio and the minimum of these three terms was chosen to replace the $\bar{\rho}_k/W_k$ term in eqn. (A1.8). As with the KIVA-II original chemistry model, this improvement still maintains the Arrhenius nature of the model by keeping the chemical kinetic calculations and not including turbulence parameters in the calculation of the reaction rate, $\dot{\omega}$. The proposed modification is made only on the calculation of reaction rate, $\dot{\omega}$ for fuel oxidation and the kinetic chemistry calculation of $NO_x$ (Zeldovich mechanism) was done separately using the NOX subroutine [section (6.1.1)]. It should therefore be noted that in the present calculations with this improved KIVA-II Arrhenius type model, $\rho_m$ used in eqn (A1.1) and eqn (A1.2) is the intermediate density of the species $m$ that has not been updated due to the kinetic reactions of NO formation. This improvement is made merely to reduce the serious uncontrollability of the original model in calculating the reaction rates of premixed engine combustion of natural gas. The improved version of this KIVA-II kinetic model will now be called the SRM-new (new single reaction rate model). The engine performance results obtained using this SRM-new are compared below with the other combustion models used in the present study in order to identify the effect of the proposed improvement. The performance of this model in calculating pollutant formation is discussed in chapter 6.
The results comparing the SRM-new model with the FFM and the EBUM [figs. (5.74) - (5.76)] give rise to an interesting issue for discussion and further study. After the modification proposed in this study, the KIVA-II SR model, which did not have the robustness to calculate premixed combustion of natural gas has not only achieved this capability but also performs better than the EBUM. The EBUM mainly considers the effects of turbulence on combustion and does not consider chemical kinetics and that can explain any difference between the performance of the EBUM and the SRM-new. The most interesting observation here is that this modified SR model (SRM-new), which does not incorporate the effects of turbulence on combustion, performing reasonably comparably with the FFM. The FFM provides a closer explanation of engine combustion in the flamelet regime and incorporates the effects of turbulence on combustion. It is reasonable, therefore, to expect any model like the SRM-new, which considers only the kinetic chemistry to give considerably inferior performance compared to the FFM. However, SRM-new has produced the pressure and the burned mass fraction variations well agreeable with the experimental data and performed well as a CFD combustion model for SI engines.

Figure (5.74). Comparison of predicted cylinder pressure (FFM, EBUM, SRM-New)
Figure (5.75). Comparison of predicted burned mass fraction

Figure (5.76). Average in-cylinder temperature with three combustion models.
Although the pressure rise is smoother compared to that produced by the EBUM, a lower pressure results with the SRM-new until the peak pressure is reached, indicating a calculated lower work output. However, very close peak pressure values have been obtained by the SRM-new and the FFM with the right arms of the pressure-crank angle diagrams being almost the same. When it comes to the burned mass fraction, the SRM-new results in an earlier consumption of reactants within the chamber but follows the experimental trace much closer than the EBUM does. As seen with the pressure - crank angle diagram, the resulting combustion is initially slower than that resulting from the FFM. The average in-cylinder temperature resulting from the SRM-new follows the same trend resulting from the FFM and again differs significantly to that produced by the EBUM.

Figures (5.77) and (5.79) give average in-cylinder temperature contours of the advancing flame at two suitable crank angle locations. It is very encouraging to find that the spherical nature of the propagating flame front has been sufficiently reproduced by the SRM-new whereas the EBUM was not successful in this regard, as seen before in figs. (4.25) and (4.26). Velocity vectors resulting from the SRM-new at those two crank angle locations are given by figs. (5.78) and (5.80) and indicate that they are comparable to those obtained with the FFM [fig. (4.11)].

These observations made here, of course, indicate that the originally available Arrhenius type kinetic chemistry model (SRM) is capable of correctly calculating natural gas fuelled SI engine combustion when upgraded to the SRM-new model by implementing the replacement proposed earlier for the $\bar{p}_k/W_k$ term in the SRM expression and then following the other suggested steps.

It is well worth studying as to how this SRM-new with turbulence effects not included in the model could perform comparably with the FFM. One possible explanation is that the levels of turbulence experienced in the engine studied here may be low enough that the effect on combustion is not very high thus both models with and without turbulence parameters perform relatively closely. It is worth recalling here that unlike the EBUM, the FFM had turbulence parameters within its formulation thus making their effect on chemical reaction rate not straightforward. The strength of the SRM-new can be established for gaseous fuel combustion in SI engines only by proper investigation and this deserves another careful look.
Figure (5.77). Average temperature contours at ~10.5°CA BTDC, SRM-new

Figure (5.78). In-cylinder velocity distribution at ~10.5°CA BTDC, SRM-new
Figure (5.79). Average temperature contours at ~4.5°CA BTDC, SRM-new

Figure (5.80). In-cylinder velocity distribution at ~4.5°CA BTDC, SRM-new
Chapter 6.

Emissions from the SI engine fuelled with natural gas

6.1. Pollutants and their formation

In IC engines, heat is released during the combustion process in order to provide useful work and in the same time many harmful pollutants are formed. Until more efficient and environmentally friendly ways of converting the chemical energy of fuels into heat energy are established, one has to develop ways to deal with these pollutants that harm human health and deteriorate the quality of the environment in which we live. However, not all combustion processes and systems produce the same amounts of pollutants per unit work done. Today’s research is heading towards finding better designs of combustion systems, fuels and strategies to minimise the emission of pollutants while maximising the heat generated (hence the work). Numerical modelling of engine combustion and formation of pollutants from these engines will continue to play a major role in this endeavour.

Pollutant formation rates in combustion processes are slow and determined by detailed kinetics. The pollutant emissions of greatest concern for IC engines are oxides of nitrogen (NOₓ) and unburned hydrocarbons (UHC), which can together contribute to photochemical smog and carbon monoxide (CO), a toxic gas. Carbon dioxide (CO₂), being a greenhouse gas, is an unavoidable product of combustion. As the combustion processes improve, complete combustion of fuels can
be obtained but with the unwanted gift of increased CO₂ emissions. One way of minimising CO₂ production from engines is using a lean burning technique where less fuel is burned. Fuels such as natural gas, whose main component is methane, is expected to give less CO₂ due to the fact that methane, among other hydrocarbons, has the least number of carbon atoms per molecule. Pollutants of secondary concern include particulate matter (primarily soot), sulphur dioxide and aldehydes. Further details on the harmful effects of various pollutants and numerical modelling of their properties and the production rates can be found in the review by Faeth (1996). Since natural gas is composed primarily of methane and other lower hydrocarbon fuels, particulate matter emissions in natural gas engines are almost non-existent and non-methane hydrocarbon emissions are extremely low. The excellent in-cylinder mixing quality of this fuel with air results in lower levels of CO emission from natural gas engines, even at cold start, compared to gasoline and diesel engines. In the current work, emphasis was given to modelling of NOₓ.

6.1.1. Nitrogen oxides

Oxides of nitrogen impact the environment in several ways; as a reactant in the production of photochemical smog, as a reactant that affects concentrations of stratospheric ozone and as a contributor to acid rain and the greenhouse effect (Bowman 1992). These factors have lead to stringent regulations on the production of nitrogen oxides in IC engines.

The formation of NOₓ in an engine is primarily a function of reaction temperature, duration and availability of oxygen and the three factors that contribute most to NOₓ formation are high combustion temperatures (needed for the high activation energy required to oxidise the stable N₂ molecule), pressure and O₂ availability. Natural gas has a lower flame temperature which tends to reduce peak NOₓ formation, but with the advanced spark timing and the increased compression ratio used to compensate for the slow flame speed of natural gas, emissions of NOₓ increases (DeLuchi et al. 1988, Heywood 1988).

The oxides of nitrogen commonly identified as NOₓ are in fact nitric oxide (NO), nitrous oxide (N₂O) and nitrogen dioxide (NO₂). Recent studies suggest that the engine combustion is not a major source of N₂O (Faeth 1996). Chemical
equilibrium considerations show that for burned gases at typical temperatures, the ratio \( \text{NO}_2/\text{NO} \) should be negligibly small for spark ignition engines (Borman and Ragland 1998). Accordingly, NO is the primary constituent in \( \text{NO}_x \) emissions from SI engines and the modelling of its formation is presented in this study.

The main sources of nitrogen oxide emissions in combustion are the oxidation of molecular nitrogen (free nitrogen in combustion air) in the post flame zone (thermal NO), the formation of NO in the flame zone (prompt NO) and the oxidation of nitrogen containing compounds (chemically bound nitrogen) in the fuel (fuel NO). The relative importance of these three sources of NO depends on the engine operating conditions and the type of fuel used. Natural gas contains insignificant levels of chemically bound \( \text{N}_2 \) and the fuel bound NO emissions are low. Prompt NO levels are also very low as the flame reaction zone in engines is extremely thin (~ 0.1 mm) at high pressures and the residence time of different species in the flame front is very short. Also since the cylinder pressure rises during most of the combustion process, the burned gases produced early in the combustion process are compressed resulting in a higher temperature than they reached immediately after combustion. NO produced from NG combustion is therefore almost solely thermal NO (Heywood 1988).

The mechanism for the formation of thermal NO was first proposed by Zeldovich et al (1947). This mechanism was modified (or extended) by Lavoie et al. (1970) by the addition of one more reaction which significantly contributes. This extended Zeldovich mechanism of formation of thermal NO consists of six principal reactions with seven species and is given by

\[
\begin{align*}
O + N_2 & \Leftrightarrow NO + N & (6.1) \\
N + O_2 & \Leftrightarrow NO + O & (6.2) \\
N + OH & \Leftrightarrow NO + H & (6.3)
\end{align*}
\]

These reactions mainly proceed in the high temperature, fuel lean, post flame regions of combustion where the required pools of \( O \) and \( N \) radicals are available (Faeth 1996). The forward rate constant for reaction (6.1) and the reverse rate constants for reactions (6.2) and (6.3) have large activation energies which result
in a strong temperature dependence of NO formation rates and to a lesser extent on the
burned gas oxygen concentrations and pressure (Bowman 1992).

The extended Zeldovich mechanism can be implemented in the CFD
code, KIVA-II, in a manner similar to the natural gas oxidation mechanism. A new
subroutine named NOX was written and called at each numerical time step in order to
calculate updated densities of each of the species (O2, N2, O, N, H, OH, NO) taking
part in the mechanism. It is known that NO formation is endothermic but some
researchers have taken this as weakly endothermic compared to the exothermic
reaction of oxidation of the fuel used. They have therefore neglected the heat of
reaction of NO formation and assumed that NO chemistry does not have a direct
influence on the fuel oxidation process (Agarval 1998, 1999). This claim was tested in
the present study and found that the NO chemistry has a significant effect on the
performance of the natural gas fuelled SI engine studied and therefore the heat of
reaction of NO formation was included in present calculations.

Figures (6.1) – (6.4) show the effect of heat of reaction of NO
formation on cylinder pressure, average cylinder temperature, burned mass fraction
and on NOx formation itself. The plots designated “No NOx heat” correspond to the
results obtained when the heat of reaction of NO formation was neglected. As these
figures indicate, if the heat of reaction of this endothermic process of NO formation is
neglected, a higher temperature resulted than when it was not neglected. This has a
direct influence on the cylinder pressure and NOx formation. It can be learned here
that it is not advisable to neglect the heat of reaction of NOx though it is weakly
endothermic compared to the main exothermic reaction of fuel oxidation.

Radicals such as N and O are needed for the production of NO. Since
these could not be obtained from the fuel oxidation reaction, it was assumed that they
were in equilibrium with their respective molecular states at the local temperature and
pressure. This is a valid assumption as during the NO formation process, the radical
concentrations achieve their equilibrium values very quickly. This equilibrium
assumption for the minor species has routinely been used with the Zeldovich kinetics
(Heywood 1988, Josefsson et al. 1998). These equilibrium reactions were given by
eqn. (2.17) in chapter 2.
Figure (6.1). Effect of heat of reaction of NO\textsubscript{x} formation on cylinder pressure

Figure (6.2). Effect of heat of reaction of NO\textsubscript{x} formation on average temperature
Figure (6.3). Effect of heat of reaction of NO\textsubscript{x} formation on burned mass fraction

Figure (6.4). Effect of heat of reaction of NO\textsubscript{x} formation on NO\textsubscript{x} emission
6.1.2. Hydrocarbons

Unburned hydrocarbons (UHC) tend to occur near the cylinder walls and in the crevices. At the cylinder walls the flame front is quenched and in the crevices fuel does not burn as the mixture is not reached by the flame. A slow flame front prevents complete combustion of the intake mixture before the exhaust valve opens giving further UHC emissions. Poor combustion quality or misfiring when running close to the lean or rich combustion limits are other causes for UHC emissions. From a natural gas engine, any UHCs appear almost entirely as methane. As methane is non-toxic and non-smog forming, generally it is not counted for HC emissions. It is reasonable to expect that advanced, dedicated NGVs will emit less non-methane HCs (NMHCs) than gasoline vehicles. NG vehicles do not emit benzene and other aromatic hydrocarbons (DeLuchi 1988, Heywood 1988, Fricker et al. 1991).

6.1.3. Carbon monoxide

CO is the obvious result of incomplete combustion. The use of NG in lean burn engines which can run leaner than gasoline engines will practically eliminate CO emissions and combustion in the NG engine can be expected to be far more satisfactory due to excellent mixing of this gaseous fuel and air. With gasoline engines, higher levels of CO can be expected at start up due to the richer mixture and poor air-fuel mixing. Due to gaseous state of NG, no fuel enrichment is needed in the NG engine during the cold start and this gives much lower CO emissions than a gasoline engine would produce at cold start (Crane and King 1992).

6.1.4. Aldehydes

In NG engines, aldehyde emissions are mainly composed of formaldehyde which is toxic if in high concentrations and is a probable human carcinogen (Gambino et al. 1992). Emission levels of formaldehyde (HCHO) from CNG vehicles are reported to be equal or less than those resulting from gasoline vehicles (Alson et al. 1988).
6.1.5. Other pollutants

NG is inherently a cleaner fuel compared with other common engine fuels. When burned, it produces the lowest levels of CO$_2$ compared to all other hydrocarbon fuels as NG has the lowest amount of carbon atoms per molecule among those fuels. Because of this high H/C ratio, NG combustion produces ~25% less CO$_2$ than gasoline or diesel fuel for the same engine efficiency. This aspect is of great importance due to the mounting concern with the greenhouse effect associated with CO$_2$. In general, NG does not contain sulphur and the sulphur oxide emissions are limited to what is formed by the combustion of lubrication oil. Solid particulate carbon can occur as a combustion product under very rich conditions. Such rich conditions, however, are not used in properly adjusted, optimised NG engines. With NG, therefore no particulate materials or smoke can be formed under normal operating conditions and there are no lead emissions. The only source of particulates in NG SI engines is lubricating oil (Alson et al. 1988, Weaver 1989, Unich et al. 1993).

6.1.6. Modelling of the formation of pollutants

Although the parametric study performed and reported in chapter 5 indicated that the modelling of a natural gas fuelled SI engine using the newly validated combustion model is a success, the next step should be to use the same modelling techniques for the calculation of the formation of pollutants from the engine. This would help establish the quality of engine combustion modelling and assure that CFD modelling of engines is a major tool for analysing emissions and the performance of an engine. Figure (6.5) shows the formation of the three main pollutants from a natural gas engine (NO$_x$, CO$_2$ and CO) within the cylinder, at the base line operating condition of the engine studied (engine speed 1500 rpm, ignition timing -32° CA BTDC, relative air/fuel ratio, $\lambda=1$ and compression ratio 13.1:1). The validated fractal flame model (FFM) has again been used here as the combustion model. In this figure, the variation of in-cylinder temperature was also included in order to understand the relationship between engine combustion and the formation of
pollutants. Figure (6.6) gives the same information when the eddy break up model (EBUM) was used as the combustion model.

A slightly higher level of CO\textsubscript{2} and a lower level of CO have been predicted when the EBUM is used compared to the results obtained with the FFM. The resulting in-cylinder temperature and NO\textsubscript{x} levels are almost the same with both models. With the FFM, the in-cylinder level of CO reaches a distinguishable peak and then drops whereas the EBUM does not result in such a clear peak. A proper validation study of these results with suitable experimental data is needed in order to establish the respective strengths and weaknesses of these two combustion models in predicting pollutant formation. Once these qualities of the combustion models are recognised, a truly meaningful numerical simulation of natural gas engines can be performed to enable the efficient designing of new combustion chambers for natural gas engines or in order to optimise the engine.

Figure (6.5). Average in-cylinder temperature and formation of the three main pollutants at base line case with the FFM
Figure (6.6). Pollutant formation at base line case when the EBUM was used

6.2. Effect of engine operating parameters on pollutant formation

6.2.1. Equivalence ratio

Running the engine fuel lean results in lower levels of emission of all three major pollutants, NO\textsubscript{x}, CO and UHC and this is seen in fig. (6.7). However, at very lean or rich conditions, beyond the combusting limits, the flame can die out giving high UHC emission levels. The equivalence ratio is the only variable, which has a significant effect on CO emission. When the mixture is rich, more CO is formed due to incomplete combustion at an environment where O\textsubscript{2} is scarce and very low CO levels result when the mixture is lean. As NO\textsubscript{x} is very much a function of burned gas temperature, at rich and lean conditions NO\textsubscript{x} formation is low and the highest level of NO\textsubscript{x} occurs at the lean side closer to the stoichiometric conditions where sufficient amounts of O\textsubscript{2} is available to combust the fuel and form NO\textsubscript{x}. 
6.2.2. Compression ratio

As the compression ratio increases, the scavenging in the engine improves and more of the exhaust is pushed out of the combustion chamber. This gives more UHC emitted in the exhaust. Lower exhaust gas temperatures will result from an increased compression ratio as more heat is converted into work, which in turn reduces the burn up of HC in the exhaust. Also with a high compression ratio, more air/fuel mixture is forced into crevices where the flame does not reach and this too, contributes to the increased UHC emission levels. NO\textsubscript{x} generation will be higher as the increased compression ratio raises the combustion temperature. With a higher compression ratio, more CO dissociation, at very low rates, can be expected (James and Garner 1995).
6.2.3. Engine speed (at constant load)

As the engine speeds up, the residual gas fraction decreases and the heat transfer per cycle is also reduced resulting in increased NO\textsubscript{x} in the exhaust. As more of the quench layer will be swept into the bulk of the charge due to increased levels of turbulence with increased speed, more HC gets burned and reduced UHC emissions can be expected in the exhaust with increased engine speed (Heywood 1988).

6.2.4. Load (at constant engine speed)

At low loads, inlet manifold pressure drops, resulting in a higher residual gas fraction. This will increase the heat transfer from the burning charge and reduces NO\textsubscript{x} emissions. At high loads, in-cylinder temperature can reach higher values thus resulting higher NO\textsubscript{x} levels. With more residual gases at low loads, combustion becomes poor and HC emission becomes high. As the load increases at a constant speed, expansion and exhaust stroke temperatures increase and the in-cylinder oxidation rate, if oxygen is available, will increase. However, as the exhaust gas flow rate increases, the residence time in critical sections of the exhaust system decreases and a reduction in exhaust port HC oxidation occurs. The net trend is for UHC concentrations to decrease modestly as load is increased (Heywood 1988).

6.2.5. Deceleration and idling

When the throttle valve is fully or almost fully closed, the engine speed becomes low resulting in a low manifold pressure. This allows more exhaust gases back into the combustion chamber during the valve overlap period and results in poor combustion. Bulk quenching of the flame is possible as the cylinder pressure is low and this indicates increased UHC levels. With more exhaust gases in and with a reduced engine speed, increased heat transfer is possible resulting in a reduced in-cylinder temperature and as a consequence reduced NO\textsubscript{x} levels in exhaust gases result (Heywood 1988, James and Garner 1995).
6.2.7. Ignition and ignition timing

The ultra-fast burning rates provided by multiple spark plugs and plasma ignition [see section (5.5.3)] produce higher combustion temperatures inside an engine combustion chamber and result in increased NO\textsubscript{x} emissions than with the other ignition system configurations at equal equivalence ratios. Improved combustion, however, will work to produce lower UHC emission levels in the exhaust (Meyer \textit{et al.} 1992).

Advanced ignition causes more recompression of the partially burned charge and increases the in-cylinder temperature, promoting knock and resulting in higher NO\textsubscript{x} levels. Retarded timing will decrease the combustion temperature but as the combustion process can not be completed before the exhaust valve closes, UHC emissions in the exhaust will be high (James and Garner 1995).

6.2.8. Residual gases and exhaust gas recirculation

The primary effect of exhaust gas recirculation (EGR) is the reduction of the burned gas temperature for a given mass of fuel and oxygen burned. This lowers the levels of NO\textsubscript{x} produced. However, residuals and EGR weaken combustion performance and UHC levels in exhaust increase. No significant effect is expected on CO emissions (James and Garner 1995).

6.3. Emission Control

NGVs can have EGR, lean burn operation, special combustion chambers and catalytic converters designed for natural gas fuel to control emissions. If a three-way catalyst is used, the engine has to run near stoichiometric conditions for the catalyst to be effective in controlling all three NO\textsubscript{x}, CO and HC emissions. EGR can be used in addition to this for further reduction of NO\textsubscript{x} emissions by effectively reducing the burned gas temperature. If lean burn operation is employed, a two-way (oxidation) catalyst, which caters only for HC AND CO, can be used. Electronic control systems for stoichiometric gasoline engines with three way catalysts have reached a high level of development and this technology is readily adaptable to
engines using NG. The basic engine control systems and sensors required for a stoichiometric NG engine control system are the same as those required for a stoichiometric gasoline system. However some fuel condition sensors (e.g. fuel temperature and pressure) may be needed to account for the greater variability in fuel conditions of NG. The key difference between lean burn and stoichiometric control systems are in the sensors and control algorithms required (Hundleby 1989, Weaver 1989, Noble and Beaumont 1991, King 1992).

6.3.1. Control of emissions of nitrogen oxides

Running an engine either very lean or very rich reduces NO\textsubscript{x} formation [see figure (6.7)], in the former case because the burned gas temperature is lowered and in the latter case because of the reduced supply of O\textsubscript{2}. Emissions of NO\textsubscript{x} can further be reduced by decreasing the burn time or lowering the engine speed as the heat dissipation is less at higher engine speeds. Also, cooling the combustion environment by adding water (maybe in the form of a spray), liquid natural gas (LNG) or exhaust gas recirculation (EGR) reduces the peak burned gas temperature and thus the NO\textsubscript{x} formation. NG engines can tolerate higher EGR rates than gasoline engines due to better performance of CNG in case of diluted combustion. NO\textsubscript{x} levels can be reasonably controlled by these methods to acceptably low levels with only a slight penalty in fuel consumption. As the NO\textsubscript{x} reduction catalyst does not work with an excess of O\textsubscript{2}, a catalyst will be ineffective in reducing NO\textsubscript{x} emissions if the engine runs lean (DeLuchi 1988, Heywood 1988). However, the lean burn engine is the next option to achieve low NO\textsubscript{x} emissions. The extensive research that has been performed on gasoline lean burn engines (Quissek et al. 1989) can successfully be applied to CNG engines. In fact, NG is an excellent fuel for lean burn engines because of its tolerance to diluted combustion as well as the high homogeneity of air-fuel mixture that can be achieved. The main problems associated with the development of lean burn engines are achieving efficient combustion at the reduced combustion temperatures, acceptable cyclic variations and a satisfactory drivability in lean conditions (Beaty et al. 1992, Unich et al. 1993). To solve these problems, more ignition energy is necessary for a lean mixture than for a stoichiometric mixture and a combustion chamber, which allows high turbulence levels and a shorter flame travel
length is needed. This way, the cyclic variability and the burning duration are reduced resulting in improved thermal efficiency (Kingston Jones and 1989, Shiells et al. 1989). The required high ignition energy can be generated by electric sparks, a pilot fuel or with the help of a separate pre-chamber. The energy provided by the pilot fuel (diesel) is usually greater than that provided by a spark plug. This allows a dual-fuel engine to operate at sufficiently lean air/fuel ratios so that intake-air throttling is not usually required, even at part engine loads (Gettel et al. 1986, Beaty et al. 1992). Staged pre-chambers, separated by orifices, have been found to reduce NO\textsubscript{x} emissions further (Crane and King 1992). Very advanced and accurate control systems for fuel and ignition are needed in order to deal with fuel composition variations and to operate lean enough to obtain low NO\textsubscript{x} without reaching the lean misfire limit (Beaty et al. 1992, Unich et al. 1993).

6.3.2. Control of emissions of unburned hydrocarbons

Increasing the temperature of exhaust gases by retarding the ignition burns UHC in the exhaust. Although a two-way or a three-way catalyst could be used with natural gas, a lower HC conversion efficiency is expected when used in natural gas engines as methane is known to be difficult to oxidise (Hundleby 1989). Multiple spark plugs and other multi-point ignition methods reduce HC emissions at lean mixtures by effectively reducing the misfire rate (Meyer et al. 1992). Staged pre-chambers, separated by orifices, have been found to reduce engine-out UHC emissions (Crane and King 1992).

6.3.3. Control of emissions of carbon monoxide

CO emissions are significantly lower with NG compared to those from gasoline engines as there is no need for fuel enrichment at cold start compared to gasoline engines and the improved lean burning conditions in transient operation. Lean burn technology is an ideal solution for reducing the emissions of CO from natural gas engines. With the amply available oxygen in a lean mixture, incomplete combustion would practically be eliminated if other necessary conditions are provided
correct. The use of a catalytic converter would further reduce any exhaust CO emissions (Hundleby 1989, Unich et al. 1993).

6.4. Parametric study with KIVA-II

After performing a parametric study and comparing the numerical results with suitable experimental results, it was indicated in chapter 4 that the predictive capability of the fractal flame model (FFM) in modelling the engine performance was sufficiently high and practical enough for numerically studying a natural gas fuelled engine, for designing new combustion chambers or in the process of optimising the engine for natural gas. It is equally necessary to establish that if this improved FFM has sufficient strength to support simulating the trends of formation of pollutants in the natural gas fuelled SI engine, so that a complete and detailed picture of the engine operation can be obtained through a single numerical simulation. During this parametric study, the combustion model constant validated for the FFM baseline case was used unchanged. The same initial conditions were applied as before.

The trends of the variations in pollutant levels at exhaust valve opening (EVO) were studied with relative air/fuel ratio (\(\lambda\)), compression ratio, engine speed and ignition timing as the operating parameters varied. As used earlier in section (5.7), the test matrix consisted of five lambda values (\(\lambda = 0.9, 1.0, 1.1, 1.2, 1.3\)), three compression ratio values (10:1, 13.1:1, 15:1), three spark timings (32°, 26°, 20° crank angles BTDC) and four speeds (1200, 1500, 1800, 2000 rpm). Only one lambda value from the fuel rich side of operation has been chosen for this study as the common practice is to use natural gas engines in the fuel lean region. Specially when lean burn engine technology is of very high interest today as a measure of controlling and reducing engine out NO\(_x\) and CO and reducing CO\(_2\) production, it is essential to concentrate the studies on the fuel lean side of engine operation.

In order to validate the results of this parametric study, they need to be compared with experiments. It is not possible to compare each of these results with experimental data as the relevant experimental data for all engine operating conditions, at which this parametric study was performed, are not available. However, the established objective of this parametric study is to examine if the improved FFM
and the CFD code as a whole are sufficiently capable of calculating the trends of pollutant formation as operating parameters varied. In order to establish this, the results from this study were compared against similar work found in literature. Experimental results obtained for engines running on gasoline have been used once here for this comparison when suitable work for natural gas fuel could not be found in the literature. This approach can be suitably justified by considering the comparison of experimental results of formation of pollutants from an engine for gasoline and natural gas by Ishii et al. (1994). They have obtained the same trends of variations for formation of each pollutant with both fuels, though quantitative differences exist [figs. (6.8) – (6.10)].

Figures (6.11) – (6.13) show the effect of varying the relative air-fuel ratio ($\lambda$) from the base line case ($\lambda=1$), on oxides of nitrogen, carbon dioxide and carbon monoxide levels at EVO (127° ATDC), as obtained from calculations. The other engine operating variables were kept the same as at the baseline case (1500 rpm, ignition at 32° BTDC, 13.1 compression ratio).

The level of NO$_x$ at EVO is the highest when air:fuel ratio is the considered lowest (i.e. when the mixture is richer) the lowest level is obtained when the mixture is fuel lean. Figure (6.14) due to Meyer et al. (1992) shows experimentally obtained trends of the variation of NO$_x$, CO and CO$_2$ emissions in exhaust with fuel:air equivalence ratio for a natural gas fuelled SI engine with three spark locations. According to this, NO$_x$ emissions attain a peak level about the stoichiometric air:fuel mixture, in the fuel lean side and drop when the mixture is rich or leaner than a specific level. This is because the highest cylinder temperature is obtained near stoichiometry, slightly towards the lean side where sufficient oxygen is available for combusting the fuel and for oxidating N$_2$ in the charge. At rich mixtures there is no sufficient oxygen available to form NO$_x$ and in the lean side, due to the amount of fuel burned being less, in-cylinder temperature is lower and hence lower NO$_x$ levels result. This trend can reasonably be seen in the present calculations [Fig. (6.11)] without a peak occurring in the lean side. The amount of NO$_x$ calculated drops as the mixture gets leaner and reaches a possible peak as mixture gets fuel richer. Lean burn engine technology is based on this principle for meeting the strict, engine NO$_x$ emissions standards.
Figure (6.8). Comparison of variation of NO\textsubscript{x} emissions (Ishii \textit{et al.} 1994)

Figure (6.9). Comparison of variation of CO\textsubscript{2} emissions (Ishii \textit{et al.} 1994)

Figure (6.10). Comparison of variation of CO emissions (Ishii \textit{et al.} 1994)
Figure (6.11). Effect of relative air-fuel ratio ($\lambda$) on cylinder NO$_x$ formation

Figure (6.12). Effect of relative air-fuel ratio ($\lambda$) on CO$_2$
Meyer et al. (1992) have experimentally observed decreasing levels of CO₂ as a percentage in exhaust, as the mixture gets fuel leaner and they have presented this result only up to stoichiometry in fig. (6.14). A more detailed picture by Ishii et al. (1994) is given in fig. (6.9) and this shows that the emission of CO₂ as a percentage in the exhaust reaches a peak level around stoichiometry. This may not be the picture of variation of CO₂ one would see if emission of CO₂ in grams were considered instead of assessing as a percentage of the exhaust. Emission of CO₂ is a direct result of the amount of fuel burned. In a real engine situation, at lean side, low amounts of fuel is burned while in the rich side, there will be more fuel, still with almost the same amount of oxygen resulting in a fairly constant level of grams of CO₂ in the exhaust. This however describes the peak of emission of CO₂ as a percentage of the exhaust, occurring near stoichiometry.
Figure (6.14) Effect of fuel:air equivalence ratio (φ), on pollutant emissions in exhaust gases from a natural gas engine, with three spark locations (Meyer et al. 1992)

It is important to be aware of the fact that the way fuel enrichment or enleanment obtained for present calculation is different to that of a real engine situation. Here, at each air:fuel ratio considered, the same total air-fuel mass was maintained instead of keeping the air mass constant. This was essential in order to maintain the same motored peak pressure for each case calculated so any comparison of pressure variations due to combustion to be meaningful. This essentially reduces the amount of oxygen in chamber if a fuel rich condition is considered thus resulting
in a lowered CO₂ level, even if it is measured by weight instead of the percentage in exhaust. This makes it possible to compare the CO₂ emission results of the present study presented in grams with those presented by Ishii et al. as a percentage of exhaust gases. The results from the present work show a peak of emitted CO₂ grams occurring around the stoichiometry and this is comparable to the trend given by Ishii et al.

Carbon monoxide is a result of incomplete combustion. If the mixture is fuel lean, the expectancy of incomplete combustion is low thus lower levels of CO can be expected as the mixture gets leaner. This is one of the reasons why lean burn engines are of interest in today’s research. Experimental observations by Meyer et al. [fig. (6.14)] and by Ishii et al. [fig. (6.10)] indicate this trend and the result from the present calculations [fig. (6.13)] is very much comparable with these and the correct trend has been captured accurately.

Figures (6.15)-(6.17) show the effect of engine compression ratio on the formation of NOₓ, CO₂ and CO emissions, as resulting from the present calculations. For this study, the other engine operating variables remained constant at the baseline case (λ = 1, 1500 rpm, ignition at 32° BTDC) while only the compression ratio is varied. The basic effect of increased compression ratio is an increased charge temperature and hence a higher peak in-cylinder temperature. This has a direct influence on NOₓ formation, which is dependent on temperature in the engine environment. Provided that sufficient oxygen is available to oxidise N₂ in the intake air, a higher temperature will result in a higher level of NOₓ formation. This trend has been experimentally observed by Takagi and Raine (1997) in their study of effect of compression ratio on a natural gas fuelled spark ignition engine at stoichiometry, as shown in fig.(6.18). It should be noted that this experimental result shows only the variation of nitric oxide (NO) and can reasonably be expected to represent the variational trends of NOₓ. This is because NO is the largest component of NOₓ emissions from an SI engine while nitrogen dioxide (NO₂) is found only in small quantities (Heywood 1988). In the results by Takagi and Raine, at a given spark timing used, NO emission level increases with increasing compression ratio, though this is a small increase. The present calculation has been able to capture this trend of variation accurately, as seen in fig. (6.15).

Thermodynamic analysis indicates that increasing compression ratio results in increasing thermal efficiency. Exhaust temperature decreases as a result of
this until the compression ratio corresponding to the maximum efficiency is reached. However, this does not indicate any effect of compression ratio on the quality of in-cylinder combustion, which is a deciding factor in determining the amount of CO₂ emitted provided that the same fuel mass is burned or the same load is considered. It can be expected to have better combustion under the influence of increased in-cylinder temperature with increased compression ratio, though this rise in temperature is not drastic. This improved combustion should produce more CO₂ and reduce CO emissions if this argument is valid. However, the resulting higher peak cylinder pressure due to increased compression ratio can affect adversely on combustion rates and also may force more gases into crevices resulting in all the mixture not being combusted or more residuals being present. When all these factors are considered, it is extremely difficult to conclude what should the exact effect of compression ratio on CO₂ and CO emissions be.

Present calculations result in a slight decrease in CO₂ levels and a slight increase in CO levels with increasing compression ratio [figs. (6.16) and (6.17)]. The equilibrium reaction of CO₂ ⇌ CO and the way the KIVA-II code was instructed to initiate chemical kinetic and equilibrium reactions in a numerical cell may also have contributed to this trend even though it is a very slight variation. It is a temperature threshold value, which signals the code for initiating chemical kinetic and equilibrium calculations and with increased compression ratio, the temperature threshold value is reached fairly early and as a result, equilibrium calculations can begin early and be sustained for longer. The only significant parameter controlling CO emissions is the charge air:fuel ratio and the effect of compression ratio on this pollutant has not been recognised as such. The present calculations suggest a slight increase in CO emission levels as the compression ratio increases, as seen in fig. (6.17). No suitable experimental data could be found for comparison. However, it should be concluded that the effect of compression ratio on CO₂ and CO emissions as predicted by the present study is not very significant. The need still remains for proper verification by comparing the predicted trends with suitable experimental data in order to appreciate if the code has been able to capture the trends of CO₂ and CO variations correctly.

Figures (6.19) – (6.27) show the effect of engine speed at constant load on pollutant formation at different ignition timing settings. General trends observed
here are a decreasing NO\textsubscript{x} emission level, an increasing level of CO\textsubscript{2} emission and a decreasing level of CO emission with increasing engine speed for a given ignition timing. As engine speed increases, the time available for complete combustion decreases and the peak cylinder pressure occurs late in the cycle, as discussed earlier in section (5.7) earlier. This results in a lowered peak average temperature within the cylinder directly influencing NO\textsubscript{x} formation. Therefore, a reduction in NO\textsubscript{x} can be expected as engine speed increases at constant load, as seen in the simulation results. It is also seen here that the variations in CO\textsubscript{2} and CO emission levels, whatever the trend seen with varying engine speed, are small and not considered significant. Also, it was not possible to find any suitable experimental data from the literature to compare the trends of the variation of these two pollutants when engine speed varied.

Figures (6.28) – (6.39) show the effect of ignition timing on the formation of the three pollutants considered here, as engine speed varied at constant load. The general trends observed from the calculations here are an increasing NO\textsubscript{x} emission level, a decreasing peak of CO\textsubscript{2} emission level and a very slightly increasing peak level of CO emission with increased advancement of ignition timing. However, there was no information about the MBT at each speed considered and the results obtained may not be comparable with those obtained for each speed at respective MBT.

NO\textsubscript{x} emissions are significantly affected by the ignition timing used. Advancing the timing so that combustion occurs earlier in the cycle increases the peak cylinder pressure, which occurs earlier and around TDC, hence a higher peak average in-cylinder temperature resulting in higher levels of NO\textsubscript{x} emissions. This trend of variation has experimentally been obtained for a natural gas fuelled spark ignited engine by Stone et al. (1996) and given by fig. (6.40) and the present calculation has produced the same trend with reasonable accuracy. As the number of different timing settings used in this study is small, it is difficult to judge if this increment of NO\textsubscript{x} level varies linearly or with a varying gradient when ignition is advanced from MBT timing. Locating the MBT at the engine speeds considered needs extra work.

Although a reduction of CO\textsubscript{2} resulted (in terms of grams) at EVO is seen with advancing the ignition timing, they reach the same level as mixture gets leaner. As engine speed increases, at each ignition timing tested, the CO\textsubscript{2} levels reach this single level at a lower value of \( \lambda \). The reduction noticed here in the CO\textsubscript{2} level
with varying ignition timing is slight, however, and only at the lowest speed tested (1200 rpm) does it show some recognisable reduction. This is also noticeable only at the fuel rich side of the mixture assessed.

As discussed earlier, CO emissions from an engine are mainly a function of air:fuel ratio and the variation of ignition timing numerically tested has not made any significant effect on the level of CO resulted in exhaust at EVO, though the variation seen is to increase CO very slightly with ignition timing advanced. This has to be so in order to have a compatibility with the slightly decreasing CO₂ emission seen when ignition timing is advanced. When combusted, carbon atoms in the hydrocarbon fuel participated in the chemical reaction have to emit as CO₂ and CO alongside the carbon present in any small quantities of unburned hydrocarbon. If the level of CO₂ is varying, the level of CO too has to vary accordingly to keep the total amount of carbon atoms emitted.

![Figure (6.15). Effect of compression ratio on formation of NOₓ](image-url)
Figure (6.16). Effect of compression ratio on formation of CO₂

Figure (6.17). Effect of compression ratio on formation of CO
Figure (6.18). Effect of compression ratio on nitric oxide emissions:
Experimental results from a natural gas, SI engine (Takagi and Raine, 1997)

Figure (6.19). Effect of engine speed on NO\textsubscript{x} emission at EVO, ignition at 20° BTDC
Figure (6.20). Effect of engine speed on NO\textsubscript{x} emission at EVO, ignition at 26° BTDC

Figure (6.21). Effect of engine speed on NO\textsubscript{x} emission at EVO, ignition at 32° BTDC
Figure (6.22). Effect of engine speed on CO\textsubscript{2} emission at EVO, ignition at 20° BTDC

Figure (6.23). Effect of engine speed on CO\textsubscript{2} emission at EVO, ignition at 26° BTDC
Figure (6.24). Effect of engine speed on CO$_2$ emission at EVO, ignition at 32° BTDC

Figure (6.25). Effect of engine speed on CO emission at EVO, ignition at 20° BTDC
Figure (6.26). Effect of engine speed on CO emission at EVO, ignition at 26° BTDC

Figure (6.27). Effect of engine speed on CO emission at EVO, ignition at 32° BTDC
Figure (6.28). Effect of ignition timing on NO\textsubscript{x} emission at EVO, 1200 rpm

Figure (6.29). Effect of ignition timing on NO\textsubscript{x} emission at EVO, 1500 rpm
Figure (6.30). Effect of ignition timing on NO\textsubscript{x} emission at EVO, 1800 rpm

Figure (6.31). Effect of ignition timing on NO\textsubscript{x} emission at EVO, 2000 rpm
Figure (6.32). Effect of ignition timing on CO₂ emission at EVO, 1200 rpm

Figure (6.33). Effect of ignition timing on CO₂ emission at EVO, 1500 rpm
Figure (6.34). Effect of ignition timing on CO₂ emission at EVO, 1800 rpm

Figure (6.35). Effect of ignition timing on CO₂ emission at EVO, 2000 rpm
Figure (6.36). Effect of ignition timing on CO emission at EVO, 1200 rpm

Figure (6.37). Effect of ignition timing on CO emission at EVO, 1500 rpm
Figure (6.38). Effect of ignition timing on CO emission at EVO, 1800 rpm

Figure (6.39). Effect of ignition timing on CO emission at EVO, 2000 rpm
6.5. Exhaust gas recirculation

It was discussed in section (6.3.1) that exhaust gas recirculation (EGR) is a well established means for controlling NO\textsubscript{x} emissions from an engine. These kind of alternative approaches to NO\textsubscript{x} control are essential when the traditional three way catalyst can not perform well enough to reduce NO\textsubscript{x} (e.g. when the engine is running very lean giving an oxidising environment in exhaust) or when additional costs involved with catalytic converters (including maintenance and/or replacement after its finite life time) are considered excessive for a particular application. As a part of the present parametric study, three levels of EGR (5\%, 10\%, 15\% of initial cylinder charge) were numerically examined for their effect on NO\textsubscript{x} formation in a natural gas fuelled SI engine. The results were then compared with the NO\textsubscript{x} levels produced when there is no EGR present. The modification to the expression for calculating the laminar burning velocity, $S_L$, when EGR is present was given by eqn. (5.1). This was an expression used for gasoline engine combustion under EGR condition (Metghalchi and Keck 1982) and used here in the absence of a suitable expression for $S_L$ for methane combustion under EGR conditions in an engine. As the main objective of
this study is to understand the trends of the formation of NO\textsubscript{x} when EGR is present, this decision to use an expression not derived for methane was justified.

Figure (6.41) shows the effect of EGR on the formation of NO\textsubscript{x} in the engine resulting from present calculations. It is seen here that the effect of increased EGR levels in the fresh charge has been to decrease engine-out NO\textsubscript{x} levels. As one would expect, the levels of NO\textsubscript{x} resulting at EVO should decrease with increasing levels of EGR in the initial cylinder charge. Morgan and Hetrick (1976) have experimentally observed this trend for a gasoline SI engine and this is given by fig. (6.42) for comparison with the trend of NO\textsubscript{x} variation obtained by the present study. It can be concluded that the calculations made have been able to capture this trend well.

However, as seen before [figs. (5.40) - (5.43)], increasing levels of EGR present in the unburned mixture has an adverse effect on the engine performance by reducing the flame speed and also by absorbing heat from the burning mixture. Therefore the suitable levels of EGR for a particular application has to be carefully chosen with the trade off between engine performance and NO\textsubscript{x} emissions in mind.

![Figure (6.41). Effect of exhaust gas recirculation on NO\textsubscript{x} formation](image-url)
6.6. Improved SRM-new model in calculating pollutant formation

It was reported in section (5.10) that the SRM-new, the improved version of the originally available chemical kinetic model in KIVA-II performed well in calculating natural gas fuelled SI engine operation. As with the two other combustion models used in the study, namely the FFM and the EBUM, it is essential to use the same modelling techniques for the calculation of the formation of pollutants from the engine with this improved SRM-new in order to establish the quality of the model. Figure (6.43) shows the formation of the NO\textsubscript{x}, CO\textsubscript{2} and CO within the cylinder, at the base line operating condition of the engine studied (engine speed 1500 rpm, ignition timing -32° CA BTDC, relative air/fuel ratio, \( \lambda \) =1 and compression ratio 13.1:1). In this figure, the variation of in-cylinder temperature has also been included in order to understand the relationship between engine combustion and the formation of pollutants. It can be seen that these trends are comparable with those resulted from the FFM and the EBUM, which were given by figs. (6.5) and (6.6).

It is convenient to compare the individual pollutant resulting from each model as given in figs. (6.44) – (6.46), so a better picture about the ability of the...
SRM-new in modelling pollutant formation could be created. Although, all three models result in almost the same level of NO\textsubscript{x}, the performance of the SRM-new is much closer to that of the FFM. This is an obvious result of the SRM-new being able to predict a peak average cylinder temperature very close to that predicted by the FFM. A similar closeness in performance between the FFM and the SRM-new can be seen in figs. (6.45) and (6.46), where the formation of CO\textsubscript{2} and CO as calculated with the three models are shown. Any difference seen in these figures is by the EBUM and surprisingly not by the SRM-new. A slightly lower level of NO\textsubscript{x} and CO and a slightly higher level of CO\textsubscript{2} have been predicted when the EBUM is used. As discussed in section (5.10), it is very interesting and encouraging to see that KIVA-II's SRM, which could not perform in an acceptable manner at all, has performed extremely well once the suggested improvement is made, comparable with the FFM in calculating both engine performance and pollutant formation. A proper validation and a parametric study on the formation of pollutants with this SRM-new improved model is essential in order to recognise the characteristics of this model and use it as a standard model for meaningful engine calculations.

Figure (6.43). Pollutant formation at the baseline case with the SRM-new
Figure (6.44). Formation of NO\textsubscript{x} compared with three combustion models

Figure (6.45). CO\textsubscript{2} formation compared with three combustion models
Figure (6.46). Formation of CO compared with three combustion models.
Chapter 7.

Summary, conclusions and suggestions for further study

7.1. Summary

The changeover from liquid petroleum fuels to natural gas can be expected to greatly reduce the emissions of carbon monoxide and reactive hydrocarbons. NG has a low propensity to soot, hence it is known to be clean burning. In order to obtain the maximum benefits achievable from natural gas as a transportation fuel for light duty applications, dedicated engines are required in place of converted gas engines. Turbocharged, lean burn, high compression ratio, dedicated engines offer the greatest improvement in the reduction of both exhaust emissions and fuel consumption. Fast burn combustion chambers with optimised shapes for NG, lean burn conditions and higher compression ratios possible with natural gas would offer higher thermal efficiencies and increased power levels compared to converted gas engines. Under mass production, the manufacture of these dedicated engines would not be costly.

The study of the effects of operational parameters on natural gas engine performance and engine emissions is of great importance in order to develop a reliable background for the mass production of dedicated engines optimised to run solely on natural gas. This research work was aimed at studying these effects using computational fluid dynamic techniques. For this, it is essential to use suitable
mathematical models for the processes that take place in an engine. In the present study, interest was mainly in the modelling of turbulent combustion in natural gas fuelled SI engines. Engine flow structure and chemistry interaction over a wide range of length and time scales is extremely important to properly describe the combustion process that take place in highly turbulent reactive flow situations as in the SI engine. Many different combustion models for the CFD modelling of SI engines have been developed over the years and these models range from simple eddy break up models to numerically expensive probabilistic models. What is most noticeable is that all these successful models have continuously been progressed over the years and their weaknesses reduced. This makes choosing a combustion model a difficult task but one has to make the choice of a model depending on the level of accuracy, available computer resources and the required level of details. The search for the ultimate model would be a never ending task.

There were two important objectives of this research work. One of them was to choose, improve, implement and validate a suitable multi-dimensional model for SI engine combustion. The other was to numerically study the effects of various engine operating parameters on the performance of a natural gas fuelled, spark ignited engine and the pollutant formation, leading towards a better understanding of the engine fluid dynamics and combustion characteristics.

In this study, it has been discussed that the flamelet models are more suitable than the other commonly used models for multi-dimensional modelling of the SI engine. Considering the fact that there is only a single model constant and that the previous applications by other researchers have been very attractive, the fractal flame model was chosen for the present study. This FFM has been improved and successfully incorporated in the CFD code, KIVA-II and validated against available experimental data. An extensive parametric study was then performed using this validated combustion model to understand how the engine operating variables (relative air:fuel ratio, compression ratio, ignition timing, engine speed) affect the engine performance. By comparing the results from this study with suitable experimental data, the global nature and the ability of this model and the CFD code, KIVA-II, as a whole to simulate the performance of a natural gas fuelled SI engine was recognised. By comparing with two other combustion models (the EBUM and the Arrhenius type chemical kinetic model that was originally available in KIVA-II),
particular strengths of this improved FFM as an engine combustion model were established (i.e. flame front contour shape, realistic burned mass fraction results, convenience in handling and the global nature of the model). Additionally, effects of exhaust gas recirculation and the engine geometry on the engine performance were studied. Necessary modifications to the KIVA-II code were done and an engine blow-by model was implemented in the code. It was found that the effect of the blow-by level considered on engine performance was not significant for this particular application. The formation of NO was modelled using the extended Zeldovich mechanism in order to understand the influence of temperature and species concentrations on the rates of formation of nitric oxide. It was recognised that neglecting the heat of formation of NO in the present engine combustion calculations is not advisable, even if it is proved to be small compared to the heat of reaction of the fuel oxidation. The equilibrium of CO₂ was used to calculate the formation of CO in the engine. An extensive parametric study was then performed in order to understand how the engine operating variables affect the pollutant formation in the engine. The parametric studies conducted with the KIVA-II CFD code incorporating various improved sub-models successfully reproduced the trends of performance and pollutants formation, which has been observed experimentally with respective engine operating parameters varied. These results indicate the effectiveness of CFD and the mathematical models of engine processes in understanding, designing and optimising dedicated natural gas engines. As an additional exercise, the originally available Arrhenius type chemistry model, which was unstable when used in the present calculations, was improved.

7.2. Conclusions

The best way to ensure that the objectives of the study are met is to look at its outcome. The conclusions reached from the present study are as follows.

(1) Flamelet models are a better choice for modelling of SI engines, which are known to operate in the flamelet regime. The predictive capability of the improved Fractal Flame Model in modelling the engine performance was sufficiently high
and practical enough for numerically studying a natural gas fuelled SI engine. Global behaviour of this improved fractal flame model when engine operating variables are changed has been encouragingly good and indicate its suitability for use in engine design work through parametric studies. Having only a single model constant and having no extra equations to solve, the FFM provides a convenient to use flamelet combustion model compared to the coherent flamelet model (CFM) and the other common, non-flamelet CFD models used for engine modelling.

(2) The fractal flame model used here is stronger than the eddy break up model in many ways. The flame contours resulting from the fractal flame model are far more realistic, the burned mass fraction results follow the experiments much closer than the eddy break up model does and the model constant, once validated, can be used unchanged over a range of operating conditions whereas the eddy break up model constants needs ‘re-tuning’ when the volumetric efficiency and/or the numerical grid used are changed. The originally available Arrhenius type chemistry model in the KIVA-II code was not capable of acceptably simulating the combustion in the natural gas fuelled SI engine studied here.

(3) One important assumption made when developing and using the fractal flame model is that a fractal nature is shown by the flame front. This assumption has been strengthened and established correct by successfully using the so developed fractal flame model in this study.

(4) The improved and validated fractal flame model is sufficiently capable of modelling the trends of formation of pollutants from the natural gas fuelled SI engine. This indicates the suitability of this model as a tool for designing new engines and assessing both performance and pollutant formation trends with various designs and operating conditions.

(5) Although the endothermic heat of reaction of the formation of nitric oxides is small compared to the exothermic heat of reaction of the fuel oxidising main
reaction, it is not advisable to neglect this in calculations of light duty, natural gas SI engines. NO\textsubscript{x} chemistry does have a considerable influence on the fuel oxidation process and hence the performance of the engine. A higher cylinder temperature resulted when the heat of reaction of NO formation was neglected than when it was included in calculations. This in turn resulted in a higher cylinder pressure and a higher rate of formation of NO.

(6) The renormalisation group theory $k$-$\varepsilon$ turbulence model used in place of the standard $k$-$\varepsilon$ turbulence model did not make any significant improvement on the results of modelling the natural gas SI engine.

(7) The effect of exhaust gas recirculation has been correctly calculated by the modified and validated fractal flame model. The trends of engine performance and pollutant formation when EGR is present have been correctly produced. This study shows that reduction of NO\textsubscript{x} is possible from natural gas SI engines with suitable levels of EGR without significantly weakening the engine performance.

(8) This study has shown the suitability of CFD modelling as a tool for testing different engine combustion chamber geometries. Although the results from the study of the effects of engine geometry on performance have not been compared with experiments, it paves a way for optimising an engine combustion chamber geometry for a particular fuel and for other requirements.

(9) KIVA-II's Arrhenius type chemical kinetic model has been improved so it is stable and usable for SI engine calculations when natural gas is used as the fuel. Although the effects of turbulence on fuel oxidation chemistry are not included in the model, it behaves surprisingly well. This improved version of the model (SRM-new) has shown a performance strength comparable with the improved and validated fractal flame model used in the present study for the base line case studied.
7.3. Suggestions for further work

The present study has indicated several areas where further work is needed or would be useful. It has paved the path for extension of much of the present work and related issues. Some of this extended work may have added to the value of the present work if the time frame had allowed their completion. As an example, the inclusion of a suitable detailed spark ignition model in the present calculations would have, no doubt, improved the quality of the work. However, framed by a suitably chosen listing of objectives, time and computational resources, a PhD research study could not undertake all such work. Therefore, only the essential aspects of the work in order to achieve the set objectives was done here leaving the space open for the addition of further work to this.

Some of the areas in which further investigation is needed are:

(1) The complete modelling of a full combusting engine cycle, starting from inlet valve opening until exhaust valve closes. This approach would give complete results as the effects of mixture preparation, turbulence and other flow properties at inlet condition, on the engine flow and combustion can properly be resolved. However, this may require simpler CFD analysis or experimentation in order to establish inlet boundary conditions, such as the level of turbulence, flow velocities, mass flow rates and air-fuel mixture quality.

(2) The criteria used to signal the onset of combustion to the CFD code and the criteria used to numerically switch the combustion calculations from laminar phase to turbulent phase need further attention. Combustion initiation in any numerical cell was signalled to the code by a temperature threshold. The effect of the choice of this threshold value needs investigation. In the present study, the switching of the combustion from laminar to turbulent phase was signalled after the flame radius had reached the integral length scale of turbulence. This transition is important and there have been several transition criteria given in the literature, as used by various researchers. Time elapsed after the spark ignition,
flame radius reaching a pre-determined value (usually the integral length scale), temperature of computational cells reaching a pre-determined threshold value or a specific amount of the intake mixture being burned are some of such criteria used by the CFD engine combustion modellers in order to signal the computer code to switch the combustion calculations from the laminar phase to the turbulent phase. A proper investigation of this would ensure that the right choice of switching criteria has been made.

(3) Suitable experimental data on the operation and the formation of pollutants on the engine tested in the present study should be collected. This would fill the gap, where there were not sufficient and/or suitable experimental data to compare the numerical results at each operating condition considered under the parametric studies made. Also, more experiments are needed at various operating conditions with the three piston geometries numerically tested to allow the results of the study to be validated and establish the global nature of the applicability of the improved and validated FFM.

(4) The effect of cylinder pressure on combustion should be included in the calculations. Increased pressure slows down combustion and can have a significant impact when the peak cylinder pressure is high. This especially becomes important when high compression ratio engines are to be studied with the validated combustion model.

(5) The improved and validated FFM must be tested for cases of very lean combustion as the present industrial trend is towards lean burn engines for reduced emissions. At very lean conditions, the flame thickness is no longer small enough to satisfy the thin flame assumption made in the flamelet combustion model development. Also, numerical tests are needed at very high levels of EGR at which bulk flame quenching is significant.

(6) The Arrhenius type chemical kinetic model originally available in KIVA-II, once improved, has proven to perform well comparable with the fractal flame model and better than the eddy break up model. This is an interesting and surprising
outcome when considering the fact that the effect of turbulence on combustion is not incorporated in this kinetic model. It arouses the users’ curiosity to know what causes this improved SRM-new model perform well as if the effect of turbulence is included. This may be an indication that the turbulence in the present engine considered has not reached high levels, at which its effect on combustion is significant and chemical kinetics modelling alone is enough to reasonably describe combustion in low or medium turbulence engines. This idea deserves a proper investigation and the performance of this SRM-new chemistry model must be tested with high turbulence engines, may be with a higher level of initial turbulence or with the suitable inclusion of turbulence enhancing features (e.g. offset piston bowl and sparks, valve shrouding) in the engine geometry. Also a parametric study with the SRM-new is needed to establish if it can perform well at various operating conditions once the model constants are fixed for a baseline case. With the kinetic model (both the original and the improved versions) in KIVA-II, only the forward reaction of fuel oxidising was used.

Some of the areas, in which extended studies may be made by the interested reader to enhance the quality of the present work are:

1. The inclusion of a detailed ignition model would be worthwhile. A proper study of different ignition techniques used in the present day natural gas engines (plasma jets, ignition gasket, multiple spark plugs and high frequency sparking etc.) can be performed with such a model. For natural gas engines, ignition is of great importance due to the high activation energy requirement of this fuel, especially for a dedicated natural gas engine to operate at optimum conditions.

2. No sufficient studies have been performed regarding the operation and the formation of pollutants at cold start of a natural gas engine. Unlike gasoline engine, no fuel enrichment is needed for natural gas engines at cold start but this is an interesting aspect to study so the suitability of natural gas as an engine fuel can further be convinced.
(3) The operation of natural gas engines at high altitudes, at high temperature environments and high humid areas are special circumstances as the inlet charge composition can vary a lot. Gaseous fuels require special arrangements to handle the variable energy content per unit volume and the variable ignition and combustion properties due to compositional changes. It is therefore useful to study the effect of mixture composition variations on engine performance and on pollutant formation. Also, it may be interesting to numerically study the fuel composition variations as natural gas composition has been found to vary considerably when taken from various origins.

(4) Injected natural gas engines are becoming popular as control of air:fuel ratio is comparatively easier with them. They may be direct injected or port/manifold injected engines with microprocessor control. It is appealing to study these engines and see if the improved fractal flame model used and validated for natural gas SI engines in the present study can be successfully used for the diffusion combustion conditions. Turbulence in direct injection natural gas engines may be modelled with the renormalisation group theory $k$-$\varepsilon$ turbulence model as the fuel jet and the bulk flow interaction is significant in those engines.

(5) In his comparison, Zhao (1994) concluded that the fractal flame model has performed better than the coherent flame sheet model. These models have been continuously improved and advanced versions of the CFM stronger than the version tested by Zhao have evolved. It is beneficial to test the improved version of the FFM used in this study with the latest versions of the CFM and other variations of the FFM such as the Peninsula fractal model by Matthews et al (1996).

(6) One of the major difficulties faced during the present numerical study is finding suitable and reliable experimental data of operation and pollutant formation of natural gas engines at various operating conditions. The CFD researcher always has to validate their results against well conducted experiments. Either, the researcher has to sacrifice some of the time available for numerical studies for conducting necessary experimentation or has to completely rely on experimental
data available from other sources. Reliability of these externally found data may not always be guaranteed or they may not be available for the required operating conditions and/or the geometry. It is therefore necessary to build a good database of reliable experimental data for natural gas engines with the operating parameters and geometrical features varied as much as the CFD research community may require.
Appendix 1.

The kinetic chemical reaction model of fuel oxidation in KIVA-II

In the CFD code, KIVA-II, procedure for evaluating the progress rate, \( \dot{\omega} \) for kinetic chemical reaction of fuel oxidation at a representative cell is as follows. It is assumed that every participating species is either inert or appears on only one side of the reaction.

The quantities \( \Omega_f \) and \( \Omega_b \) will be calculated as follows.

\[
\Omega_f = k_f \prod_m \left( \frac{\bar{\rho}_m}{W_m} \right)^{a'_m} \tag{A1.1}
\]

\[
\Omega_b = k_b \prod_m \left( \frac{\bar{\rho}_m}{W_m} \right)^{b'_m} \tag{A1.2}
\]

where \( k_f \) and \( k_b \) are forward and backward rate coefficients respectively. These are assumed to be of general Arrhenius form and calculated using eqn.s (2.13) and (2.14). Here the reaction orders \( a'_m \) and \( b'_m \) need not equal \( a_m \) and \( b_m \) (the integral stoichiometric coefficients of the reaction and used in eqn. (2.10) earlier) so that empirical reaction orders can be used. Then, for this reaction, KIVA-II identifies the
species, whose density is in greatest danger of being driven negative by checking the quantity,

\[ W_m \frac{(b_m - a_m)(\Omega_f - \Omega_b)}{\rho_m} \]  \hspace{1cm} (A1.3)

is a minimum. This identified species is called the reference species, \( K \) for the reaction in question. Once the species \( K \) is identified, the following terms will be calculated.

\[ \Lambda_{Top} = \tilde{\rho}_k + \Delta t \cdot W_k \left[ b_k \Omega_f + a_k \Omega_b \right] \]  \hspace{1cm} (A1.4)

\[ \Lambda_{Bot} = \tilde{\rho}_k + \Delta t \cdot W_k \left[ a_k \Omega_f + b_k \Omega_b \right] \]  \hspace{1cm} (A1.5)

The quantities in square brackets in eqn.s (A1.4) and (A1.5) give the formation and destruction of the species \( K \) during the reaction, respectively and therefore \( \Lambda_{Bot} > \Lambda_{Top} \). According to usual practice, reaction rate \( \dot{\omega} \) is given by

\[ \dot{\omega} = \Omega_f - \Omega_b \]  \hspace{1cm} (A1.6)

However, in KIVA-II, this will be calculated using an additional factor in order to always keep \( \tilde{\rho}_k > 0 \) and is given by

\[ \dot{\omega} = \frac{\tilde{\rho}_k}{\Lambda_{Bot}} \left( \Omega_f - \Omega_b \right) \]  \hspace{1cm} (A1.7)

When re-arranged, this becomes

\[ \dot{\omega} = \frac{\tilde{\rho}_k \left( \frac{\Lambda_{Top}}{\Lambda_{Bot}} - 1 \right)}{\Delta t \cdot W_k (b_k - a_k)} \]  \hspace{1cm} (A1.8)
Appendix 2.

Some indices and scales commonly used in SI engine related calculations

The statistical measure of the largest sized eddies is the integral length scale, $L$. The smallest sized eddies are identified by the Kolmogorov length scale, $\eta$ which is given by

$$\eta = \left( \frac{\nu^3 L}{u'^3} \right)^{1/4}$$

where

$\nu$ the kinematic viscosity

$u'$ the turbulent intensity

When the flame thickness is less than $\eta$, then the system is described as a locally laminar premixed flame, embedded in a turbulent flow (i.e. the flamelets).

The turbulent Reynolds number is given by

$$Re_T = \frac{u'/L}{\nu}$$

Laminar flame speed, $S_L$ is given by
where $\delta$ is the laminar flame thickness.

Eddy turn over time (the macroscopic time scale) for turbulent eddies, $t_0$ is given by

$$t_0 = \frac{L}{u'},$$

the chemical reaction time, $t_L$ is given by

$$t_L = \frac{\delta}{S_L},$$

and the Kolmogorov time scale, $t_K$ is given by

$$t_K = \frac{v}{\sqrt{\epsilon}}$$

where $\epsilon$ is the dissipation rate of turbulent energy.

The Damköhler number, $Da$ is given as the ratio between the eddy turn over time, $t_0$ and the chemical reaction rate, $t_L$

$$Da = \frac{L/u'}{\delta/S_L}$$

The Karlovitz number, $Ka$ is given as the ratio between the chemical reaction rate, $t_L$ and the Kolmogorov time scale, $t_K$

$$Ka = \frac{\delta/S_L}{(v/\epsilon)^{1/2}}$$
For very high values of the Damköhler number (e.g. $10^3 - 10^4$), chemistry is very fast compared with the turbulence and reaction sheets are observed. According to the relationship among $Re_T$, $Da$, $L$, and $\delta$, which is given by

$$\sqrt{Re_T \cdot Da} \propto \frac{L}{\delta},$$

the reaction sheet concept is associated with large values of $\frac{L}{\delta}$.

The Lewis number, $Le$ is given by

$$Le = \frac{\lambda}{D \rho c_p}$$

where

$D$ mass diffusivity
$\rho$ density
$c_p$ specific heat capacity at constant pressure
$\lambda$ thermal conductivity

The Prandtl number, $Pr$ is given by

$$Pr = \frac{\nu \rho c_p}{\lambda}$$

The Schmidt number, $Sc$ is given by

$$Sc = \frac{\nu}{D_0}$$

where $D_0$ is the binary diffusion coefficient for the vapour into the ambient gas.
The Wobbe number, $WN$, which is a measure of the interchangeability of gaseous fuels is given by

$$WN = \frac{HHV}{\sqrt{\rho_f}}$$

where $HHV$ is the higher heating value of the fuel.

The octane number, $ON$ ranks fuels according to their anti-knock properties. Isooctane is arbitrarily set at 100 and $n$-heptane, which is more prone to knock, is arbitrarily set at zero. The octane number is the percentage of isooctane in the isooctane and $n$-heptane mixture, which most nearly matches the knock performance of the test fuel. The research octane number, $RON$ is obtained by testing the fuel at 125°F inlet air with 13° spark advance at 600 rpm. The motor octane number, $MON$ is obtained by testing the fuel at 300°F inlet air with 19° - 26° spark advance at 900 rpm. The $RON$ is greater than the $MON$ and the difference between these two is termed sensitivity of the fuel. By definition, sensitivity is zero for the reference fuels.

As methane has a $RON$ of around 130, which is beyond the octane scale, another index named methane number, $MN$ is defined. In this scale, methane is arbitrarily assigned a $MN$ of 100 with hydrogen, which is very sensitive to knock, having a $MN$ of zero. The methane number of the test fuel is the percentage of methane in the most nearly matching mixture of methane and $n$-heptane.

The cetane number, $CN$ ranks the fuels according to their ignition delay when undergoing a standard test. Cetane ($n$-hexadecane) is one of the fastest igniting hydrocarbon fuels and is assigned a $CN$ of 100. Isocetane (heptamethylnonane) ignites slowly and is arbitrarily assigned a $CN$ of 15. The $CN$ of the test mixture at specified test conditions is defined by

$$CN = \% \text{Cetane} + 0.15(\% \text{Isocetane})$$
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