Predictions of explosions and fires of natural gas/hydrogen mixtures for hazard assessment

This item was submitted to Loughborough University's Institutional Repository by the/an author.

Additional Information:

- A Doctoral Thesis. Submitted in partial fulfilment of the requirements for the award of Doctor of Philosophy of Loughborough University.

Metadata Record: [https://dspace.lboro.ac.uk/2134/6354](https://dspace.lboro.ac.uk/2134/6354)

Publisher: © Christopher Mumby

Please cite the published version.
This item was submitted to Loughborough’s Institutional Repository (https://dspace.lboro.ac.uk/) by the author and is made available under the following Creative Commons Licence conditions.

For the full text of this licence, please go to:
http://creativecommons.org/licenses/by-nc-nd/2.5/
Predictions of Explosions and Fires of Natural Gas/Hydrogen Mixtures for Hazard Assessment

By

Christopher Mumby

A doctoral thesis submitted in partial fulfilment of the requirements for the award of degree of doctor of philosophy of Loughborough University

April, 2010

Department of Chemical Engineering
Abstract

The work presented in this thesis was undertaken as part of the safety work package of the NATURALHY project which was an integrated project funded by the European Commission (EC) within the sixth framework programme. The purpose of the NATURALHY project was to investigate the feasibility of using existing natural gas infrastructure to assist a transition to a hydrogen based economy by transporting hydrogen from its place of production to its place of use as a mixture of natural gas and hydrogen. The hydrogen can then be extracted from the mixture for use in fuel cells or the mixture used directly in conventional combustion devices. The research presented in this thesis focused on predicting the consequences of explosions and fires involving natural gas and hydrogen mixtures, using engineering type mathematical models typical of those used by the gas industry for risk assessment purposes.

The first part of the thesis concentrated on modifying existing models that had been developed to predict confined vented and unconfined vapour cloud explosions involving natural gas. Three geometries were studied: a confined vented enclosure, an unconfined cubical region of congestion and an unconfined high aspect ratio region of congestion. The modifications made to the models were aimed at accounting for the different characteristics of a natural gas/hydrogen mixture compared to natural gas.

Experimental data for the laminar burning velocity of methane/hydrogen mixtures was obtained within the safety work package. For practical reasons, this experimental work was carried at an elevated temperature. Predictions from kinetic modelling were employed to convert this information for use in models predicting explosions at ambient temperature.

For confined vented explosions a model developed by Shell (SCOPE) was used and modified by adding new laminar burning velocity and Markstein
number data relevant to the gas compositions studied. For vapour cloud explosions in a cubical region of congestion, two models were used. The first model was developed by Shell (CAM2), and was applied using the new laminar burning velocity and other composition specific properties. The second model was based on a model provided by GL Services and was modified by generalising the flame speed model so that any natural gas/hydrogen mixture could be simulated.

For vapour cloud explosions in an unconfined high aspect ratio region of congestion, a model from GL Services was used. Modifications were made to the modelling of flame speed so that it could be applied to different fuel compositions, equivalence ratios and the initial flame speed entering the congested region.

Predictions from the modified explosion models were compared with large scale experimental data obtained within the safety work package. Generally, (apart from where continuously accelerating flames were produced), satisfactory agreement was achieved. This demonstrated that the modified models could be used, in many cases, for risk assessment purposes for explosions involving natural gas/hydrogen mixtures.

The second part of thesis concentrated on predicting the incident thermal radiation from high pressure jet fires and pipelines fires involving natural gas/hydrogen mixtures. The approach taken was to modify existing models, developed for natural gas.

For jet fires three models were used. Fuel specific input parameters were derived and the predictions of flame length and incident radiation compared with large scale experimental data. For pipeline fires a model was developed using a multi-point source approach for the radiation emitted by the fire and a correlation for flame length. Again predictions were compared with large scale experimental data. For both types of fire, satisfactory predictions of the flame length and incident radiation were obtained for natural gas and mixtures of natural gas and hydrogen containing approximately 25% hydrogen.
Acknowledgements

I wish to thank the following for their help along the way;

Prof. Geoff Hankinson (Supervisor),
Dr. Barbara Lowesmith (Project Leader),
Dr. Phil Cleaver (GL Industrial Services UK Ltd.),
Mr. Mike Johnson (GL Industrial Services UK Ltd.),
Dr. Jonathan Puttock (Shell Global Solutions),
Mr. Les. Shirvill (Shell Global Solutions),
Prof. Mike Fairweather (Leeds University).

I wish to thank the following for their support;

Sinead Robertson, my fiancé,
My Mum and Dad and Sister,
My Grandma, and Granddad that couldn’t be here to see me finish,
Catalina Spartaru, fellow PhD. student, working on the NATURALHY safety work package, for technical and moral support.
# Table of Contents

1 Introduction ......................................................................................... 1

1.1 The contribution of Hydrogen to the energy economy .......................... 2
1.2 NATURALHY ................................................................................. 8
1.3 Hazards and Risk ............................................................................ 12
1.4 Explosions and Fires Involving Natural Gas/Hydrogen Mixtures .......... 15
   1.4.1 Experimental Work ................................................................. 15
   1.4.2 Objectives and Structure of the Thesis ..................................... 15

2 Predicting Large Scale Explosions ................................................. 20

2.1 Introduction ..................................................................................... 20
2.2 Description of a Gas Explosion ....................................................... 20
2.3 Explosion Hazards .......................................................................... 23
2.4 Modelling Explosion Events ........................................................... 24
2.5 Review of Existing Engineering Explosion Models ......................... 27
   2.5.1 Empirical Models ................................................................. 28
      2.5.1.1 TNT equivalency ............................................................. 28
      2.5.1.2 TNO multi-energy ......................................................... 29
      2.5.1.3 Baker-Strehlow ............................................................. 30
      2.5.1.4 Shell CAM2 ................................................................. 31
   2.5.2 Phenomenological Models ....................................................... 33
      2.5.2.1 Shell SCOPE ................................................................. 33
      2.5.2.2 CLICHE ................................................................. 34
      2.5.2.3 GL’s compact explosion model ........................................ 35
      2.5.2.4 GL HAREM ................................................................. 37
   2.5.3 Other models ........................................................................ 38
   2.5.4 Note on CFD models ............................................................... 38
2.6 Assessment of Explosion Predictions by Comparison with Experimental Data ................................................................. 40
   2.6.1 Variability of explosions and the analysis of pressure data from explosion experiments ................................................................. 40
   2.6.2 Predictive capability of explosion models .................................. 41
2.7 Factors to consider when modelling explosions .................................. 42
   2.7.1 Initial Conditions ................................................................... 43
   2.7.2 Laminar and Turbulent Burning .............................................. 44
      2.7.2.1 Laminar Burning ......................................................... 44
      2.7.2.2 Turbulent Burning ......................................................... 46
   2.7.3 Stretch and Instability ............................................................. 50
3 Determining Burning Velocity ................................................. 63

3.1 Introduction ........................................................................ 63
3.2 Burning Velocity Determination and Important Parameters ... 64
3.3 Methodology for Correction of Initial Temperature .......... 66
  3.3.1 Temperature Correction of Laminar Burning Velocity ...... 67
  3.3.2 Temperature Correction of Markstein Number ............... 68
3.4 Results of Temperature Correction ................................... 69
  3.4.1 Burning Velocity .............................................................. 69
  3.4.2 Markstein Numbers ........................................................... 76
3.5 Discussion ........................................................................ 78
  3.5.1 Sources of Correlations for Laminar Burning Velocity .... 78
    3.5.1.1 Andrews and Bradley [1972] for methane .................... 79
    3.5.1.2 Sharma et al. [1981] for methane ................................. 79
    3.5.1.3 Lijima and Tadao [1986] for methane/hydrogen mixtures ... 80
    3.5.1.4 Stone et al. [1998] for methane ................................. 80
    3.5.1.5 Gu et al. [2000] for methane ........................................ 80
    3.5.1.6 Elia et al. [2001] for methane ...................................... 81
    3.5.1.7 Yu et al. [1986] for methane (also propane) and hydrogen .. 81
    3.5.1.8 Laio et al. [2004] for natural gas ................................. 82
    3.5.1.9 Huang et al. [2006] for natural gas, hydrogen and mixtures . 83
    3.5.1.10 Coppens et al. [2007] for methane/hydrogen mixtures .... 83
  3.5.2 Comparison of laminar burning velocity correlations at standard temperature and pressure ........................................... 84
    3.5.2.1 Methane and natural gas ............................................. 85
    3.5.2.2 Methane/hydrogen mixtures ....................................... 86
  3.5.3 Comparison of temperature correction correlations .......... 88
    3.5.3.1 Burning velocity of methane at 360K ............................ 89
3.6 Conclusions ..................................................................... 91

4 Confined Vented Explosions .................................................... 93

4.1 Introduction ..................................................................... 93
4.2 Experiments .................................................................... 93
4.3 Modelling Methodology .................................................... 97
  4.3.1 Model Inputs ................................................................. 99
4.4 Results – Comparison of predictions with data ................. 105
  4.4.1 Predictions of flame exit speed and maximum internal overpressure ................................................................. 106
  4.4.2 Flame Speed and Blast Decay ....................................... 108
    4.4.2.1 INDEXP 13 ............................................................... 110
    4.4.2.2 INDEXP 6 ............................................................... 111
5 Compact Cubic Explosion................................................. 118

5.1 Introduction 118
5.2 Experiments 118
5.3 Modelling Methodology 121
  5.3.1 CAM2 .............................................................................. 121
     5.3.1.1 Source Pressure Model .............................................. 122
     5.3.1.2 Blast Decay Model ...................................................... 125
     5.3.1.3 Model Implementation and Usage .............................. 128
  5.3.2 Compact Congested Explosion Model (CCEM) 128
     5.3.2.1 Flame Speed Model .................................................... 129
     5.3.2.2 Flame Speed Model Modifications for CCEM ............... 130
     5.3.2.3 Source Overpressure Model ....................................... 134
     5.3.2.4 Drag ........................................................................ 137
     5.3.2.5 Blast Model ............................................................... 138
     5.3.2.6 CCEM Model Implementation and Usage .................... 141
5.4 Results – Comparison of predictions with data 143
  5.4.1 Comparison of predicted explosion overpressure against
     experimental data ................................................................ 143
  5.4.2 CAM2 – Detailed Results .............................................. 145
  5.4.3 CCEM – Detailed Results .............................................. 151
5.5 Conclusions 156

6 Pipe Rack with Initial Confinement................................. 160

6.1 Introduction 160
6.2 Experiments 160
6.3 Modelling Methodology 169
  6.3.1 Flame Speed within HAREM ........................................... 169
  6.3.2 Modification to the Flame Speed Model ......................... 170
     6.3.2.1 Comments on Ignition Conditions ............................... 171
     6.3.2.2 Maximum Flame Speed .............................................. 172
     6.3.2.3 Maximum Flame Speed with Incoming Explosion Ignition 174
     6.3.2.4 Flame Acceleration .................................................... 175
  6.3.3 Source Overpressure Model within HAREM .................. 176
  6.3.4 Blast Decay Model within HAREM ............................... 178
  6.3.5 Model Implementation and Usage ................................. 178
6.4 Results – Comparison with experimental data 180
  6.4.1 Predictions for explosions where the flame reaches a stable
     speed (non-accelerating flames) ............................................ 183
     6.4.1.1 Discussion of flame speed predictions .......................... 189
     6.4.1.2 Discussion of overpressure predictions ....................... 191
6.4.2 Predictions for explosions where the flame continues to increases its speed (accelerating flames) ............................................. 192
6.4.2.1 Discussion of flame speed predictions ......................................... 200
6.4.2.2 Discussion of overpressure predictions ........................................ 201
6.5 Conclusions 202

7 References ............................................................................................................ 204

8 Predicting Large Scale Gas Fires .............................................................. 216
8.1 Introduction 216
8.2 Fire 216
8.3 Fire Types 217
8.4 The Effect of Fire 220
8.5 Emission of Thermal Radiation 221
8.5.1 Modelling Radiant Transfer ............................................................. 222
8.5.2 Surface Emitter Models ................................................................. 224
8.5.3 Point Source Approach ..................................................................... 225
8.6 Approaches to Modelling Fires 227
8.6.1 Empirical Models .............................................................................. 228
8.6.2 Phenomenological Models .............................................................. 229
8.6.3 Note on CFD models ...................................................................... 230
8.7 Assessment of Fire Predictions by Comparison with Experimental Data 232
8.8 Conclusions 233

9 Predicting Large Scale Jet Fires ............................................................... 235
9.1 Introduction 235
9.2 Experiments 235
9.3 Modelling Methodology 238
9.3.1 Multi Point Source Model .............................................................. 238
9.3.1.1 Description of the Flame and Radiative Characteristics ............. 238
9.3.1.2 Fraction of heat radiated for methane/hydrogen mixtures ............ 242
9.3.1.3 Computer Implementation of the Model and Application to the NATURALHY Jet Fires ................................................................. 246
9.3.2 Johnson et al. [1994] ..................................................................... 247
9.3.2.1 Flame Geometry ......................................................................... 248
9.3.2.2 Gas Jet Properties ....................................................................... 251
9.3.2.3 Radiative Characteristics ............................................................. 252
9.3.2.4 Computer Implementation of the Model and Application to the NATURALHY Jet Fires ................................................................. 254
9.3.3 GL Model JBurn [2006] ................................................................. 255
9.3.3.1 Flame Geometry ......................................................................... 255
9.3.3.2 Radiative Characteristics ............................................................. 256
9.3.3.3 Application to the NATURALHY tests ........................................ 256
9.4 Results – Comparison of predictions with experimental data 257
  9.4.1 Multi Point Source Model ........................................................ 257
    9.4.1.1 Flame geometry ................................................................. 257
    9.4.1.2 Incident Radiation ............................................................... 259
  9.4.2 Johnson et al. [1994] .............................................................. 267
    9.4.2.1 Flame Geometry ................................................................. 267
    9.4.2.2 Incident Radiation ............................................................... 268
  9.4.3 GL JBurn [2006] ..................................................................... 276
    9.4.3.1 Flame Geometry ................................................................. 276
    9.4.3.2 Incident Radiation ............................................................... 277

9.5 Discussion and Conclusions 285
  9.5.1 Flame Geometry ................................................................. 285
  9.5.2 Incident radiation ................................................................... 289

10 Predicting Fires Following High Pressure Gas Pipeline 290

10.1 Introduction 290
10.2 Experiments 290
10.3 Modelling Methodology 294
10.4 Results – Comparison of Predictions with Experimental Data 295
  10.4.1 Flame Geometry ................................................................. 296
  10.4.2 Fraction of Heat Radiated ....................................................... 299
  10.4.3 Predicting Incident Radiation (Test 1) ..................................... 301
    10.4.3.1 Incident radiation at specific locations ................................ 301
    10.4.3.2 Incident radiation at all locations at 20s intervals ............... 304
  10.4.4 Predicting Incident Radiation (Test 2) ..................................... 307
    10.4.4.1 Incident radiation at specific locations ................................ 308
    10.4.4.2 Incident radiation at all locations at 20s intervals ............... 310
10.5 Conclusions 314

11 References ........................................................................ 315

12 Overall Conclusions ........................................................... 320

12.1 Predicting Explosion Hazards involving Natural gas/Hydrogen Mixtures 320
  12.1.1 Recommendations for future work on explosion models ........ 322
12.2 Predicting Fire Hazards for Natural Gas/Hydrogen Mixtures 323
  12.2.1 Recommendations for future work on fire models ............... 324

APPENDIX A Explosions ....................................................... 325

  A.1 Burning Velocity Data 325

APPENDIX B Fires .................................................................. 333
B.1 Extended Jet Fire Predictions - Johnson et al. 94 333
  B.1.1 Test 1 .......................................................... 333
  B.1.2 Test 2 .......................................................... 334
  B.1.3 Test 3 .......................................................... 334
  B.1.4 Test 4 .......................................................... 335
  B.1.5 Test 5 .......................................................... 336
  B.1.6 Test 6 .......................................................... 336

B.2 Extended Jet Fire Predictions - GL JBurn 337
  B.2.1 Test 1 .......................................................... 337
  B.2.2 Test 2 .......................................................... 339
  B.2.3 Test 3 .......................................................... 341
  B.2.4 Test 4 .......................................................... 342
  B.2.5 Test 5 .......................................................... 344
  B.2.6 Test 6 .......................................................... 345

APPENDIX C  Gas Properties ........................................ 347

  C.1 Equation of State 347
  C.2 Thermodynamic 347
  C.3 Transport 348
    C.3.1 Viscosity ...................................................... 348
    C.3.2 Thermal Conductivity ..................................... 349
    C.3.3 Mass Diffusion .............................................. 349
List of Figures

Figure 2-1: Illustration of the combustion process, with central ignition ........22
Figure 3-1: Temperature exponent, $m$, variation with equivalence ratio, $\Phi$, using the GRI kinetic mechanism .............................................................. 70
Figure 3-2: Temperature exponent, $m$, variation with equivalence ratio, $\Phi$, using the Konnov kinetic mechanism ............................................................. 70
Figure 3-3: Graph showing how calculated adiabatic flame temperature, $T$, for methane varies with equivalence ratio, $\Phi$ ...................................................... 72
Figure 3-4: Graph showing the laminar burning velocity, $u_l$, as a function of equivalence ratio, $\Phi$, displaying experimental results at 360K and temperature correction applied using power laws derived from Konnov and GRI mechanisms- for methane ............................................................................. 74
Figure 3-5: Graph showing the laminar burning velocity, $u_l$, as a function of equivalence ratio, $\Phi$, displaying experimental results at 360K and temperature correction applied using power laws derived from Konnov and GRI mechanisms- for 90% methane 10% hydrogen ............................................. 74
Figure 3-6: Graph showing the laminar burning velocity, $u_l$, as a function of equivalence ratio, $\Phi$, displaying experimental results at 360K and temperature correction applied using power laws derived from Konnov and GRI mechanisms- for 80% methane 20% hydrogen ............................................. 75
Figure 3-7: Graph showing the laminar burning velocity, $u_l$, as a function of equivalence ratio, $\Phi$, displaying experimental results at 360K and temperature correction applied using power laws derived from Konnov and GRI mechanisms- for 50% methane 50% hydrogen ............................................. 75
Figure 3-8: Flame thickness variation with equivalence ratio, $\Phi$, in the laminar regime at 360K and 298K .............................................................................. 77
Figure 3-9: Markstein number, $M_a$, variation with equivalence ratio (ER) for (a) methane, (b) 90:10, (c) 80:20 and (d) 50:50 fuel gas compositions ............... 78
Figure 3-10: Comparison of laminar burning velocity at 298K for methane/natural gas ............................................................................................................. 86
Figure 3-11: Comparison of correlations in the literature for laminar burning velocity of methane with %v/v hydrogen addition ............................................. 87
Figure 3-12: Comparison of correlations for laminar burning velocity at 298K with %v/v hydrogen addition from the literature and the work in this chapter. 88
Figure 3-13: Comparison of the literature and current work of the temperature exponent, m, varying with equivalence ratio ............................................. 89
Figure 3-14: Comparison of derived values for laminar burning velocity at 360K (by applying correlations found in the literature) and the Leeds laminar burning velocity data obtained at 360K ............................................. 90
Figure 4-1: External photograph of the confined vented explosions experiment [Lowesmith, 2007] .................................................................................. 94
Figure 4-2: Schematic of test rig showing pipework congestion arrangement [Lowesmith, 2007] .................................................................................. 94
Figure 4-3: Plan view showing pressure transducer locations (squares) [Lowesmith, 2007] .................................................................................. 95
Figure 4-4: Plan and sectional views showing IP locations (stars) [Lowesmith, 2007] .................................................................................. 96
Figure 4-5: Flow chart describing the modelling steps undertaken within SCOPE [Puttock et al. 2000] ............................................................................. 99
Figure 4-6: Correlation for turbulent burning velocity for methane, and 20% and 50% hydrogen addition to methane [Fairweather et al, 2006] ......... 104
Figure 4-7: Comparison of flame speed at the vent of the enclosure from SCOPE predictions and experiments (data from [Lowesmith, 2007]) ........ 107
Figure 4-8: Comparison of maximum internal overpressure from SCOPE predictions and experiments (data from [Lowesmith, 2007]) ............. 108
Figure 4-9: (a) INDEXP13: Flame Speed; (b) INDEXP13: Maximum overpressure outside chamber (data from [Lowesmith, 2007]) .............. 110
Figure 4-10: (a) INDEXP06: Flame Speed; (b) INDEXP06: Maximum overpressure outside chamber (data from [Lowesmith, 2007]) .............. 111
Figure 4-11: (a) INDEXP08: Flame Speed; (b) INDEXP08: Maximum overpressure outside chamber (data from [Lowesmith, 2007]) .............. 112
Figure 4-12: (a) INDEXP11: Flame Speed; (b) INDEXP11: Maximum overpressure outside chamber (data from [Lowesmith, 2007]) .............. 113
Figure 4-13: (a) INDEXP10: Flame Speed; (b) INDEXP10: Maximum overpressure outside chamber (data from [Lowesmith, 2007]) .................... 114
Figure 4-14: (a) INDEXP14: Flame Speed; (b) INDEXP14: Maximum overpressure outside chamber (data from [Lowesmith, 2007]) .................... 115
Figure 5-1: Photograph of the rig used in the compact congested experiments [Roberts et al., 2006] .................................................................................... 119
Figure 5-2: Diagram of a ‘breaking’ pressure wave................................. 140
Figure 5-3: Predicted source overpressure summary: (a) Shell CAM2; (b) CCEM; against experimental data (data from [Roberts et al., 2006]) ............ 144
Figure 5-4: Source overpressure increase with hydrogen addition .......... 145
Figure 5-5: NatHy_02 – 100% methane - CAM2 and experimental (data from [Roberts et al., 2006]) overpressure-distance graph ..................................... 147
Figure 5-6: NatHy_04 - 75:25 CH4:H2 - CAM2 and experimental (data from [Roberts et al., 2006]) overpressure-distance graph ..................................... 148
Figure 5-7: NatHy_03 – 50:50 CH4:H2 - CAM2 and experimental (data from [Roberts et al., 2006]) overpressure-distance graph ..................................... 149
Figure 5-8: NatHy_05 - 25:75 CH4:H2 - CAM2 and experimental (data from [Roberts et al., 2006]) overpressure-distance graph ..................................... 150
Figure 5-9: NatHy_01 - 100% hydrogen - CAM2 and experimental (data from [Roberts et al., 2006]) overpressure-distance graph ..................................... 151
Figure 5-10: CCEM flame speed profile results for all tests ..................... 152
Figure 5-11: NatHy_02 - 100% methane – CCEM and experimental (data from [Roberts et al., 2006]) maximum overpressure with distance .......... 154
Figure 5-12: NatHy_04 - 75:25 CH4:H2– CCEM and experimental (data from [Roberts et al., 2006]) maximum overpressure with distance .......... 154
Figure 5-13: NatHy_03 – 50:50 CH4:H2 – CCEM and experimental (data from [Roberts et al., 2006]) maximum overpressure with distance .......... 155
Figure 5-14: Test NatHy_05 - 25:75 CH4:H2 – CCEM and experimental (data from [Roberts et al., 2006]) maximum overpressure with distance .......... 155
Figure 5-15: Test NatHy_01 - 100% hydrogen – CCEM and experimental (data from [Roberts et al., 2006]) maximum overpressure with distance .... 156
Figure 5-16: Predicted flame speed for 90% and 95% hydrogen added to methane......................................................................................... 158
Figure 5-17: 90% hydrogen 10% methane – maximum overpressure with
distance and data for 100% hydrogen ................................................. 159
Figure 5-18: 95% hydrogen 5% methane – maximum overpressure with
distance and data for 100% hydrogen ...................................................... 159
Figure 6-1: Photograph of external congested region and initial confined
enclosure [Lowesmith, 2008] ....................................................................... 161
Figure 6-2: Photograph of the rig for the high aspect ratio vapour cloud
explosion experiments [Lowesmith, 2008] ................................................... 161
Figure 6-3: Plan and elevation view of ionisation probes [Lowesmith, 2008]
(‘IP’: ionisation probe, ‘R’: pipe rack)............................................................ 162
Figure 6-4: Plan view of pressure transducers [Lowesmith, 2008] (‘T’:
pressure transducer, ‘R’: pipe rack)............................................................. 162
Figure 6-5: Pressure trace from a transducer within the congested region
showing multiple pressure peaks produced by interaction of the flame with
successive piperacks (R#) [Lowesmith, 2008] .............................................. 181
Figure 6-6: VCE 01: predicted and experimental [Lowesmith, 2008] flame
speed with distance ..................................................................................... 184
Figure 6-7: VCE 01: predicted and experimental [Lowesmith, 2008] maximum
overpressure with distance .......................................................................... 184
Figure 6-8: VCE 02: predicted and experimental [Lowesmith, 2008] flame
speed with distance ..................................................................................... 185
Figure 6-9: VCE 02: predicted and experimental [Lowesmith, 2008] maximum
overpressure with distance .......................................................................... 185
Figure 6-10: VCE 04: predicted and experimental [Lowesmith, 2008] flame
speed with distance ..................................................................................... 186
Figure 6-11: VCE 04: predicted and experimental [Lowesmith, 2008]
maximum overpressure with distance.......................................................... 186
Figure 6-12: VCE 09: predicted and experimental [Lowesmith, 2008] flame
speed with distance ..................................................................................... 187
Figure 6-13: VCE 09: predicted and experimental [Lowesmith, 2008]
maximum overpressure with distance.......................................................... 187
Figure 6-14: VCE 10: predicted and experimental [Lowesmith, 2008] flame
speed with distance ..................................................................................... 188
Figure 6-15: VCE 10: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance .......................................................... 188
Figure 6-16: VCE 12: predicted and experimental [Lowesmith, 2008] flame speed with distance ..................................................................................... 189
Figure 6-17: VCE 12: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance .......................................................... 189
Figure 6-18: VCE 03: predicted and experimental [Lowesmith, 2008] flame speed with distance ..................................................................................... 193
Figure 6-19: VCE 03: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance .......................................................... 193
Figure 6-20: VCE 05: predicted and experimental [Lowesmith, 2008] flame speed with distance ..................................................................................... 194
Figure 6-21: VCE 05: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance .......................................................... 194
Figure 6-22: VCE 06: predicted and experimental [Lowesmith, 2008] flame speed with distance ..................................................................................... 195
Figure 6-23: VCE 06: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance .......................................................... 195
Figure 6-24: VCE 08: predicted and experimental [Lowesmith, 2008] flame speed with distance ..................................................................................... 196
Figure 6-25: VCE 08: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance .......................................................... 196
Figure 6-26: VCE 11: predicted and experimental [Lowesmith, 2008] flame speed with distance ..................................................................................... 197
Figure 6-27: VCE 11: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance .......................................................... 197
Figure 6-28: VCE 13: predicted and experimental [Lowesmith, 2008] flame speed with distance ..................................................................................... 198
Figure 6-29: VCE 13: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance .......................................................... 198
Figure 6-30: VCE 14: predicted and experimental [Lowesmith, 2008] flame speed with distance ..................................................................................... 199
Figure 6-31: VCE 14: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance .......................................................... 199
Figure 8-1: Photograph of a jet fire [Lowesmith, Apr, 2008].........................219
Figure 8-2: Photograph of the fireball stage of a pipeline fire in progress
[Lowesmith, Aug, 2008] .....................................................................................220
Figure 9-1: Schematic of horizontal jet fire experiment arrangement with target in view [Lowesmith, Apr, 2008] ......................................................................236
Figure 9-2: Photograph of a jet fire experiment [Lowesmith, Apr, 2008] ......238
Figure 9-3: Diagram of the multi-point source model .................................239
Figure 9-4: The calculated value of $F$ from the experimental data [Lowesmith, Apr, 2008] and how $F$ changes with the number of point sources...........242
Figure 9-5: The fraction of heat radiated value for methane addition to hydrogen................................................................................................................245
Figure 9-6: The fraction of heat radiated derived from experimental data...246
Figure 9-7: Diagram of flame shape and dimensions [Chamberlain, 1987] . 248
Figure 9-8: Comparison of predicted and observed [Lowesmith, Apr, 2008]
flame length ..................................................................................................258
Figure 9-9: Predictions using multi point source model for Test 1..............261
Figure 9-10: Predictions using multi point source model for Test 2............262
Figure 9-11: Predictions using multi point source model for Test 3............263
Figure 9-12: Predictions using multi point source model for Test 4............264
Figure 9-13: Predictions using multi point source model for Test 5............265
Figure 9-14: Predictions using multi point source model for Test 6............266
Figure 9-15: Comparison of flame lengths from experiments [Lowesmith, Apr, 2008] and predictions.................................................................268
Figure 9-16: Prediction using the Johnson et al. [1994] model for Test 1 ....270
Figure 9-17: Prediction using the Johnson et al. [1994] model for Test 2 ....271
Figure 9-18: Prediction using the Johnson et al. [1994] model for Test 3 ....272
Figure 9-19: Prediction using the Johnson et al. [1994] model for Test 4 ....273
Figure 9-20: Prediction using the Johnson et al. [1994] model for Test 5 ....274
Figure 9-21: Prediction using the Johnson et al. [1994] model for Test 6 ....275
Figure 9-22: Comparison of flame lengths from experiments [Lowesmith, Apr, 2008] and predictions.................................................................277
Figure 9-23: Prediction using the JBurn model for Test 1 ............................279
Figure 9-24: Prediction using the JBurn model for Test 2 ............................280
Figure 9-25: Prediction using the JBurn model for Test 3 ............................281
Figure 10-17: Test 1 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations, 80s after rupture 306
Figure 10-18: Test 1 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations, 100s after rupture .................................................. 306
Figure 10-19: Test 1 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations, 120s after rupture ................................................................. 307
Figure 10-20: Test 2 – Photograph of the fire at time of 4.80s ..................... 308
Figure 10-21: Test 2 – Comparison of incident radiation predictions and experimental data [Lowesmith, Aug, 2008] at R13, 76m to the south .......... 309
Figure 10-22: Test 2 – Comparison of incident radiation predictions and experimental data [Lowesmith, Aug, 2008] at R13, 76m to the south .......... 309
Figure 10-23: Test 2 – Comparison of incident radiation predictions and experimental data [Lowesmith, Aug, 2008] at R13, 76m to the south .......... 310
Figure 10-24: Test 2 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations at 20s ..................... 311
Figure 10-25: Test 2 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations at 40s ..................... 311
Figure 10-26: Test 2 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations at 60s ..................... 312
Figure 10-27: Test 2 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations at 80s ..................... 312
Figure 10-28: Test 2 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations at 100s .......... 313
Figure 10-29: Test 2 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations at 120s ............. 313
## List of Tables

Table 3-1: Details of changing parameters of combustion has on the laminar burning velocity .......................................................... 71
Table 3-2: Fitted correlations for the temperature corrected laminar burning velocity to 298K ........................................................................... 76
Table 3-3: Comparison of correlations for laminar burning velocity and initial temperature changes (where available) ......................................................... 85
Table 4-1 Confined vented explosion experimental parameters [Lowesmith, 2007] .............................................................................................................. 97
Table 4-2: Summary of area blockage ratio (ABR) calculations ................... 102
Table 5-1: Compact congested rig parameters [Roberts et al., 2006] .......... 120
Table 5-2: Compact congest experimental programme of different fuel compositions [Roberts et al., 2006] .............................................................. 121
Table 5-3: Summary of explosion overpressures from CAM2 predictions and experiments (data from [Roberts et al., 2006]) .............................................. 146
Table 5-4: Summary of explosion overpressures from CCEM predictions and experiments (data from [Roberts et al., 2006]) ............................................. 153
Table 6-1: Test condition matrix ................................................................... 164
Table 6-2: Test conditions and summary of observations ......................... 168
Table 6-3: SCOPE predictions at enclosure vent ........................................... 182
Table 6-4: Comparison of predicted and measured maximum flame speeds for tests with non-accelerating flames (data from [Lowesmith, 2008]) .......... 190
Table 6-5: Comparison of predicted and measured maximum overpressure for tests with non-accelerating flames (data from [Lowesmith, 2008]) .......... 191
Table 9-1: Jet fire experimental conditions and visible flame length [Lowesmith, Apr, 2008] ................................................................................ 237
Table 9-2: Calculated value of $F$ from experimental data (based on 100 point sources) ....................................................................................................... 243
Table 9-3: Experimentally observed [Lowesmith, Apr, 2008] and predicted flame length ........................................................................................................ 257
Table 9-4: Experimental observed [Lowesmith, Apr, 2008] and predicted flame lengths ................................................................. 267
Table 9-5: Surface Emissive Power (SEP) values ................................................. 268
Table 9-6: Experimental observed [Lowesmith, Apr, 2008] and predicted flame lengths ......................................................................................................... 277
Table 9-7: Calculated value of $F$ used in JBURN ............................................. 278
Table 9-8: Predicted flame length with varying hydrogen addition to natural gas ................................................................................................. 287
Table 10-1: Pipeline fire test conditions [Lowesmith, Aug, 2008] ................. 292
Table 10-2: Fuel properties ............................................................................... 295
### Glossary

Glossary of acronyms and word used throughout this thesis:

<table>
<thead>
<tr>
<th>Abbreviation / Acronym / Words</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABR</td>
<td>Area Blockage Ratio</td>
</tr>
<tr>
<td>Advantica</td>
<td>Advantica Ltd. Formerly British Gas Research and Technology division and now Germanischer Lloyd (GL) Industrial Services.</td>
</tr>
<tr>
<td>ALARP</td>
<td>As Low As Reasonably Practical</td>
</tr>
<tr>
<td>CAM2</td>
<td>Shell’s Congestion Assessment Method version 2.</td>
</tr>
<tr>
<td>CCEM</td>
<td>GL’s Compact Congested Explosion Model</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>DDT</td>
<td>Deflagration to detonation transition</td>
</tr>
<tr>
<td>DOI</td>
<td>Digital Object Identifier</td>
</tr>
<tr>
<td>EC</td>
<td>European Commission</td>
</tr>
<tr>
<td>EMERGE</td>
<td>EC funded project on Extended Modelling and Experimental Research into Gas Explosions</td>
</tr>
<tr>
<td>ER</td>
<td>Equivalence Ratio</td>
</tr>
<tr>
<td>EU</td>
<td>European Union</td>
</tr>
<tr>
<td>GL</td>
<td>Germanischer Lloyd refers to the Industrial Services division in this thesis. Former brand names include Advantica (see above) and British Gas Research and Technology.</td>
</tr>
<tr>
<td>HAREM</td>
<td>GL’s High Aspect Ratio Explosion Model</td>
</tr>
<tr>
<td>HSE</td>
<td>Health and Safety Executive</td>
</tr>
<tr>
<td>HSL</td>
<td>Health and Safety Laboratory</td>
</tr>
<tr>
<td>MERGE</td>
<td>EC funded project on Modelling and Experimental Research into Gas Explosions</td>
</tr>
<tr>
<td>Abbreviation / Acronym / Words</td>
<td>Description</td>
</tr>
<tr>
<td>-------------------------------</td>
<td>-------------</td>
</tr>
<tr>
<td>MPS</td>
<td>Multi Point Source</td>
</tr>
<tr>
<td>NG</td>
<td>Natural gas</td>
</tr>
<tr>
<td>Overpressure</td>
<td>The difference between the pressure generated by an explosion and atmospheric pressure</td>
</tr>
<tr>
<td>PDE</td>
<td>Partial Differential Equation</td>
</tr>
<tr>
<td>QRA</td>
<td>Quantified Risk Assessment</td>
</tr>
<tr>
<td>SCOPE</td>
<td>Shell Code for Overpressure Prediction in Gas-Explosions</td>
</tr>
<tr>
<td>Stoichiometry</td>
<td>Condition at which the amount of fuel and oxidiser gives complete combustion</td>
</tr>
<tr>
<td>SEP</td>
<td>Surface emissive power</td>
</tr>
<tr>
<td>TNO</td>
<td>Netherlands Organisation for Applied Scientific Research</td>
</tr>
<tr>
<td>UK</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>VBR</td>
<td>Volume Blockage Ratio</td>
</tr>
<tr>
<td>VCE</td>
<td>Vapour cloud explosion</td>
</tr>
</tbody>
</table>
The availability of fossil fuels for continued future use is known to be limited. As the world’s population and demand for more energy increases we need to find ways to meet this demand. This is hampered by the increasing effort required to extract oil and gas from the ground, although with new technology and investment even greater quantities can be extracted. The amount of fossil fuels left may eventually be too little or too difficult or costly to extract. Furthermore, it is also widely agreed that the product carbon dioxide produced by combustion of fossil fuels is contributing to increasing the temperature of the earth (the greenhouse effect [Le Treut et al., 2007]). With our increased demand for fossil fuels as economies grow this effect can only seemingly increase. It is thus inevitable to look to create a more sustainable and cleaner future. Hydrogen is seen as an alternative energy carrier to the portfolio of fossil fuels, allowing sustainable energy sources (such as solar generated electricity) to become portable. It is suggested that a move should be made towards a hydrogen economy, in which sustainable sources of energy are harnessed to produce hydrogen as soon as possible.

Natural gas is a widely used fossil fuel, consisting primarily of methane along with some higher hydrocarbons that vary depending upon the point of extraction. Natural gas exists naturally in the ground and is extracted and processed to remove some of the higher hydrocarbons. It is the cleanest burning fossil fuel and widely used in industry and domestic appliances. There is a vast infrastructure of pipelines that connects many homes and industries to a supply of natural gas. The storage, distribution and end use of natural gas
is well understood due to many decades of experience and knowledge. To have a hydrogen economy on the scale of the current natural gas/fossil fuel economy poses many challenges which need to be solved, not least being the production of hydrogen from renewable sources. Another challenge is the transport of hydrogen from its point of production to its point of use. It is proposed that to assist the transition to a hydrogen economy, hydrogen is introduced into the current natural gas transmission and distribution system. This proposition is the focus of a major European Commission (EC) funded project called the NATURALHY project.

This chapter outlines the background to the problems of the sustainability of fossil fuels and the role it is envisaged that hydrogen can play in alleviating the problem. The NATURALHY project is introduced, before focussing on the safety aspects in particular. This work forms part of the safety work package of the NATURALHY project, which addresses the hazards and risks associated with using the current gas infrastructure to transport natural gas/hydrogen mixtures. Following this chapter, the thesis is split into two parts, Part A concerned with predicting explosion hazards and Part B concerned with predicting fire hazards. Each part has an opening chapter including a presentation of the problem and a literature review, before additional chapters which cover different hazard scenarios. For each hazard scenario, the predictive model used is presented, modified/developed as necessary and then the results compared with experimental data taken from the experimental programme on explosions and fires also undertaken by Loughborough University as part of the safety work package of the NATURALHY project.

1.1 The contribution of Hydrogen to the energy economy

Fossil Fuels
Currently, most of the energy consumed originates in the form of fossil fuels. Fossil fuels are a natural resource formed from dead organisms over millions
It is widely agreed that, due to the increasing build up of carbon dioxide in the air, produced by human activity, the greenhouse effect is creating a warmer world. This is commonly referred to as (human induced) climate change. Because of this, and following the Kyoto Protocol, many governments are looking to reduce their countries carbon dioxide emissions to help the "stabilization of greenhouse gas concentrations in the atmosphere at a level that would prevent dangerous anthropogenic interference with the climate system" [UNFCC, 1997]. Further political interest comes from the Intergovernmental Panel on Climate Change (IPCC), and the recent UK government Stern review on the economics of climate change. It is important that the government remains informed of the current state of emissions and new technologies that may reduce them.

Mankind has a dependence on fossil fuel, and it is an integral part of all national economies. Any change in the supply and price of energy has an effect on all. There are many places around the globe where there are known oil and/or gas reserves, some of these may be in the process of being worked, nearly fully extracted or just mapped. The UK has in the past met its demand for natural gas completely from the North Sea reserves. However, these reserves are becoming depleted and nowadays some natural gas is being imported via the European continent (particularly in high demand periods,
such as winter). It is expected that to meet our increasing demand for energy more gas will need to be imported. Thus the energy supply becomes dependent on other countries and sources, where politics may have an important role for the security of supply.

Natural gas, of which methane is its main component, when burnt releases the least amount of carbon dioxide compared to other hydrocarbons (and fewer other pollutants such as oxides of nitrogen and sulphur) and as a consequence is been used increasingly to replace such fuels as coal.

Currently, the main source of natural gas is from oil fields or natural gas fields on and off-shore, but it has been proposed that methane can be obtained from sources like cow manure and land fill sites that release methane as a natural by-product. Natural gas is widely used in industry and in the domestic environment, including power generation, industrial and domestic heating and cooking, and is even used to power vehicles. It is transported through a vast network of pipelines to industry, businesses and homes.

**Hydrogen**

It is suggested that hydrogen is a suitable energy carrier for sustainable energy sources. It is the most abundant element in the universe, and is clean producing no greenhouse gases when burnt. The main combustion product is water. A reaction of hydrogen in air also produces nitrogen oxides (NO$_x$) due to the high temperatures, which also contribute to the greenhouse effect and other environmental factors such as acid rain$^1$ [Badr and Probert, 1993]. Even though hydrogen is the most common element it is not found naturally on our planet by itself. Most hydrogen is contained in other compounds such as water and hydrocarbons. Thus it is not a primary energy source. A number of problems need to be addressed and solutions found to introduce hydrogen as a viable energy carrier on a large scale. Topics include: producing hydrogen, transport, storage, and end use of hydrogen. At all stages safety must be high priority.

$^1$ In some cases the NO$_x$ emissions for hydrogen may be higher than for methane, so careful combustion design is required.
To obtain hydrogen it must be extracted from hydrogen containing molecules. Currently, the most common way of producing hydrogen is by steam reforming of methane [Balat, 2009]. Currently this is the most economical but the process still produces greenhouse gases. Another potential method is water electrolysis which does not produce greenhouse gases. However, it uses electrical energy which would need to be generated using renewable sources to be sustainable and avoid production of carbon dioxide. At this time new ‘green’ sources of electricity could prove to be considerably more expensive than more ‘conventional’ means. Other methods of producing hydrogen also include: coal gasification (which makes town gas that contains primarily hydrogen and carbon monoxide); biological fermentation that uses biological process such as enzymes and bacteria to produce hydrogen; chemical production such as the reaction of aluminium, sodium hydroxide and water, or via the use of heat (thermochemical).

The amount of hydrogen needed for mass consumption in homes and businesses on the scale of the current hydrocarbon economy would place great demands on renewable sources of electricity for electrolysis systems. [Norbeck et al., 1996]. Some people doubt its role as a universal energy carrier, “hydrogen can never compete with its own energy source” [Bossel, 2006]. Bossel argues that, in terms of efficiency, for non-mobile applications, electricity is the most desirable form of energy to produce and transport. Bossel’s answer to the question “does the hydrogen economy make sense” is never, due to the “parasitic losses”. There exist many ways to obtain electrical energy, which can be centrally produced and then distributed, or generated closer to the point of use. The greatest benefit to be gained from using electricity as an energy carrier is that once created, the energy is used directly and not used to create another form of energy, such as breaking up water to form hydrogen. However, currently it is difficult to store electricity making it a difficult option for transport and other portable applications. European Commission funded initiatives that focus on the role of hydrogen in the future, include: HYWAYS looking at a roadmap to a hydrogen economy; HYSAFE
looking at the safety of hydrogen; NATURALHY looking at the part that the
natural gas system can play in a transition towards the hydrogen economy.

The use of hydrogen is currently being heavily researched, for example the
following European Commission funded 6th framework projects HYSafe,
HYWAYS, HYLIGHTS, HYAPPROVAL, European Hydrogen and Fuel Cell
Technology Platform, and STORHY [European Commission, 2004].

Applications include fuel cells, and direct combustion mostly for vehicle
applications. Fuel cells use hydrogen (from storage) and oxygen taken from
the atmosphere to produce electricity. This is done at a much higher efficiency
than burning fossil fuels, up to 60% efficient compared to 20-30%. At the
present stage of development, the energy lost is in the form of heat. Fuel cells
are seen by many to be the future of our portable energy needs, they are
scalable meaning they can be used in small electronic devices, domestic
environments and industry, and they are clean. In addition, the heat from a
fuel cell can be used, creating a combined heat and power (CHP) device.

Another important topic that needs to be addressed is the infrastructure of a
hydrogen economy, this involves how hydrogen will be transported and
stored. Furthermore, there are social and economic issues that must be
addressed for hydrogen to proceed successfully. These issues include: public
perception about safety, ease of use, and the cost of hydrogen over the cost
of traditional sources of energy. Initially the cost may put the technology out of
the reach of the majority. Areas affected include replacements for home
heating, new vehicles using hydrogen, the ease of obtaining hydrogen and the
filling up of vehicle fuel tanks. It may be these issues that will determine how
successful and quickly the transition to a hydrogen based economy will
happen.

Storage of hydrogen is currently a problem. By mass it has a higher energy
density, but its energy to volume ratio is lower than for fossil fuels. This means
it is usually stored under immense pressure or low temperature to increase
the volumetric energy density [Strubel, 2008]. However, these involve extra
processes on the gas which expend energy, thereby, reducing the overall
efficiency of the system. Two other approaches to the storage of hydrogen are, compounds with hydrogen (hydrides) and through chemical reaction producing pure hydrogen, and by a specially designed container that ‘absorbs’ hydrogen that can then be extracted later.

The transportation and distribution of hydrogen, whether by pipeline, similar to the natural gas system, or by vehicular transport as a compressed gas or liquefied gas is not so simple. As stated previously, the volumetric energy density of hydrogen is lower, so high pressures will be needed. This increases the power consumption to generate the high pressure. Existing pipeline systems may not be able to handle the presence of hydrogen due to the affect of the hydrogen on the pipeline material as well as the increase in pressure above the original design specification, that is, for natural gas. Another approach is local production, sometimes called distributed production, where hydrogen is produced near to where it is used requiring many facilities. If electrolysis was used then any plant could be placed near a water source, meaning many towns could have a local source of hydrogen, providing a potentially greater security of energy supply. This would also increase the efficiency of the transportation of hydrogen, requiring less power, either through shorter lengths of pipeline or distance for vehicular transport.

Hydrogen has different properties to current fuels with which we are familiar. To use hydrogen in everyday life, with the same safety and ease that we are accustomed to with carbon based fuels, has many challenges, including preconceptions people have about the safety of hydrogen. Hydrogen is the lightest element, has a high diffusivity, it is very reactive and easy to ignite. Small flames of hydrogen are invisible in most cases (apart from heat haze). Also the burning velocity is very high which can lead to violent explosions. Hydrogen is easy to ignite and is flammable over a wide range of concentrations. Hydrogen is known to affect many storage materials, through embrittlement and also leaks more readily out of imperfections. Hydrogen is much less dense than air (1/14th) and so will readily ascend due to buoyancy. In open or well ventilated spaces, this may well prevent build up of flammable mixtures. The large differences in properties between hydrogen and
conventional fuels will have an effect on the hazards and the risk that the gas poses. New codes and regulations for safe usage will be required.

Concerns have also been raised concerning a build up of hydrogen in the atmosphere due to small leaks in hydrogen systems, and the effects that this will have on the atmosphere [CALTECH, 2003].

1.2 **NATURALHY**

The aim of the NATURALHY project is “to prepare for a hydrogen economy by using the existing natural gas system as a transition catalyst”. The NATURALHY project is co-financed by the European Commission through the Sixth Framework Programme (2002-2006) for research, technological development and demonstration (RTD). Work commenced in 2005 and was planned to take 5 years. This large integrated project has a budget of approximately 17 million Euros and 39 partners.

To achieve the aim of the project, potential barriers stopping the introduction of hydrogen as an energy carrier will be identified and attempts made to remove them. It is envisaged that if it is shown to be feasible to introduce hydrogen into the natural gas pipeline system the adoption of hydrogen as an energy carrier may be accelerated, and the cost benefits by using existing assets will be huge. Furthermore, it is proposed that the new fuel mixture of natural gas and hydrogen may be used directly, or the hydrogen used as a pure gas after separation. It is envisaged that it will be possible to add a certain amount of hydrogen before significant problems arise. Thereafter, further hydrogen addition will require increasing modification and hence cost.

The NATURALHY project states its objectives as;

1. To define the technical conditions under which hydrogen can be accommodated in the existing natural gas system with acceptable risks, to avoid leakage and significant degradation of the system and consequences for the end users.
2. To analyse the socio-economic aspects of transitional natural gas/hydrogen systems and compare these with current natural gas and related systems.

3. To carry out life cycle assessment as a means of comparing the major resource inputs and environmental outputs of current natural gas and related systems.

4. To develop innovative devices (membranes) to separate hydrogen from natural gas/hydrogen mixtures.

5. To motivate all stakeholders in the whole chain from production up to and including end use to welcome hydrogen.

6. To assess the current situation of standards and regulations regarding natural gas/hydrogen mixtures and to identify necessary modifications and to initiate required changes.

7. To develop a Decision Support Tool for the assessment of the suitability of an existing natural gas system (transmission, storage, distribution, end user infra structure and end user appliances) for mixtures of natural gas and hydrogen and to develop models to determine the economic and environmental aspects of the whole chain from sustainable hydrogen production up to and including end user appliances.

To carry out the research, the project has been divided into work packages. This enables the work to be split into research interest areas and delegated to the most appropriate researcher. There are eight different work packages, each focusing on a different aspect of the infrastructure for natural gas and hydrogen mixtures. Each one defines a list of tasks to achieve its objective. The list of work packages is as follows.

1. **Life cycle and social economic assessment** (Leader: Loughborough University, UK)

   Evaluates the social and economic costs associated with the projects aims over the whole life cycle of the system. This will be done in three stages, assessing the current system, one with a mixture of natural gas and hydrogen, and finally a purely hydrogen system.
2. **Safety** (Leader: Loughborough University, UK)
   This work package focuses on how the addition of hydrogen to the natural gas infrastructure may change the risk to the general public, and what may be a safe quantity of hydrogen to add without the need to make significant changes to the existing infrastructure. The work described in this thesis is part of this work package and contributes to several of the tasks. More information regarding this matter is provided later in this section.

3. **Durability** (Leader: GDF Suez, France)
   Aims to establish an acceptable hydrogen content that can be mixed into the natural gas system given any change it has on the characteristics of the system including transmission, distribution and end uses. This work also feeds into the safety work package as it involves work on the frequency of a hazardous event occurring, from the failure of the infrastructure.

4. **Integrity** (Leader: DBI Gas- und Umwelttechnik GmbH, Germany)
   Determines how integrity management will need to incorporate the change of operating a system using a mixture of the natural gas and hydrogen. This will provide all the information needed by pipeline operators to effectively manage their systems and to do so safely.

5. **End use** (Leader: Oxford University, UK)
   Assesses what affect hydrogen will have on existing natural gas appliances and end uses. Further, there is work underway to develop membranes for the separation of hydrogen from the mixture. This will enable a hydrogen market to start, as soon as there is a readily available source of the gas.

6. **Decision support tool** (Leader: Instituto de Soldadura e Qualidade (ISQ), Portugal)
   A software decision tool will be developed for the assessment of the suitability of a natural gas system to have hydrogen introduced into it as a natural gas and hydrogen mixture. This draws on the results of all the other technical work packages (1-5).

7. **Dissemination** (Leader: Exergia, Greece)
   This work package focuses on making the results of the NATURALHY
project available to the public. This may be an important step in the public and industrial acceptance of introduction of hydrogen into society.

8. **Project management** (Leader: Gasunie, The Netherlands)
   Manages the 39 partners that make up the project.

The NATURALHY project does not address the issue of where and how hydrogen may be produced but concentrates on assessing the feasibility of using the existing natural gas infrastructure to transport hydrogen as a mixture with natural gas.

**Safety work package**
The work described in this thesis forms part of the safety work package (WP2) led by Loughborough University. Currently, the risks of natural gas are well understood as much experimental and modelling work has been carried out by gas companies to understand and reduce the risks, for example Selby and Burgan [1998]. However, by adding hydrogen to natural gas the behaviour and properties of the gas mixture may be different to natural gas and hence change the risks. The objectives of the safety work package is to identify and quantify the changes in consequences and level of risk resulting from accidental releases of natural gas/hydrogen mixtures compared with those of natural gas.

The objectives of the safety work package will be achieved by revisiting the major hazard scenarios studied with natural gas and performing an experimental test programme using natural gas (or methane) and hydrogen mixtures. Concurrent with the experimental programme is a modelling activity in which models, developed and validated for natural gas, are further developed and modified for natural gas/hydrogen mixtures. The results of the natural gas/hydrogen experiments will be compared with existing natural gas experimental data and with the model predictions. Any differences between model predictions and experimental data can then be identified and resolved and the models incorporated into risk assessment methodologies. Changes in the level of risk as the proportion of hydrogen is increased will determine the
amount of hydrogen that can be added before the risk becomes unacceptable.

The safety work package is structured into 12 tasks:

1. Parameters of natural gas and hydrogen mixtures including combustion in air
2. Gas Build-up and Explosions in Confined/Vented Enclosures
3. Vapour Cloud Explosions in Congested Regions
4. High Pressure Jet Fires
5. Pipeline Fires
6. Comparison with natural gas and hydrogen Data and Predictions
7. Failure and Ignition Frequency Assessment
8. Leakage Assessment
9. Modification of Risk Assessment Methodology
10. Implementation of Risk Assessment Methodology
11. Assessment Guidance
12. Work Package Co-ordination

The work described in this thesis contributes to the modelling activities of tasks 2 to 6.

1.3 **Hazards and Risk**

Producing, processing, transporting, storing, and utilising any flammable substance constitutes a hazard. A hazard is a situation that has the potential to cause damage and/or loss. Damage may be to life, or to property and the surrounding environment. Damage to life may incur loss of quality of life, loss of earnings, or even loss of life. Damage to property can involve loss in monetary terms (loss of value of assets, cost to rebuild, loss of earnings). In addition, there is possibly, loss of reputation. Risk is a function of the likelihood that a particular hazard is realised and the severity of the consequences. Fundamentally, it is defined mathematical as a function of the frequency of an untoward event (such as the rupture of a high pressure gas pipeline) and the consequences (such as loss of life following ignition of the released gas).
The frequency with which an untoward event might occur is usually investigated using fault tree analysis. To determine the probability of failure attributable to the failure modes considered, historical data is often used. Once an untoward event has occurred, the sequence of subsequent events is usually explored using event tree analysis. The combination of both fault tree analysis and event tree analysis is used to give the frequency with which a consequence might occur, such as the number of lives lost per year.

Hazard analysis is a process that is carried out to assess the safety of hazardous activities. Hazard analysis comprises two parts, hazard identification and risk assessment. For particularly hazardous activities, risk assessment is usually carried out in a quantitative way called quantitative risk assessment (QRA). It is important to be able to quantify risk, in particular so that different hazardous activities can be compared. The frequency of a particular consequence is normally expressed as how many times it may occur in a given time period, such as per year.

It is vital that the risk is understood and managed by industry. Risk can be managed by preventing or reducing the likelihood of an untoward event, reducing the impact or providing protection from the impact of the untoward event. This is accomplished by following, standards, regulations and best practice.

Unfortunately risk cannot be completely eliminated, but there are general criteria as to what is an acceptable level of risk. These are set by the regulator, in the case of the UK this is the Health and Safety Executive (HSE). The HSE have set acceptability criteria and use the concept called ALARP which stands for As Low As Reasonably Practicable. Three regions are defined: (1) a region where the risk is too high so as to be considered intolerable so the risk HAS to be reduced; (2) a region where the risk is sufficiently low that it is (broadly) acceptable; (3) the region in-between call the ALARP region. In the ALARP region the facility owner is obliged to reduce the risk to as low as is reasonably practical. Reasonably practical is determined by means of a cost benefit analysis. To reduce risk you must either reduce the
frequency of it happening or the consequences of it happening. It is generally accepted that the best way to reduce risks is to reduce the consequences; this concept is called Inherent safety.

Two categories of risk can be considered: individual risk and societal risk. Individual risk is calculated by considering a single person positioned indefinitely at a particular location. Societal risk is a measure of the effect of an activity on society as a whole. Societal risk is often displayed as a FN curve, which is the Frequency of N of more casualties plotted against the Number of casualties.

When undertaking a risk assessment it is important to look at many cases. This is necessary because there may be many different potential accident scenarios and the prevailing conditions may change throughout time, for instance atmospheric, operating conditions and populations present. These conditions may change from day to day or even season to season. Each scenario may have a different probability associated with it and produce a different consequence. As a requirement, therefore, QRA techniques may need to be applied multiple times for different cases to determine the profile of risk. It will also determine the situation that produces the worse scenario, which is often the most important scenario to identify and understand. Furthermore, because many cases need to be considered, the assessors may not have time for lengthy detailed computational runs therefore engineering type models are most desirable. Detailed computational runs, such as computational fluid dynamic (CFD) models, can take many days to complete, require high expertise in the use of such software and afterwards may still need calibration against experiments. Engineering type models are easier to use by the assessor, take less time to run and are validated using experiments of the same type as the scenario under consideration, meaning that much of the uncertainty of the fundamental physics are embodied in the calibration (this is discussed further in Chapter 2).

Use of materials that pose a hazard are regulated in the U.K. by the HSE and the Environment Agency. Industries that involve use of large quantities of a
hazardous material are subject to the Control of Major Accident Hazards Regulations 1999 (COMAH). A requirement of COMAH is that a safety report is required which demonstrates that all necessary measures have been taken to minimise the risks posed by the operations with regard to the environment and local populations.

1.4 **Explosions and Fires Involving Natural Gas/Hydrogen Mixtures**

Confined vented explosions, vapour cloud explosions, jet fires and pipeline fires are possible incidents that could arise due to leakage of gas from containment. The circumstances under which an escape of gas results in a particular type of incident (explosion or fire), can be simplified to delayed and immediate ignition. Explosions and fires are the two most important incidents to be understood and to assess during risk assessments associated with natural gas infrastructure.

1.4.1 **Experimental Work**

Within the NATURALHY project an experimental programme on explosions has been carried out for three different geometries. These were; confined vented enclosures, unconfined compact congested regions of pipework and unconfined congested regions with a large aspect ratio (simulating piperacks). The long pipe-rack explosions were ignited by means of an initial confined vented explosion. Two types of fires were studied: high pressure jet releases representing punctures in above ground plant or pipework and releases representing the rupture of an underground high pressure pipeline. These represent scenarios pertinent to natural gas infrastructures and have been studied previously for natural gas only releases.

1.4.2 **Objectives and Structure of the Thesis**

The aim of this thesis is to predict the hazards posed by explosions and fires involving natural gas/hydrogen mixtures using the kind of model usually used
for risk assessments. The frequency or probability of the event happening and
the subsequent effects of the consequences of explosions and fires are not
explored. The technical work described in this thesis is split into two parts.
Part A is a study of the prediction of explosions and Part B is a study of the
prediction of fires.

Existing engineering models were used and extended in this work. The
availability of validated engineering models has two main benefits. The first is
that the risk assessor can run many different parameters and conditions in a
relatively short space of time. The second is that a validated formulation
includes effects that are difficult to model in a more sophisticated CFD model
due to the complexity or incomplete physical understanding of the problem.

For explosions, predictions of the maximum overpressures generated are
needed as these give rise to the greatest consequences. Pressure can cause
damage to many things depending on its magnitude, duration and rate of rise.
This includes damage to structures and life. This is why it is important to
determine the maximum overpressure. Hydrogen is known to detonate readily
but in a mixture with natural gas this effect is unknown, this is a specific
question and was one of the objectives of the safety work package of
NATURALHY.

Hence, the objective of Part A of this thesis is to use existing models of gas
explosions, which were developed and validated for use with hydrocarbons
(usually natural gas), and then apply them to predict the consequences of
natural gas/hydrogen explosions. By comparison with the large scale
experimental data produced within the NATURALHY project, the performance
of the models can be assessed. Where necessary, modifications and
extensions to the models, which specifically address the different
characteristics and behaviour of hydrogen, are made and predictions of
maximum overpressure and flame speed (where possible) from the revised
model are compared with the experimental data.
For fires, the thermal radiation incident upon a target is needed, and this normally involves predicting the size of the fire. Radiation can have an effect on; structures weakening them and maybe causing collapse, and on life where in severe cases it can cause burns to the skin. Thus it is very important to be able to quantify the incident radiation levels around a fire. Small jet fires involving hydrogen are known to be virtually invisible and do not radiate much heat Before the NATURALHY project, little was known regarding the characteristics of large natural gas/hydrogen jet fires.

The objective of Part B of this thesis is to use existing engineering models to predict the flame size and incident radiation field produced by fires involving natural gas/hydrogen mixtures. In particular, the effect of hydrogen in the mixture on the radiative characteristics of the flames is considered.

Discussion and conclusions from the work are included at the end of each chapter and an overall conclusion is provided at the end of the thesis.

The overall objective of this thesis is to extend the applicability of consequence models, used in risk assessment within industry, to natural gas/hydrogen mixtures. The models can then be used to quantify the change in risk presented to the public if hydrogen is introduced into the gas network.
PART A

Explosions

In this part of the thesis the topic of explosions is studied.
## Nomenclature

Symbols used in this part of the thesis:

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_p$</td>
<td>Specific heat capacity at constant pressure</td>
<td>J mol$^{-1}$ K$^{-1}$</td>
</tr>
<tr>
<td>$D$</td>
<td>Mass diffusion coefficient</td>
<td>m$^2$·s$^{-1}$</td>
</tr>
<tr>
<td>$E$</td>
<td>Expansion ratio</td>
<td></td>
</tr>
<tr>
<td>$Ka$</td>
<td>Karlovitz stretch factor (Introduced Eq (2-4))</td>
<td>-</td>
</tr>
<tr>
<td>$L$</td>
<td>Markstein Length</td>
<td>m</td>
</tr>
<tr>
<td>$Ma$</td>
<td>Markstein number (Introduced Eq (2-6))</td>
<td>-</td>
</tr>
<tr>
<td>$M$</td>
<td>Laminar burning velocity initial temperature exponent</td>
<td>-</td>
</tr>
<tr>
<td>$u_l$</td>
<td>Stretched laminar burning velocity</td>
<td>ms$^{-1}$</td>
</tr>
<tr>
<td>$u_{L0}$</td>
<td>Un-stretched laminar burning velocity</td>
<td>ms$^{-1}$</td>
</tr>
<tr>
<td>$S_L$</td>
<td>Stretched laminar flame speed</td>
<td>ms$^{-1}$</td>
</tr>
<tr>
<td>$S_{L0}$</td>
<td>Un-stretched Laminar Flame Speed</td>
<td>ms$^{-1}$</td>
</tr>
</tbody>
</table>

Greek symbols used in this part of the thesis:

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Gamma$</td>
<td>Ratio of gas specific heat capacity</td>
<td>-</td>
</tr>
<tr>
<td>$\delta_{L0}$</td>
<td>Un-stretched Flame thickness</td>
<td>m</td>
</tr>
<tr>
<td>$\delta_L$</td>
<td>Stretched flame thickness</td>
<td>m</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Thermal Diffusivity</td>
<td>m$^2$·s$^{-1}$</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Area blockage or porosity of a grid</td>
<td>-</td>
</tr>
<tr>
<td>$\Phi$</td>
<td>Equivalence Ratio</td>
<td>-</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>Flame Stretch Factor, eq (2-3)</td>
<td>-</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density</td>
<td>kg·m$^{-3}$</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Kinematic viscosity</td>
<td>m$^2$·s$^{-1}$</td>
</tr>
</tbody>
</table>
2 Predicting Large Scale Explosions

2.1 Introduction

In this chapter a review of explosion models, typically used in industry, is carried out. The focus has been on more recent models rather than some of the older techniques. Briefly, the basics for modelling are addressed, and then a review of current explosion models, focusing on empirical and phenomenological models, which are the models most widely used by industry for risk assessment purposes.

2.2 Description of a Gas Explosion

An explosion is a sudden and forceful release of energy, where the violence depends on the rate of release of energy. The energy released in the explosion process is in the form of chemical and physical/mechanical energy. The source of energy may be potential energy (gas under pressure) and chemical energy (exothermic chemical reaction). In the safety work package, explosions of different compositions of gases are studied where the energy of the explosion is derived solely from chemical energy of gaseous fuels (once ignited).

If gas were to escape from containment and given the right local conditions, the gas may build up in some region. Through dispersion, air will be entrained into the gas and thus there is potential for the fuel-air mixture to become flammable. For the mixture to be a hazard the concentration of fuel in the
mixture needs to be within a particular range, defined by the flammability limits of the fuel, outside these limits the mixture will not react [Tite, 2001]. An explosion in this situation is initiated some time after the gas started to escape and thus there is an inventory of fuel-air available for the explosion.

An explosion consists of a thin reacting region, known as a flame, propagating into a combustible mixture away from the ignition source. The flame surface is influenced by the flow field ahead of the flame. There are two modes in which the flame can propagate, a deflagration and a detonation. In a deflagration the propagation velocity of the flame is sub-sonic with respect to the reactants. A detonation is where the flame travels as a shock wave coupled with a reacting wave releasing energy to sustain the leading shock wave. As guidance, the detonation velocity is of the order of more than 1.5 km/s [Moen, 1993; Groethe et al., 2007] whereas deflagrations propagate at a velocity an order of magnitude less. Detonations result in high and destructive overpressures. A deflagration can also result in high overpressure and may lead to transition to a detonation, if acceleration of the flame is sustained.

Briefly, in an explosion the flame is a thin sheet of combustion propagating into reactants and leaving combustion products in its wake (see Figure 2-1). The flame speed propagates at the local burning velocity plus the speed of the gases behind the flame (i.e. the combustion products). The flow field ahead of the flame influences the behaviour of the flame. In particular turbulence ahead of the flame will increase the burning velocity (locally) which may change the shape of the flame. Turbulence may be caused by instabilities but primarily by obstacles as expansion of the combustion products pushes the unburnt gas around them. The flame surface, as it propagates, generates pressure in front of it, and, in general the faster the propagation the greater the pressure generated. Pressure is generated due to the inertia of the gas in front of the flame. As the flame accelerates, the pressure waves coalesce and may produce a shock wave. The faster a flame travels the greater is the disturbance that is generated in the flow ahead which will lead to higher burning velocities and increase in the flame speed. This is a feed-back
mechanism and has been called the Shchelkin mechanism [Shell SCOPE help, Ledin, 2002].

Figure 2-1: Illustration of the combustion process, with central ignition

Gas explosions can generally be grouped into two categories, confined explosions and unconfined vapour cloud explosions.[Ledin. 2002]

In confined explosions there is a high degree of confinement due to walls, ceilings and floors but the confinement may contain vents that allow gas to exit. The pressure generated in this type of explosion comes from the confinement and is related to the ratio of the temperature of the burnt and unburnt gases. For natural gas this is approximately 8 [Tite, 2001]. The pressure rise in an enclosure is due to the fact that the hot combustion products want to expand, but because of the confinement there is nowhere for the gas ahead of the flame to go. As the volume is constant, the pressure rises. In real scenarios however, there is likely to be some sort of vent through which gas can escape, or the overpressure generated may cause part of the enclosure to fail thus limiting the extent to which the pressure can rise within the enclosure. However in such cases, unburnt gas mixture can be pushed through a vent followed by the flame resulting in a further explosion outside of the enclosure. These are generally termed confined vented explosions.
Unconfined explosions are defined as those explosions that involve a vapour cloud that exists in a region of low confinement. The overpressure generated in this scenario is a function of the flame speed. If the vapour cloud is in an unobstructed region in free space, that is, one without obstacles (pipes and vessels) that form congestion, then the overpressures generated are negligible. However, if the vapour cloud is in a region with congestion then the overpressures generated can be very significant. It is widely recognised [van den Berg, 1985] that significant overpressures are only generated in unconfined regions where the flammable cloud engulfs a region of congestion. This is because the obstacles are the mechanism by which the flame can accelerate to high speeds and it is the flame speed and, consequently, the rate at which fuel is consumed and hence the rate at which energy is released that generates overpressure.

2.3 Explosion Hazards

Explosions cause an increase in pressure. This is known as overpressure which is the increase in the pressure above the undisturbed atmosphere pressure. Generally the higher the overpressure generated the more damage is caused. For particularly strong explosions, shock waves can occur where the pressure almost instantaneously rises from ambient to the overpressure value. There is no warning for an observer in free space as no pressure information travels ahead of the shock front.

The main damage from an explosion is as a result of the overpressure generated. However, there is also radiation from the flame but this, in general, is insignificant compared to the overpressure and usually ignored in safety calculations. Different levels of overpressure have different consequences. If the overpressure is significant, it can damage or destroy structures constructed from various materials such as brick, glass and steel. Furthermore, overpressure can harm humans. As the flame front propagates and generates overpressure, a pressure wave travels away from the flame. The overpressure wave (sometimes called blast wave) can also cause objects
to move possibly becoming missiles which can cause further damage to structures and harm to people.

During an explosion, the reaction converts the fuel and oxidiser, which in most common scenarios is air, into products which do not contain air. This poses a problem for individuals in an area through which a flame front has passed as there will be no air to breath and suffocation can occur. Furthermore, high temperature flames also produce nitrogen oxides (NOₓ) which is harmful to the environment and to health. Different reactions will produce varying degrees of nitrogen oxides.

However, the principles hazard of explosions is the overpressure generated. It is known how overpressure damages many materials and structures and this information has been compiled into databases [Mannan, 2005].

There are ways to mitigate against events that may lead to an explosion (prevention) and methods to try and reduce the consequences if the incident takes place (protection) [Mannan, 2005]. There are two ways to provide mitigation, passive and active, the former being something that is inherent in the mitigation concept and active where something is actively monitored and then a response is made as appropriate. In the beginning good design can help in reducing the likelihood of failure of containment, and the magnitude of the consequences of an event happening. This concept is known as inherent safety and an example of this is reducing the inventory of the hazardous substance which would reduce the magnitude of a resulting fire or explosion. If an event happens active methods include water deluge to extract energy from a fire or explosion, and passive methods may include low pressure relief panels to limit the build up of overpressure in a confined enclosure.

2.4 Modelling Explosion Events

An explosion is the result of a violent release of energy from a combusting mixture. It is an unwanted event. Therefore, it is desirable to have an understanding of explosions and be able to predict such explosion events.
Predictions allow safety assessors to design facilities or assess existing facilities and give recommendations on how to mitigate explosions and reduce the risk.

As previously stated one of the most important explosion parameter to be predicted is the overpressure generated. This depends on a number of other factors;

- Fuel properties
  - The reactivity of the fuel, often characterised by the burning velocity
  - The oxidant
  - The concentration of the fuel in the fuel-oxidant mixture (stoichiometry)
- Ignition source – type and location.
- Confinement and area available for venting.
- Initial background condition, pressure, temperature but more significantly background turbulence in the flammable mixture.
- Congestion, the amount, shapes and sizes of obstacle in the gas cloud.
- Size of the gas cloud and plant.

There are three main approaches to modelling [Ledin, 2002];

- **Empirical or correlation type models**
  These are based on the observation of experiments, whereby a correlation is obtained by analysis of the experimental data. Usually the correlation is tied specifically to the range of experiments upon which it is based and thus to model something different may require the performance of new experiments a new correlation. These methods are often conservative as a precaution against the estimations involved.

- **Phenomenological or Integral models**
  These models simplify the essential physics and geometry behind a problem, thereby replacing the real system by an idealised one. This type of model is based much more on the actual physics behind a process than an empirical approach, but does not have the same
degree of complexity as computational fluid dynamics (CFD) models. Consequently, phenomenological models have much faster run times than CFD models. Although phenomenological models are based on the essential physics it is still necessary to calibrate certain parts of the model to account for the simplifications.

- **Computation Fluid Dynamics (CFD)**
  Computation Fluid Dynamic (CFD) modelling is based as closely as possible on the actual physics and the actual geometry and predicts the fluid flow. However, computer runtimes are, generally, very long (often taking may days [Fairweather and Woolley, 2009]) and the memory requirement is very high [Ledin, 2002]. CFD uses computational techniques to solve, numerically, a set of simultaneous differential equations that describe a system, which can not be solved analytically. CFD programs have three parts to them, a pre-processor, a solver and a post-processor. However, due to their complexity it takes, even an experienced user, considerable time to input all the data and parameters to set up the model before a solution can be attempted. For these reasons their use as a hazard assessment tool is limited, but their use in design is important. When undertaking a safety study, many assessments are needed to be carried out for different scenarios so a short runtime is important.

CFD is an all encompassing name which ranges from solving a partial differential equation (PDE) in one dimension to a much more complex set of PDEs in three dimensions and time. Although CFD codes are based as close as possible on the actual physics they remain approximations and, similar to phenomenological models, require empirical data to evaluate parameters contained with the PDEs. CFD codes that solve the full differential equations are called advanced models. If some simplification of the geometry is made, such as modelling processes that occur at a length scale less than the grid spacing rather than fully resolving the geometry by using a refined the grid, then the model is called a ‘simple’ CFD code.
There are various ways to approximate the PDEs for incorporation into a computer program, called the discretisation method. There are three discretisation techniques, finite difference (FD), finite volume (FV) and finite element (FE). A mesh or grid is defined where the discrete locations (nodal points) used for solving the discretised equations are defined. These can take different forms depending on the geometry and accuracy required at various locations. CFD codes provide a numerical answer at every nodal point of the mesh and such results are capable of visualising the progression of a process variable with time.

In this work it is engineering models that are the subject of investigation. An engineering model is defined as a model takes only minutes to run. These include empirical and phenomenological models described above, but in general not CFD codes. Engineering models are designed for commonly addressed hazard scenarios, enabling an assessment of the level of the hazard to be obtained quickly.

An engineering model encompasses many processes in its formulation, and thus these processes do not need to be addressed separately. The inputs for these type of models are much simpler, and usually adopt an idealised geometry to represent a complex scenario. Because of this, many assumptions have to be made and then the model is generally only applicable within these range of assumptions. The output is a parameter of interest but an engineering model is generally not capable of providing intermediate variables that may be provided by CFD codes.

2.5 Review of Existing Engineering Explosion Models

Here, a survey of available explosions models is presented for empirical and phenomenological models. The survey concentrated on engineering models and did not include CFD models, for the reasons given in Section 2.4, and because this fulfilled the scope of work defined for the safety work package of NATURALHY by Loughborough University. Some CFD modelling of
explosions was performed by Leeds University as part of the safety work package. Some comments on CFD models are noted in Section 2.5.4.

The Health and Safety Laboratory (HSL) Fire and Explosion science group recently produced a comprehensive document entitled “A Review of State-of-the-Art in Gas Explosion Modelling” [Ledin, 2002], which reviewed the current available models ranging from empirical to full CFD codes and the current accuracy of these models.

2.5.1 Empirical Models

2.5.1.1 TNT equivalency

The TNT equivalency model is an empirical model that was first introduced by Brasie and Simpson, 1968 [Lees, 2005, p17/154]. This model assumes that a gas explosion can be approximated by an explosion involving a high charge explosion of TNT. However, there are significant differences between gas and TNT explosions:

1. larger volume and extent of gas/air cloud,
2. lower overpressure at the centre of the gas/air explosions,
3. different shape, in the near field, of the blast wave, and
4. longer duration of the blast.

These differences become more significant as the gas explosion becomes weaker.

Briefly, the mass of TNT that is equivalent to the mass of fuel gas in the cloud must be determined. This involves determining a yield factor, and another factor to introduce the fact that many common hydrocarbon fuel gases have higher heats of combustion than TNT. A graph is then used to read off the peak overpressure with distance. There are various modifications to this model which reflect differing ways in which the yield factor is determined, and for differing graphical correlations, see Lees [2005, p17/156].
Many authors have cited concerns over the applicability of this model for gas explosions due to the difference in behaviour between gas and high charge explosions [van den berg, 1984]. In addition, the effect of geometric congestion on a gas explosion is not taken into account [Bjerketvedt et al., 1997]. Consequently, it is recommended that the TNT equivalency model is not used to simulate gas explosions.

2.5.1.2 **TNO multi-energy**

The TNO multi-energy method [van den Berg, 1985] is considered a better alternative to the TNT equivalency model [Mercx et al, 2000]. It can be used to estimate the blast from gas explosions with variable strength. The concept is based on the observation that the explosive potential of a vapour cloud is primarily determined by the congestion within the vapour cloud. That is, uncongested unconfined vapour clouds generate very little overpressure, but with increasing confinement and congestion the overpressure generated increases. The model uses graphs depicting pre-calculated numeric simulations of blast waves from centrally ignited spherical clouds, with constant velocity flames.

Two characteristics are needed by the model to apply the blast graphs, both of which can be difficult to determine sensibly [Ledin, 2002]; a charge size, which is the heat of combustion of the flammable mixture actually contributing to the blast; and a charge strength which represents the explosion overpressure produced, and is a number between 1 and 10, with 10 being a detonation. A combustion energy scaled distance is defined and used when reading the curves presented on the graphs. A non-dimensional maximum over-pressure and positive phase duration with scaled distance is read from the ten respective curves on the graphs.

It is often difficult to determine a sensible charge strength and charge size. There have been two projects, GAME [Eggen, 1998] (guidance on the application of the multi-energy method) and GAMES [Mercx et al, 1998] which investigated the practical application of the multi-energy method, providing
specific recommendations for the charge size and charge strength.

TNO also developed two other models preceding the above; the TNO shock wave model or Wiekema model and the TNO correlation model [Lees, 2005]. The Wiekema model uses the fact, that given the pressure-time profile, it is possible to derive the energy of an explosion [Strehlow et al. 1973]. The model inverts this result, using as an input the energy available to obtain the pressure time profile. Further, the TNO model estimates the radius of circles defining a particular level of damage.

### 2.5.1.3 Baker-Strehlow

This model was first developed by Baker, Tang, Scheier and Silva (1994) [Ledin, 2002] but later extended by Baker et al.[1998]. The model includes a number of steps to determine the blast pressures. The model is a combination of the blast (and impulse) curves of Strehlow's spherical model [Strehlow et al., 1979], in which the curves are based on the flame Mach number, and the TNO multi-energy method for determination of the source energy. The scaled distance is the same as in the TNO multi-energy method. To use the Baker-Strehlow curves requires the flame speed to be determined, and 27 combinations of fuel reactivity, confinement and obstacle density are presented to determine the flame Mach number. This is used to identify the curve to be used from the Strehlow et al. blast curves.

To assess a particular facility it is necessary to identify:

- the potential explosion sites (PES) where gas may accumulate and be ignited,
- fuel reactivity,
- confinement and
- congestion.

Ledin [2002] reports that the Baker-Strehlow model is fast and easy to use, takes into account basic geometric congestion and confinement, and can handle multiple ignition points. Ledin also concludes that the model tends be over conservative.
2.5.1.4 Shell CAM2

Shell Congestion Assessment Method (CAM) was first published by Cates and updated by Puttock [1995] to become version 2. This model is applicable to unconfined congested explosions of approximately cubic proportions of the congested region. The model was further extended by Puttock [1999] to include a smooth function\(^2\) for the source overpressure and this version is referred to as Shell CAM2. Shell CAM2 was the first model to estimate the source overpressure by using guidelines to include the layout of the site and the fuel type.

Shell CAM2 includes a decision tree to give a reference pressure [Puttock, 1995], which can then be multiplied by a fuel factor to include the effect of fuel type. A fuel factor of 1 is used for propane as this was the original basis for the model. The fuel factor is determined using fractal\(^3\) scaling theory of Taylor and Hirst [1998] and a table of factors for common fuels is presented. The last step is to use the given equations to calculate the pressure-distance curve away from the source congested region.

The original formulation of pressure decay is presented in [Puttock, 1995] but a new formulation is further presented [Puttock, 1999]. The original formulation is based on acoustic pressure decay (inverse distance law). However, it was found that beyond a certain distance the pressures predicted are higher than what is observed during experiments. This was attributed to the faster decay due to dissipation in a shock front that is formed. Puttock [1999] goes on to state that “if the multi-energy hypothesis were correct, then beyond the transition point the pressure at a given distance would be

---

\(^2\) A smooth function is defined as a function with derivatives that are continuous functions.

\(^3\) Fractal: a curve or geometric figure, each part of which has the same statistical character as the whole (Compact Oxford English Dictionary, 2002, Oxford University Press). A famous example is the Mandelbrot set.
independent of source pressure”. This can be seen in the multi-energy curves where they coincide after the transition point (curves of strength 6 and above).

In the absence of comprehensive pressure field measurements, CFD calculations were performed using a spherical piston with a prescribed velocity history to determine the free field pressure decay. This method is very similar to the TNO method which assumes a constant velocity piston but differs by using an accelerating piston with a prescribed velocity history. Puttock [1999] explains that, the constant velocity piston develops a shock sooner, so starting the more rapid pressure decay sooner than for a real source. Equations fitting the calculations are presented. In comparison with the TNO multi-energy method, the shape is similar but the faster decay starts later due to the more realistic piston behaviour. This method provides better predictions when overpressures of 1 bar or more are predicted at the source.

Puttock [1999] introduces a function for the source overpressure that gives a continuous values with the input variables. The source overpressure equation includes terms for the following: fuel scaling; number of rows of obstacles, spacing of the rows and the size of the obstacles in a row. The equation is then fitted to a database of hundreds of experiments carried out by Shell, TNO and as part of the European Commission funded project MERGE [Mercx, 1994]. An expression is also presented to provide a limit to the overpressures predicted by this expression, and this is called the Severity index. This prevents the predicted overpressures becoming excessively large (and unrealistic) and, when applied, provides a limit of about 8 bar to the source overpressure calculated. Mixtures of obstacles of different sizes are also accounted for through the obstacle complexity factor; this is a factor for each of four different ranges of obstacle sizes. In addition, allowance can be made for sharp edged obstacles.

Other parameters have been added, these are: high aspect ratio (long, narrow) areas of plant which are accounted for through an ‘effective’ length; guidance on detonation probability; partial filling; and non-central ignition.
2.5.2 Phenomenological Models

2.5.2.1 Shell SCOPE

The Shell Code for Overpressure Prediction in Gas-Explosions (SCOPE) which was developed for explosions in confined vented enclosures began with the work of Cates and Samuels [1991]. The model is now in its fourth version. Version 3 is described by Puttock et al. [2000].

The model takes an idealised environment in the form of a rectangular confined vented enclosure and solves a set of one dimensional differential equations describing the pressure. The enclosure contains a homogenous gas-air mixture and obstacles are represented as a series of grids normal to the main flow direction, the ignition is on the back wall of the enclosure at the opposite end to the vent. After ignition the flame front is modelled as being hemispherical in shape, initially expanding until the edge of the flame front reaches the walls of the enclosure.

The unburnt mass is monitored using expressions for its rate of consumption by the flame and its mass flow out through the vent. Self-acceleration of the flame is taken into account. Self acceleration occurs as the expanding laminar flame develops wrinkles in the flame front that increase the flame area and the rate of fuel consumption. Puttock et al. [2000] discuss the region in which self acceleration is applicable. This was achieved by analysing experimental results. Good agreement was found for methane by stopping self-acceleration after 3m of flame propagation from the point of ignition, and for propane after 2m of flame propagation. This occurs when the actual burning velocity reaches two and a half times the laminar burning velocity.

The turbulence model in SCOPE is semi-empirical. The turbulent burning velocity is expressed by a smooth transition between two turbulent burning velocity functions, one applicable at low turbulence intensity and another at high turbulence intensity. The turbulence level is calculated by an expression that is a function of the drag that a grid exerts on the incoming flow. The drag of a grid of obstacles depends on the drag coefficient of a cylinder (which
depends on the flow velocity and Reynolds number) and the blockage ratio. The model can also take into account sharp edged obstacles and takes into account grids with differing obstacle sizes through an ‘obstacle complexity’ factor.

The vent flow model is based on the equation for standard compressible vent flow [Richardson et al., 1999], and can handle side and rear venting configurations. However, no consideration of the distortion of the flame shape by the side vents is included in the model. Outside the enclosure SCOPE can predict the external explosion (as it keeps track of the mass of unburnt gas flowing through the vent), where the vapour cloud is idealised with a simple, symmetrical shape.

Gas information is stored in an electronic data file, and a separate method within the software can be used to generate new gas data files based on mixtures of gases. The model has been validated using over 300 experiments, carried out using vented enclosure of different volumes ranging from 2.5 m$^3$ to 550 m$^3$.

### 2.5.2.2 CLICHE

The CLICHE model was developed by British Gas Research and Technology Division (now known as GL Industrial Services, or GL for short). The CLICHE model is designed to model confined vented explosions and is an acronym for Confined Linked CHamber Explosion [Catlin, 1990]. CLICHE is based on earlier work of Fairweather and Vasey [1982], and Chippett [1984] but extends these methods to add the ability to model a series of linked chambers (rooms) [Ledin, 2002]. Pressure gradients occur as a result of the drag of obstacles on the flow field ahead of the flame.

The model applies the conservation laws to each chamber for mass and internal energy, assuming uniform properties within each chamber. Momentum changes are assumed to happen at the vent of adjacent chambers. Equations from each chamber form a system of ODEs which are computed numerically.
The model is interfaced with a detailed geometry database, such as may be used for a CFD simulation. CLICHE extracts the information it needs from this source. Of particular importance is the variation of area blockage along the path of the flame from the ignition source to the vent. A combustion model determines the mass burning rate of the flame and this describes the flame acceleration given the changing flame shape, obstacle drag and turbulence. CLICHE has a more sophisticated flame shape than the earlier work on which it is based which used analytical expressions. The flame area is computed numerically and includes effects of flame elongation and flame folding through obstacles. Since the flame area is calculated numerically it enables a variety of ignition positions to be modelled. Turbulence levels are calculated using the mean flow velocity of the unburnt gas through obstacles ahead of the flame to determine the characteristics of the wake [Catlin, 1990].

The laminar burning velocity is described by a correlation which is a function of flame radius. Turbulent burning is taken into account using a correlation, based on dimensionless groups, which has been calibrated against many experimental measurements. The model assumes the laminar flamelet concept and takes into account quenching of flamelets by the strain field.

There is a separate model for the external explosion of vented fuel based on observations of Catlin [1991]. Catlin found that the external explosion depends on the magnitude and history of the flame exit velocity.

### 2.5.2.3 GL’s compact explosion model

This model is described by Cleaver and Robinson [1996] and Cleaver et al. [1997] of GL Industrial Services (formerly Advantica and British Gas Research and Technology Division). The model is designed to provide predictions for compact congested geometries.

The compact explosion model was developed for cubic congested geometries and validated against the EC funded MERGE (Modelling and Experimental
Research into Gas Explosions) experiments [Cleaver and Robinson 1996]. The approach taken was similar to Deshaies and Leyer [1981] where the flow is assumed to be incompressible and the flame represents a piston. This results in a non-dimensional algebraic equation relating the overpressure at the flame front to the flame velocity history (which includes the effect of geometry) and thermodynamic properties of the gas.

The model uses incompressible one-dimensional conservation of mass and momentum. The drag force is also included. To use this model the flame speed history (profile) is needed. In the second paper Cleaver et al. [1997] presents a non-dimensional flame speed profile correlation for the specified geometry produced from analysis of the MERGE experiments. To use this correlation a maximum attained flame speed is needed and this is calculated through a correlation, whereby the effects of fuel reactivity and congestion are introduced. The effect of congestion on the production of turbulence and hence flame speed is embodied in the correlation. It can sometimes be difficult to determine a flame speed, as the speed on any part of the flame surface may be different to other parts thereby distorting the shape of the flame surface. In extreme cases different parts of the flame may be moving in the same general direction but at vastly different speeds making any one flame speed value difficult to apply.

A predictive method for the blast wave is presented by Cleaver et al. [1997]. They argue that a general pressure wave can be described by the relationships used to describe the propagation of a shock wave in still air. This methodology does not make any assumptions about the shape of the pressure wave from the explosion source. It also, correctly, predicts the ‘shocking up’ of a wave form as it propagates away from the source.

The implementation of this model is achieved in three stages. Firstly, a flame speed profile must be determined using a correlation as described above. Secondly, the flame speed profile is used within the source overpressure model to predict the pressure history (with time) at the flame front. Thirdly, the
source overpressure is used to predict the propagation of the pressure waveform away from the region in free space.

2.5.2.4  **GL HAREM**

This model extends GL’s compact explosion model (see previous section) for geometries that have high aspect ratios, that is, regions where one direction is much longer (five times) than the other two [Humphreys, 1999; Humphreys, 2000]. HAREM is an acronym of High Aspect Ratio Explosion Model. The congestion is assumed to be ideal, that is the congestion can be simulated using regular arrays of obstacles.

For the different geometry used in HAREM a different flame speed correlation to that used in the compact explosion model is presented. This correlation is again non-dimensional and describes the shape of the flame speed profile through the congested region. The HAREM model assumes that the flame speed achieves a maximum speed that remains constant through the remainder of the congested region. (GL found that using an experimental velocity history profile, where the flame speed continuously changes between grids, did not improve the overpressure predictions). Another parameter is introduced into the HAREM model which is the acceleration distance, or the distance the flame speed takes to reach the maximum flame speed. A new correlation for the maximum flame speed and acceleration distance is also used.

The source overpressure model used in HAREM is also modified from the form described in the compact explosion model. Unlike the spherical geometry where the flow can be reduced to a one dimensional problem (as was done in the compact explosion model), the fluid flow in this geometry is not completely planar or spherical. The GL Technical Report states that the pressure drop will be of a similar form to the spherical case, as in the compact explosion model. The Technical Report presents an extended version of the compact explosion model overpressure model with additional factors and powers to take into account the geometry.
The blast wave decay model used in HAREM is the same as used in the compact explosion model.

2.5.3 Other models

Dorofeev [2006] presents a model to predict the acceleration of a flame through unconfined congestion, taking into account the flame size including the effects of: flame folding; the laminar burning velocity; expansion ratio; and turbulent burning velocity. The author presents an argument for changing the expansion ratio as a way of accounting for loss of push from thermal expansion because burnt products are being vented. The model was compared with data from experiments involving different hydrocarbons and data from hydrogen explosion experiments [Molkov et al., 2005] and good agreement was found.

Tite [2002] presents some predictive methods for determining the overpressure generated in confined vented and completely confined enclosures without congestion. The methods presented are closely linked to the experimental configuration upon which they are based. As the explosion progresses there are various features that can be found in the pressure-time traces depending on the position of the flame and whether or not the enclosure has failed allowing venting. There are up to four discernable stages. The methods presented by Tite each predict one of the maximum values of a particular pressure trace feature. The models were developed prior to the 1980’s, and nowadays improved models exist, for example GL’s CLICHE and Shell’s SCOPE.

2.5.4 Note on CFD models

Although outside the scope of this thesis, it should be noted that there are a number of CFD models which have been developed for predicting gas explosion events.
Well known examples of ‘simple’ CFD codes (see Section 2.4) include EXSIM (Tel-Tek, Norway and Shell Global Solutions, UK), FLACS (http://www.gexcon.com/) and AutoReaGas (originally Century Dynamics Ltd. and TNO, now trademark ANSYS, http://www.ansys.com/) [Ledin, 2002]. Generally these codes do not fully resolve the geometry and small scale obstacles are not fully described. Instead the turbulence generated by such small scale obstacles is accounted for by the so called Porosity/Distributed Resistance (or PDR) method, which represents the obstacles by a volume porosity, area porosity and a drag coefficient which feeds in the k-ε turbulence model. These kind of CFD codes also tend to have fixed cell sizes for computation which can lead to problems in the reaction zone if the cells are not small enough. This can also result in grid independence issues.

Advanced CFD codes include CFX-4 (now CFX, http://www.ansys.com/), COBRA (Mantis Numerics Ltd.), NEWT (Engineering Department of Cambridge University) and REACFLOW (Joint Research Centre of the European Union in Ispra, Italy) which use adaptive meshes or automatic grid refinement methods to allow more accurate description of the geometry and the reaction zone to be assessed in more detail. Some codes have also improved on the k-ε turbulence model, by various methods. CFX-4 includes a Reynolds Stress turbulence model.

As part of NATURALHY project safety work package Leeds University have been developing and using the COBRA CFD code for confined vented and vapour cloud explosions. A Reynolds Stress turbulence model was incorporated within COBRA as part of this work and found to perform significantly better than the k- ε approach in cases of high turbulence [Fairweather and Woolley, 2008; Fairweather and Woolley, 2009].

Another CFD code is called OPENFOAM (http://www.openfoam.com/) which is an open source project providing the code openly to any user. OPENFOAM contains many solvers and sub models that can be used in a modular fashion and is open to extension and development. Bauwens et al. [2010] have used
OPENFOAM to perform numerical simulations of vented confined explosions with good results.

2.6  **Assessment of Explosion Predictions by Comparison with Experimental Data**

When comparing predictions of explosion behaviour (especially maximum overpressure) with experimental data, two factors must be considered. Firstly, the variability of measured maximum overpressure from apparently identical explosions and secondly the degree of accuracy realistically expected from explosion models.

2.6.1  **Variability of explosions and the analysis of pressure data from explosion experiments**

Measurements of overpressures generated during explosions often include short duration spikes which can give a misleading representation of the true overpressure and such short duration variations are not applicable to structural response [Shearer et al., 2000]. For this reason, it is usual to apply some form of rolling average to the pressure traces generated during explosion experiments typically of the order 0.1-1.5 ms [Lowesmith, 2007; Lowesmith, 2008; Evans et al., 1999; Selby and Burgan, 1998]. This then allows a more realistic comparison of measured and predicted maximum overpressures.

Evans et al. [1999] reported a series of nominally identical explosion experiments in order to assess the repeatability of the measured values of pressure at a number of locations throughout a test rig, representing an offshore module at full scale. In this case, a 1.5 ms rolling average was applied to the pressure traces prior to identification of the maximum overpressure at each measurement location. The variability of the pressure measurements at each location across 5 or 6 nominally identical experiments was quantified by statistical analysis. It was found that significant variation can
be expected and that the variation in peak pressure at an individual location
could vary between 0.71 and 1.41 of the mean value across the series of
experiments (based on encompassing 90% of the data). Furthermore, this
variability was not random, that is to say, if the pressure was higher at a
particular location during one experiment, then it would tend to be higher at all
locations for that experiment.

The experiments discussed above involved a very large test rig with a
complex mix of confinement and congestion of varying sizes and shapes. The
resulting flame speeds and overpressures were high (typically more than 1
bar). The variability of overpressure during less severe explosion events is
expected to be less. Analysis of two pairs of similar (although not identical)
experiments conducted within the NATURALHY project support this view
[Lowesmith, 2008]. Performing a statistical analysis in the same manner as
Evans et al. [1999] on a pair of experiments which involved a high speed
flame and high overpressures, the variation of peak pressure was between
0.65 and 1.54 of the mean, which not dissimilar to the findings of Evans et al.
[1999]. However, for a pair of similar experiments involving a lower speed,
lower overpressure explosion, the variation was 0.82 to 1.22.

The conclusion is that some significant variation in overpressure can be
experienced from apparently identical explosion events, especially when high
speed flames, and hence high overpressures are generated. This will be a
factor when assessing the predictive capabilities of an explosion model.
Ideally predictions should be conservative and allow for the potential natural
variability in the explosion event itself.

2.6.2 Predictive capability of explosion models

A study of the predictive capability of explosions models, both CFD and
phenomenological, [Selby and Burgan, 1998] showed that significant
differences between predictions and data can also be expected. It is
noteworthy that the criteria used to assess model performance was the ability
to predict within a factor of 2 (or 0.5) of the measured value, and that neither
CFD nor simpler models showed a clear predictive accuracy. Also, CFD models did not perform any better than the simpler models. Indeed, predictions from CFD models were found to show significant variation when only minor changes were made to the input data.

Newer work [Ledin, 2002] reviewing the predictive performance of a range of available empirical and phenomenological models suggests that the predictions of phenomenological and CFD models are “generally fairly good (to within a factor of two)” from the experimental observations, again confirming that this criteria is realistic for the assessment of explosion models. The authors also state that “small changes, or inaccuracies in the representation of the geometry, can lead to over predictions in one case and under predictions (or vice versa) when the geometry changes have been implemented”.

The developers of the widely used CFD codes FLACS state that they are content if the predictions are within +30% of experimental data whilst considering them acceptable if within a factor of two [Ledin, 2002].

The accuracy of predictions is also complicated by the fact that they are generally tuned to the experiments against which they are validated against, and when used for ‘blind’ predictions for a new situation the accuracy of the predicted results reduce [Selby and Burgan, 1998].

To conclude, predictions of overpressure can be considered satisfactory if within a factor of two of experimental observations. Ideally predictions should be conservative, so within 100% and 200% of measured values is preferred. Such an approach would also encompass the variability of the actual data itself when limited large scale data is available.

### 2.7 Factors to consider when modelling explosions

In this section some of the key parameters which need to be considered when modelling explosions are identified. How these parameters are addressed
within the explosion models may affect the ability of the model to be used to predict explosions involving natural gas/hydrogen mixtures, since the model may have been developed based on empirical correlation from experiments involving natural gas. The factors considered below are:

- Initial conditions (prior to ignition);
- Laminar and turbulent burning characteristics;
- Flame stretch and instability;
- Flame acceleration by obstacles;
- Potential for transition to detonation.

### 2.7.1 Initial Conditions

The initial conditions prior to an explosion, that is to say, the nature and extent of the gas/air mixture, can affect the severity of an explosion. Within this study and generally for the purposes of risk assessment, a uniform, (usually close to stoichiometric) concentration gas/air mixture is assumed to exist throughout the entire geometry being considered, as this will generate the worst case, highest overpressure. If the gas/air accumulation is smaller in volume, not close to stoichiometric or non-uniform, the overpressures will tend to be lower [Johnson and Cleaver, 2002]. A reduced volume results in lower overpressures due to scale effects and a non-uniform or lean or rich gas/air mixture will produce a lower flame speed and hence lower overpressures.

In real situations, the gas/air accumulation formed (in particular its extent and concentration) is affected by the degree and nature of the ventilation to the region where the gas/air mixture is forming, which in turn is related to the ambient wind speed. In low ventilation situations, the buoyancy of the gas may also affect the location and concentration of the gas/air accumulation and buoyancy induced ventilation may contribute to lowering gas concentrations [Lowesmith et al., 2009; Tite, 2001].

In some circumstances, with low wind speeds (<3 m s⁻¹) the atmospheric conditions can affect the formation of the gas/air mixture. Pasquill atmospheric
stability criteria define the variation in the temperature gradient of the atmosphere close to the ground [Pasquill, 1968] which can then either assist or hinder the dispersal of the gas.

Once ignition occurs, any influence of atmospheric conditions is negligible. Indeed, Evans et al. [1999] showed that during a series of seemingly identical large scale explosion experiments, although there was significant variation in the results, no correlation with air temperature, relative humidity or ambient air pressure was found. Furthermore, the EC funded project EMERGE [Mercx, 1997] conducted vapour cloud explosion experiments where the gas/air accumulation was subjected to a region of high turbulence (considerably more than would be generated by wind turbulence or atmospheric stability considerations) and found that, overall, the explosion overpressures were not significantly affected.

It is therefore concluded that, although atmospheric conditions can affect the location, extent and concentration of the gas/air accumulation (which in turn affects the overpressure generated following ignition), for a given gas/air mixture, the atmospheric conditions do not affect the explosion event following ignition or the resulting overpressures generated.

### 2.7.2 Laminar and Turbulent Burning

#### 2.7.2.1 Laminar Burning

It is necessary to determine the speed with which a flame propagates through a homogeneous flammable mixture. The flame propagation can be broken into two distinct categories, laminar burning, and turbulent burning. For any state, there exists a speed of propagation that depends on the local flow conditions. The actual burning velocity is a measure of the velocity with which the flame burns into the fresh un-burnt mixture.

The laminar burning velocity can be determined experimentally or by theoretical and computational means. To model fundamentally the combustion
process, the intermediate reactions need to be known. Modern theory and computation allows the conservation equation to be solved for all the intermediate reactions to provide solutions for the independent variables such as volume fraction of species, temperature through the flame and laminar burning velocity. This can be done using software such as Sandia Laboratories Chemkin code (now licensed to Reaction Design Software). However, this method is time consuming [Kuo, 2005]. Also chemical kinetics is itself a research field that is continually evolving more accurate solutions.

The laminar burning velocity represents the reactivity of a mixture; more reactive substances have a faster rate of reaction and a higher laminar burning velocity. Indeed, it was found by theory in the 19th century that the laminar burning velocity, \( u_i \), is dependent on the square root of the product of thermal diffusivity, \( \alpha \), and reaction rate, \((RR)_T\), [Kuo, 2005],

\[
\begin{align*}
u_i \propto \sqrt{\alpha (RR)_T} \\
(2-1)
\end{align*}
\]

Many parameters affect the value of the laminar burning velocity, including the type of fuel and its reactivity, the quantity of fuel, the oxidiser, and the initial pressure and temperature.

Conveniently, it is possible to correlate the laminar burning velocity against the equivalence ratio for fixed initial conditions (pressure and temperature). The equivalence ratio, \( \Phi \), is an important parameter and is defined as, the ratio of the number of moles of fuel (F) to oxidiser (O) in the fuel-air mixture over the ratio of fuel to oxidiser required for complete combustion (or stoichiometric conditions),

\[
\Phi = \frac{\left(\frac{F}{O}\right)}{\left(\frac{F}{O}\right)_{stoich}}
\]

Once a correlation has been obtained for particular values of pressure and temperature, further correlations can be found to account for changes in the laminar burning velocity for different values of pressure and initial
temperatures, see for example Metghalchi and Keck [1982] and later in Section 3.3.

*Flame speed*

The flame speed is the speed at which the flame front, or flame surface, propagates with respect to a fixed observer. The burning velocity is constant for the given equivalence ratio, fuel and state, but the flame speed can be affected by flame area which can change due to instability and stretching and strain effects. It can be calculated phenomenologically from the laminar burning velocity (assumed constant over the flame surface), the expansion factor and the area correction factor [Harris, 1993]. As a flame propagates, the fresh mixture is burnt and thus its temperature increases, causing thermal expansion to occur which has the effect of pushing the flame front thereby increasing its speed. The (volume) expansion factor is calculated as the ratio between the density of fresh and burnt gases.

The flame area has an important effect on the flame speed since an increase in flame area means a larger surface area for combustion to take place and hence an increase in the rate at which unburnt gases are consumed. A propagating flame can exhibit ‘wrinkles’ on its surface leading to an increased flame area and combustion rate. This makes calculating the flame surface area difficult [Harris, 1993].

2.7.2.2 *Turbulent Burning*

The turbulent burning velocity is much more difficult to define and measure. Many flows are turbulent, in which flow properties are unsteady and seem to vary chaotically. There also exists a region between laminar flow and fully turbulent flow called the transition region which is also an important flow regime [Versteeg and Malalasekera, 1995]. Turbulence begins to develop after a certain Reynolds number is reached. The Reynolds number is an important parameter and is defined as the ratio of the inertia forces to the viscous forces.
Turbulence is a three dimensional process, and due to the chaotic nature of turbulence an accurate calculation of the flow is computationally very expensive. CFD can be employed to directly solve the conservation equations, and is the most computationally intensive. Turbulence models are frequently used to try and introduce turbulence into the conservation equations by including extra partial differential equations to close the system. One of the most well known turbulence models is the k-ε model [Versteeg and Malalasekera, 2007]. There is no complete model that describes all the features of turbulence, many models have deficiencies that are known and models are often applied to specific situations.

In turbulent flows, there exist important length and time scales. Turbulent energy is contained in areas of random and swirling motion called eddies. The energy is transferred to smaller and smaller eddies in an energy cascade until, at the smallest scale, the eddies are dissipated by the damping effect of viscosity. There are three important length scales; the integral scale which represents the scale of the largest energy containing eddies; the Taylor microscale where eddies become affected by viscous forces, and the Kolmogorov microscale where the eddies start to dissipate due to the viscosity of the fluid.

Turbulence increases the mixing of heat, mass and momentum, effectively increasing the corresponding diffusion coefficients. This increases the speed of propagation of the flame [Kuo, 1986, p405]. There are various approaches to modelling turbulence and its effects. Currently, there is no model that gives good predictions over a wide range of conditions,

Turbulent premixed flames can be characterised by their apparent behaviour and can be represented by the Borghi diagram [Warnatz et al., 2001]. The diagram is a plot of the ratio of turbulence intensity to laminar flame speed against the ratio of the integral length scale to the laminar flame thickness. The plot is divided into different regions representing laminar flames, wrinkled flames, torn flames, island formation of the flame and ideally stirred reactor.
This can be important to know as some models are specific to a particular mode found on the diagram. Peters [2000] also presents a similar diagram.

**Approaches to Turbulent Burning**

What is important is how turbulence affects the flame speed, which will then affect the overpressures generated. Damköhler [Lewis and von Elbe, 1961; Warnatz et al., 2001] was the first to propose effects that turbulence has on the burning velocity. He proposed that, if the turbulence is of fine scale, the eddy size and mixing length are smaller than the flame thickness, and the effect of the these small eddies is to enhance the transport processes in the flame. He also proposed that, if the eddies are much larger than the flame thickness, then an increase in the flame velocity is caused by an increase in the flame area (the turbulent flame area) by the eddies distorting the laminar flame. It is possible in very turbulent flows that the flame may extinguish, this is called quenching.

The laminar flamelet model describes a turbulent flame as an ensemble of laminar flame sheets in a turbulent flow [Peters, 2000] that are undergoing stretching (strain and curvature) effects (see also Section 2.7.3). A correlation for turbulent burning velocity in terms of flame stretch is presented by Bray [1990] which is valid for Lewis numbers below 1.3. The Lewis number is a dimensionless number defined as the ratio of thermal diffusivity to mass diffusivity, it is used to characterize fluid flows where there is simultaneous heat and mass transfer by convection. The correlation is based on over 1600 experiments. This was further extended by Bradley et al. [1992] to include the Lewis number in the correlation, as the stretching mechanism is influenced by the Lewis number. It is difficult to measure turbulent burning velocities accurately and there is significant scatter in the correlations.

The SCOPE (version 3) model from Shell [Puttock et al., 2000] uses two correlations, one for low turbulence and one for high turbulence with a relationship that provides a smooth transition between the two. They performed a new fit on the correlations given by Bray [1990] and Bradley et al. [1992] to extend to larger length scales and higher Reynolds numbers, than
are found in laboratory experiments but that are present in large scale explosions. The new fit includes the Karlovitz number (Equation (2-4)) and the Markstein number (Equation (2-6)) which replaces the Lewis number in Bradley et al. It is noted by Peters [2000] that turbulence at high Reynolds number is intermittent and this will cause local flow variations with time and thus the local turbulent burning velocity will vary.

Some models for turbulent burning velocity have been based on fractals representing the wrinkled geometry of a flames surface [Gulder, 1990]. These models only work for low turbulence where the scale of turbulence has the effect of increasing the diffusion coefficients and wrinkling the flame surface. The concept uses fractal methodologies to calculate the wrinkled flame area for the cross sectional area of the flow. This gives, as suggested originally by Damkolher, the ratio of turbulent flame area to cross sectional area, which can be used to determine the ratio of turbulent flame velocity to laminar flame velocity. The predictions of models of this type agree well with experimental data for low turbulent intensities.

At high turbulence levels the effect of turbulence is to distort the flame front rather than increase the diffusion processes. A flame in which high turbulence levels exist has high levels of flame stretch which can lead to (localised) quenching.

It is important to assess the level of turbulence present or generated by obstacles, to determine the turbulent burning velocity. Furthermore, it is important to note that turbulence levels may vary from place to place. Also, unless constantly generated, turbulent eddies will eventually decay through the energy cascade and viscous dissipation. The effect of obstacles is considered further in Section 2.7.4.
2.7.3 Stretch and Instability

Stretch
A flame propagating into a non-uniform and unsteady flow field is subjected to strain and curvature effects leading to a change in the flame area and thickness [Kuo, 2005, p471]. A stretched flame can have a reduced flame thickness and flame speed. Karlovitz and Markstein initiated the study of stretched flames and showed that aerodynamic stretching and preferential diffusion causes instabilities in the flame front. It can be applied to flame stabilization, determining laminar flame speed, flammability and turbulent flame modelling. It can be manifested as curvature and aerodynamic strain.

The flame stretch factor, $\kappa (s^{-1})$, is defined as the relative rate of change of flame surface area, $A_F (m^2)$, with time, $t (s)$,

$$\kappa = \frac{1}{A_F} \frac{dA_F}{dt} \quad (2-3)$$

The flame stretch factor takes into account the change of flame surface area due to flame strain and curvature. The Karlovitz number [Kuo, 2005], $Ka$, is a dimensionless stretch factor, it is calculated by the following expression,

$$Ka = \frac{\delta_{L_0}}{S_{L_0}} \kappa \quad (2-4)$$

where $\delta_{L_0}$ is the flame thickness and the subscript $\theta$ means the value at unstretched conditions, and $S_{L_0}$ is the unstretched flame speed. The flame thickness is a measure of the scale over which diffusion of mass and heat occurs.

As the flame velocity, $S_L$, is affected by flame stretch, it was found that this effect can be quantified by a linear relationship between the unstretched flame speed, $S_{L_0}$, and stretch factor, $\kappa$, [Tseng et al., 1993],

$$S_L = S_{L_0} - L\kappa \quad (2-5)$$

The Markstein length, $L$ (m), is the constant of proportionality for the flame stretch factor; it is a measure of the response of the flame to stretch. Negative values of $L$ increase the flame speed and the flame is said to be unstable, while positive numbers decrease the flame speed and stabilise the flame. The
Markstein length is determined from experimental measurements. It has been shown to be independent of whether the flame stretch is manifested as strain or curvature [Kuo, 2005]. The stretch parameters can be decomposed into values for strain and for curvature [Gu et al., 2000].

The Markstein number, $Ma$, is a dimensionless number and represents the sensitivity of laminar burning velocities to flame stretch. It is defined as the Markstein length divided by the characteristic (unstretched) flame thickness, [Halter et al., 2005],

$$Ma = \frac{L}{\delta_L}$$  \hspace{1cm} (2-6)

The flame thickness, in this work, is defined as [Gu et al., 2000],

$$\delta_L = \frac{\nu}{u_f}$$  \hspace{1cm} (2-7)

where $\nu$ is the kinematic viscosity. Other author’s have different definitions of the flame thickness (e.g. Halter et al. [2005], Tseng et al. [1993]).

There is a linear relationship between the stretched laminar flame speed, and the Karlovitz ($Ka$) and Markstein ($Ma$) numbers [Tseng et al., 1993; Kuo, 2005],

$$\frac{S_{L0}}{S_L} = 1 + MaKa$$  \hspace{1cm} (2-8)

The Markstein number as a function of equivalence ratio can be correlated as a straight line, although with a degree of scatter.

**Instability**

The Lewis number of a flame describes the importance of thermal diffusion to mass diffusion across the reaction zone, it is a dimensionless number defined as the ratio of thermal diffusivity to mass diffusivity. It is used to characterize fluid flows where there is simultaneous heat and mass transfer by convection. The Lewis number is assumed unity in many analyses as it represents the equality of flux of energy due to diffusion of fuel molecules and the equal, but opposite, flux due to thermal conduction [Bradley et al., 1992]; this leads to a constant enthalpy flame.
As a flame progresses, a number of instabilities can develop altering the shape of the flame and the alteration of the flame speed. These instabilities can be hydrodynamic and thermo-diffusive [Clarke, 2002], the results of these effects depend on the Lewis number, being greatest when the Lewis number is not equal to one. Thermo-diffusive effects arise from the preferential diffusion of reactants over thermal transport leading to an increase in flame area and wrinkling [Marley and Roberts, 2005] and seen a cellular structure on the flame surface developing.

2.7.4 Flame Acceleration by Obstacles

A flame is heavily influenced by the flow conditions it passes through. Under some circumstance the flame speed can reach orders of magnitude higher than in its laminar un-perturbed state. Factors that affect the flame speed include the ignition source, flow instability, and turbulence in the flow field.

Immediately after ignition the flame development is transient and may be influenced by the ignition source. After some time the influence of the ignition source may have dissipated, and propagation depends on the prevailing flow conditions. From a low-energy spark (point ignition) the flame surface will propagate out spherically increasing in speed until it reaches a steady state, assuming a quiescent (at rest) atmosphere. Actually what can be found to happen is that wrinkling in the flame surface occurs even in laminar flow [Puttock et al., 2000] caused by hydrodynamic and diffusive-thermal instabilities [Mercx et al., 1995].

It is also well known that congestion (obstacles) in the path of a flame creates turbulence which causes the flame to accelerate, [eg. Mashri et al., 2000]. In unconfined explosions it is obstacle congestion that creates the turbulence that causes the flame acceleration that leads to high flame speeds and significant overpressure. As a flame propagates the gas ahead of the flame is pushed forward. If this flow encounters any solid body the turbulent intensity can increase in the wake created by the body (turbulence may already be
present in the flow ahead of the flame). The turbulence may decay by viscous forces but if other obstacles are encountered the turbulent intensity may keep increasing, leading to large increases in the burning velocity and thus the flame speed. Obstacles also have the effect of distorting the flame surface, which normally increase the surface area. This has the effect of increasing the mass burning rate of the flame which also may increase flame speed [Moen et al., 1980]. Other important parameters are the size of the obstacles, their shape/profile, their spacing from other obstacles in the same grid, and the spacing of the grids.

Obstacles and congestion cause increases in the flame speed, however outside congested regions the flame may slow down as turbulence decays (assuming a deflagration). Consideration of the gas and likely scenarios can lead to the design of a safe separation distance between two areas of plant (that is two areas of congestion). This can prevent the flame reaching too high a speed and hence too high an overpressure.

When gas accumulations occur in regions where there are pipes and structural supports, these areas of congestion are very important to the severity of an explosion which may result. A good description of the geometry of the obstacles is needed to give good predictions. However, the geometry is often idealised within models due to its complexity. This means that the scenario is analysed to obtain either parameters that represent the whole volume, or represent a series of grids within the volume where local average properties can be defined.

As fluid flows relative to a solid body the solid body exerts a force on the oncoming flow caused by viscous action, this resistive force is called drag. The drag is composed of pressure and friction (surface) drag. There is an associated dimensionless coefficient, the drag coefficient which is a function of the flow Reynolds number and obstacle shape. The point of separation is the point on the surface of solid body where the boundary layer separates from the surface. This is important, as in the ‘wake’ of the object, or behind the point of separation, large turbulent eddies are formed. The influence of the
The turbulent wake of an object depends on how fast the eddies are dissipated by viscous forces and how far downstream the turbulence exists.

The cascade of turbulent energy from the largest eddies to many small eddies, ending in complete dissipation, can be described as an energy spectrum. Thus to determine the distance required for eddies to dissipate it is necessary to determine when the large eddies are eventually dissipated which corresponds to when the turbulent kinetic energy has dissipated. The decay of turbulent kinetic energy can be determined phenomenologically, based on the turbulent energy spectrum [Skrbek and Stalp, 2000] as original considered by Kolmogorov in 1941.

Changing the size and shape of an obstacle may increase the drag and the turbulence generated, thus increasing the flame speed. If there are many obstacles then their location relative to each other is important [Bjerketvedt et al., 1997]. For example, as a flame travels through a congested region consisting of regular arrays of pipes arranged normal to the path of the flame (sometimes referred to as a pipe-rack), then ‘fingering’ occurs, that is, between the pipes is the only place for the flame to propagate resulting in ‘jets’ of flame thereby increasing the flame surface area. If the following pipe array has the same configuration then these flame ‘fingers’ will pass between the pipes in the next array. If the pipes in adjacent arrays are staggered, then these flame ‘fingers’ will interact more effectively with the obstacle and the process of turbulence generation is enhanced, increasing more rapidly the flame area thereby accelerating the flame and increasing the overpressures.

The SCOPE model of Shell [Puttock et al., 2000] calculates the turbulence generated by a grid of obstacles by taking generation to be proportional to the product of the square root of the grid drag coefficient and the gas flow velocity through the grid. To take into account the fingering mechanism of the flame front, the authors used a CFD package to simulate the behaviour of the flame as it passed through an obstacle grid, and drew a simple correlation from the results. The model can also deal with staggered or offset obstacle grids, this is
termed obstacle complexity. It takes account of this effect by increasing the flame area.

### 2.7.4.1 Grids

Generation of nearly isotropic (uniform in all directions) turbulence can be achieved by placing a regular grid perpendicular to the flow stream. A grid is a regular structure of solid boundaries, such as a sequence of pipes of the same size and spacing between them. They may also be called tube bundles or even rod screens. Work has been done on the behaviour of flow through grids [Roach, 1987]. When flow passes through a grid there is a pressure drop across the grid, and turbulence is generated downstream.

As fluid flows through a screen a (static) pressure drop occurs, resulting in a drag force on the screen. The drag force [Blevins 1984, pp309], $F_d$, is related to the pressure drop across the screen, $p_1-p_2$ (pressure upstream - pressure downstream), and the area of the screen, $A_s$,

$$F_d = (p_1-p_2)A_s \quad (2-9)$$

An important dimensionless number is associated with grids and this is the porosity or area blockage ratio, $\beta$, defined as the ratio of the area available for fluid to or flow through over the total area. The velocity through a screen, $U_m$, is always higher then the incoming velocity, $U$, for incompressible flow this can be written as,

$$U_m = U/\beta \quad (2-10)$$

There is an expression to calculate the pressure loss across a screen

$$\frac{p_1 - p_2}{1/2 \rho U^2} = K(\beta, Re) \quad (2-11)$$

where $\rho$ is the fluid density, $\beta$ is the porosity, $Re$ is the Reynolds number, and $K$ is a function of porosity and Reynolds number. For turbulent flows $K$ is mostly independent of Reynolds number. Tables of values of the pressure loss function, $K$, for some common screens can be found in Table 10-17 Blevins [1984, pp314]. As the flow through a screen approaches the speed of sound the effect of compressibility increases the pressure loss.
Roach [1984] presents correlations to determine the turbulent intensity downstream of a grid, and the length scales involved.

### 2.7.4.2 Potential for Transition to Detonation

Up to now the discussion on explosions has been concerned with subsonic explosions called deflagrations. There is an even more potent explosion mode called detonation, were the combustion front propagates at supersonic speed. Once initiated the flame will propagate at a constant speed which can be estimated by calculating the Chapman-Jouget (C-J) detonation velocity [Kuo, 2005]. A deflagration to detonation transition (DDT) can occur when the flame accelerates up to the local speed of sound in the mixture resulting in a shock wave ahead of the flame. This can be achieved by turbulence increasing the flame speed which increases the turbulence which increases the flame speed further. A shock wave acts as a piston compressing the gas and thus raising its temperature. Once the temperature has reached the auto ignition temperature (AIT) of the mixture, it auto ignites forming a detonation wave [James, 2001]. Furthermore, similar to flammability limits, detonation can only occur between a lower and upper gas concentration, these detonation limits are subject to variations due to experimental configurations [Kuo, 2005].

Hydrogen is known to readily detonate, whereas it is practically impossible to detonate methane. However, the relative difficulty of detonation of a mixture of methane and hydrogen is unknown. Recent experimental work by Chaumeix et al. [2007] showed that by adding up to 60% methane to hydrogen resulted in detonation but the methane has an inhibiting effect. For instance the detonation speed fell from 2551 m/s for 100% hydrogen to 2180 m/s for a 40% hydrogen 60% methane mixture, both at an equivalence ratio of 0.75. The detonation cell size was also observed to increase.

The modelling of the transition between a deflagration and a detonation is extremely complex and outside the limits of the engineering models being studied here which are all based on deflagration. However, awareness of the
potential for a transition to detonation must be borne in mind for natural gas/hydrogen mixtures in cases where models predict high flame speeds.

### 2.8 Properties of Natural Gas and Hydrogen

The properties of hydrogen relating to its combustion and its interaction with materials differ significantly to those of natural gas. Therefore, adding hydrogen to natural gas may have a significant impact on the hazard the mixture presents compared to natural gas alone. The mixture which has been called “Hydrothane” by [Abdel-Aala et al., 2005], may prove to be much more hazardous, perhaps by increasing the likelihood of accidental release, or by increasing the damage caused by a fire or explosion.

Hydrogen is the lightest element and its properties are significantly different to gases that are commonly used. Over the centuries since the industrial revolution hydrocarbon based fuels have been used and their properties are understood. However, hydrogen has not been widely studied in the context of its use as an energy carrier and very little work has been undertaken on mixtures of methane and hydrogen. The basic properties of hydrogen [Abdel-Aala et al., 2005] are given below:

- Least dense of all the elements, it is the lightest element making it very buoyant meaning that, after release into the atmosphere it will rise faster than other gases
- Diffuses quicker than other gases
- Colourless, odourless and non-toxic
- Flammability range is wide (4 - 75 %/v/v)
- Ignition energy is very low (0.02 mJ)
- Burning velocity is highest of any gas
- Detonation is known to be possible

Some of these properties may indicate that hydrogen may be more hazardous than natural gas. It may appear that incidents involving hydrogen might be more likely than with other gases. However, some of the properties of
hydrogen may work in its favour. Drawing on experience from the aerospace industry, it has been suggested [Carcassi and Fineschi, 2005] that hydrogen could be safer than methane: “its deflagration can always be mitigated, if not prevented, and detonation can certainly be avoided”. Hydrogen has a low ignition energy compared with methane increasing the probability of ignition, much wider flammability limits again increasing the probability of ignition. The high diffusivity has two effects, it means that the hydrogen reacts very fast when combusting, but it means it diffuses fast which may increase the safety. Hydrogen is known to detonate readily, therefore the behaviour of methane/hydrogen mixtures must be understood. It should be noted that hydrogen has been used in various industries around the world with good success. The concern of introducing hydrogen into the natural gas infrastructure is that hydrogen will no longer be confined to industrial sites but will be brought into the public environment.

Hydrogen combustion is sometimes treated as a special case as its properties are so different to gaseous hydrocarbon fuels. For example the Soret effect [Kuo, 2005, p480], a phenomenon in which a temperature gradient in a mixture of substances gives rise to a concentration gradient, is a significant process in hydrogen that is mostly ignored for hydrocarbons. Natural gas consists mainly of methane as its main component, along with heavier hydrocarbons such as Ethane, Propane and Butane and very small amounts of other impurities. The exact composition of the gas varies from country to country and depends on where the gas comes from. Interestingly many models and experiments described in the literature are performed using methane. Even though methane is the prime component of natural gas the higher hydrocarbons present may affect some of its properties. For example, the mixture’s average molecular weight will be higher; typically natural gas has an average molecular weight of 19.5 g/mol compared with 16 g/mol for methane. In practice, the difference between the behaviour of natural gas and methane has been found to be quite small, within experimental errors, and methane has proved to be a good approximation to high methane containing natural gas, such as that used in the UK [Huang et. al., 2006].
Mixtures

Yu et al. [1986] added small amounts of hydrogen to methane and propane and obtained a linear correlation for the laminar burning velocity represented by adding to the pure hydrocarbon laminar burning velocity, the amount of hydrogen added, multiplied by a constant. Their experimental method tried to take measurements where flame stretch could be subtracted out from the calculations.

Halter et al. [2005] studied the effects of adding hydrogen to methane-air mixtures, they found that hydrogen increased the laminar burning velocity and decreased the flame thickness. They compared their results with Yu et al. [1986] and found that their results were being overestimated possibly due to the experimental arrangement. Halter et al. also present results calculated using the CHEMKIN™ software package from Reaction Design. They showed the laminar burning velocity displayed the same trends as the experimental results but were higher.

The Markstein length (see Section 2.7.3) was seen to decrease with increasing hydrogen addition and increase with equivalence ratio. The reduction in Markstein length reduces the dependence of the laminar flame speed on flame stretch. It was also found by Jackson et al [2003] that the Lewis number was reduced by adding hydrogen to methane, again reducing the sensitivity of the laminar flame speed to flame strain rates. Thus, hydrogen addition has a stabilising effect on methane. Even with a higher burning velocity the flame stretch effect is reduced, and thus flame speeds will not increase proportionally with the increase in burning velocity.

In a recent study by Huang et. al. [2006] the laminar burning velocities and Markstein lengths of natural gas – hydrogen – air mixtures were measured for various additions of hydrogen and for different equivalence ratios. Huang et al. found that the work of Halter et al. [2005] had underestimated the burning velocity, when compared to other available data in the literature. Huang et al. proposed a correlation for calculating the increase in burning velocity with percentage hydrogen addition.
As described in Chapter 5, explosion work has been carried out by Shell Global Solutions, using a cubic, unconfined congested rig [Roberts et al, 2006]. The mixtures used were 100% methane to 100% hydrogen with 3 equally spaced intermediate mixtures containing; 25%, 50% and 75% hydrogen. The aim was to determine the overpressures generated by these mixtures in an experimental setup that was well understood, having been used in previous studies involving methane.

Interestingly, the difference in maximum overpressure (measured at the edge of the congestion region) involving 75% hydrogen and that involving 100% hydrogen was nearly 4 bar, while the difference in maximum overpressure between the experiment involving 75% hydrogen and the experiment with methane was only 0.6 bar. This shows that the increase in maximum overpressure is clearly not linear with hydrogen addition. Adding just 25% hydrogen increased the maximum overpressure by 20mbar from the maximum overpressure in the methane experiment, which was a very small increase. The maximum overpressure increased by 320mbar for 50% hydrogen from the methane experiment which was more significant. Adding 75% hydrogen increased the maximum pressure by 620mbar (0.6bar) from the methane experiment which again was a significant increase. This implies that by adding 25% hydrogen to natural gas, the overpressures generated should result in only slightly higher overpressures being generated compared with natural gas. Roberts et al. [2006] further conclude that 10% hydrogen addition is not likely to make any difference to the overpressure within experimental errors. Roberts et al. [2006] present a graph that shows that overpressure can be correlated with the mass of hydrogen in the mixtures, for the experiments undertaken.

By adding hydrogen to natural gas, thermodynamic and transport properties change. Intensive thermodynamic properties can generally be calculated by summing the contributions of each component of the mixture, assuming an ideal gas. Transport properties can be calculated from kinetic theory and the properties of mixtures can be calculated by empirical formulae [Bird et al,
2002]. The method of calculating values used in the models of this work can be found in APPENDIX C.

2.9 Conclusions

Explosion models (empirical, phenomenological and CFD type) have been developed and, in many cases, validated against experimental data from large scale explosion experiments involving hydrocarbons as the fuel, providing a predictive capability for explosion overpressure within a factor of two.

The focus of this study is engineering models (empirical and phenomenological) which are used for routine hazard assessment within the oil and gas industry. There appears to be few publications relating to such models in recent years possibly for two main reasons. Firstly, much research was completed in the 1990’s and the models validated against large scale data which became available at that time and secondly because the models are held by individual companies who may not wish to publish details of model development to retain commercial advantage for consultancy work. The development of CFD codes is ongoing, especially within academia.

Both the empirical and phenomenological models often make use of empirical correlation based on the results of experiments using hydrocarbons (usually natural gas), for various important parameters, for example flame speed. This means that they will be unsuitable for predicting natural gas/hydrogen explosions without alternative correlations or, ideally, by generalising correlations such that the fundamental properties of the fuel are included in the correlation, thereby broadening their applicability.

It has been identified that key fuel properties in this respect are the laminar and turbulent burning velocities and the parameters which describe the response to flame stretch. Therefore in Chapter 3, particular attention is paid to determining the burning velocity and Markstein numbers for methane/hydrogen mixtures. These will be used later in Chapters, 4, 5, and 6 when modifying and extending the engineering models so that predictions of
methane/hydrogen explosions can be undertaken by generalising and extending the models developed only for natural gas.
3.1 Introduction

The local burning velocity of a fuel/oxidant mixture is a very important and fundamental parameter for modelling combustion processes. It describes the velocity at which the combustion progresses. For the current work it is a fundamental parameter for both explosion and fire modelling. It is an important way of determining how the fuel behaves and how severe an explosion or fire may be. Determining this parameter accurately can be achieved from experiments or theoretical models of varying complexity.

As part of the safety work package of NATURALHY, one of the partners, Leeds University, have undertaken work to measure the laminar and turbulent burning velocities of methane/hydrogen/air mixtures [Fairweather et al, 2006]. This work involved both experiments and detailed kinetic modelling (laminar only), for pure methane and mixtures with compositions of (in terms of added hydrogen by volume) 10%, 20% and 50%. Unfortunately, it was necessary to undertake the experimental work at an elevated temperature of 360K. For accidental releases of gas from the network, leading to a fire or explosion hazard, the burning velocity at normal atmospheric temperature is required. Consequently, it was necessary to establish a method by which the laminar burning velocity could be determined at other values of initial temperature, such as normal room temperature, from the data provided by Fairweather et al.

In this Chapter, factors influencing burning velocity are considered and a methodology for temperature correction presented. This is then applied to
temperature correct the experimental data to an initial temperature of 298K. The results are then compared with data from the literature, where possible.

### 3.2 Burning Velocity Determination and Important Parameters

The laminar burning velocity can be defined as “the velocity of the unburned gases normal to the combustion wave surface as these gases move into the combustion front” [Kuo, 2005, p449]. To determine its value there are various methods, which fit into one of two categories; experimental and theoretical modelling. There are various modelling techniques varying in complexity, ranging from a complex solution of a system of the chemical kinetic equations to phenomenological models.

Performing experiments for a fuel/oxidant mixture over a range of equivalence ratios (the equivalence ratio is the ratio of fuel to oxidant over that ratio for complete combustion) to determine the laminar burning velocity enables one to fit a curve to the data. This provides a relatively easy way of determining the laminar burning velocity for a given fuel/oxidant and equivalence ratio.

There are severe problems when attempting to use the most fundamental theoretical methods. They require considerable CPU time, and in addition the detailed chemical kinetic reactions are not fully understood or indeed known. Moreover, because the details of the intermediate chemical species are not fully understood the predications often have to be validated against experiments. The benefit of adopting this approach is that it gives one the detailed internal structure of the flame, including temperature and chemical species profiles.

Classical laminar burning velocity theories attempt to model the physical and chemical processes involved [Kuo, 2005, p449]. An important result of these theories is that the laminar burning velocity, \( u_l \), is proportional to the square root of the product of thermal diffusivity, \( \alpha \), and reaction rate, \( (RR)_T \).
It is found that the following have an effect on the laminar burning velocity [Kuo, 2005, p496]:

- **Mixture ratio**
  This is the ratio of fuel to oxidant and is often described by the equivalence ratio (see Equation (2-2)). The effect of varying the amount of fuel in a mixture is that the temperature of the flame varies. For hydrocarbons the peak temperature of the flame occurs slightly on the rich side (more fuel than oxidiser) [Law et al., 2006] as does the maximum laminar burning velocity. Further, there are limits on the ratio of fuel to oxidiser outside of which no combustion can occur. These are termed the lower and upper flammability limits (often abbreviated to LFL and UFL). The burning velocity is linked to the flame temperature, which depends on the mixture, through the reaction rate.

- **Pressure**
  The effect of the initial pressure varies depending on the reaction.

- **Initial temperature**
  The effect of increasing the initial temperature is to increase the laminar burning velocity

In a chemical reaction there are many intermediate steps between the reactants and complete creation of the products. In between many intermediate molecules and atoms, which are called free radicals, are created and then react with each other to form new particles, until such a time that the reaction chain finishes with the creation of the final products. Understanding the intermediate reactions is difficult and different authors have published different steps, two well known sets for small hydrocarbons are the GRI mechanism [Smith et al., 1999] and Konnov [Konnov, 2000] as used in the Leeds modelling work.

The more free radicals there are, the more chance there is of promoting the chain (they are called chain carriers) and the reaction rate is quicker. This
effect can also be seen with light free radicals such as H atoms, as they diffuse quickly to the place of reaction. Thus, adding hydrogen to a combustng mixture increases its burning velocity [Kuo, 2005, p502].

### 3.3 Methodology for Correction of Initial Temperature

The initial temperature of a fuel gas and oxidant mixture is an important parameter that has an effect on the laminar burning velocity. The higher the initial temperature, the faster the reaction rate is and since the laminar burning velocity is proportional to the square root of the reaction rate (Equation (2-1)), the laminar burning velocity increases.

Work by Metghalchi and Keck [1982] to determine the laminar burning velocity for four different fuels at different initial temperatures and pressures produced a good fit in the form of a power law,

\[
\dot{u}_{lb} = \dot{u}_{la} \left( \frac{T_b}{T_a} \right)^m \left( \frac{P_b}{P_a} \right)^n \]  

(3-2)

where \(m\) and \(n\) are real numbers and depend on the equivalence ratio. \(\dot{u}_{lb}\) is the burning velocity at \(T_b\) and \(P_b\), and \(\dot{u}_{la}\) is the burning velocity at \(T_a\) and \(P_a\), in SI units. Metghalchi and Keck [1982] found that the constants \(m\) and \(n\), given the experimental scatter for four fuels, were constant, that is, \(m\) and \(n\) appear to be independent of the fuel.

Metghalchi and Keck [1982] also presented another relation, based on the thermal theory of laminar flame propagation by Zeldovich and Frank-Kamenetskky, in which they make use of the Arrhenius rate equation. The Arrhenius rate equation can be used to determine the reaction rate, \(k\), which gives the number of collisions which results in a reaction per second,

\[
k = A e^{-\frac{E_A}{RT}} \]  

(3-3)

where \(A\) is a pre exponential factor that depends on the reactants (s\(^{-1}\)), \(E_A\) is activation energy that depends on the reactants (J per mole), \(R\) is the universal gas constant, and \(T\) is the temperature (K) that the reaction takes place at. The resulting relation is as follows,
\[ u_{lb} = u_{la} \left( \frac{T_b}{T_a} \right)^a \left( \frac{P_b}{P_a} \right)^n \exp\left( -\frac{E_a}{2RT} \right) \]  

(3-4)

They state that although the fit is as good as the power law Equation (3-2), the parameters vary much more widely with equivalence ratio making it more difficult to correlate. Hence Equation (3-2) is much easier to use.

### 3.3.1 Temperature Correction of Laminar Burning Velocity

The Leeds laminar burning velocity data [Fairweather et al., 2006] was carried out at initial temperatures of 360K. The aim is to use this data to evaluate the laminar burning velocity at 298K. This temperature was chosen as it is a typical ambient temperature and so relevant to situations where an accidental escape of gas has occurred. Additionally, it allows comparison with the literature as many reported laminar burning velocities are at this value. To achieve this, Equation (3-2) will be fitted using results from kinetic modelling and then applied to the experimental data.

Leeds University performed kinetic modelling at four temperatures of 250, 300, 330 and 360K using the Sandia PREMIX code and Chemkin software to solve the complex chemical kinetics of the combustion process. The chemical kinetic mechanisms used were taken from two sources, GRI-Mech [Smith et al., 1999] and Konnov [Konnov, 2000].

The complete set of laminar burning velocity data obtained during the experiments and the predictions from the kinetic modelling work were made available in Microsoft Excel format. The process of determining the power law relationship was undertaken separately for the GRI and Konnov mechanisms, as the kinetic modelling predictions are dependent on the mechanism used and cannot be compared directly.

The predicted laminar burning velocity from the kinetic modelling was plotted against the scaled temperature, which is the ratio of the temperature at which the prediction was made, \( T_b \), over the temperature at which the laminar
burning velocity is required, $T_a$. This was done for each of the four fuel compositions (0, 10, 20 and 50% v/v hydrogen addition to methane) for the same equivalence ratio on the same graph. This was repeated for different equivalence ratios from 0.6 to 1.7 in 0.1 steps. Microsoft Excel was then used to plot a power trend line through each series of data. This provided a relationship in the form,

$$y = Ax^k$$

(3-5)

The values $A$ and $k$ correspond to $u_{la}$ and $m$ in Equation (3-2), and $x$ is $(T_b/T_a)$. The pressure dependence is omitted since all the work was performed at atmospheric pressure. Hence,

$$u_{lb} = u_{la} \left(\frac{T_b}{T_a}\right)^m$$

(3-6)

Once these constants had been determined, Equation (3-6) was rearranged to give,

$$u_{la} = \frac{u_{lb}}{\left(\frac{T_b}{T_a}\right)^m}$$

(3-7)

Equation (3-7) can then be applied to the experimental values of laminar burning velocity obtained by Fairweather et al at 360K to obtain values of laminar burning velocity at 298K.

### 3.3.2 Temperature Correction of Markstein Number

The Markstein length is also an important parameter in flame propagation, describing the influence of a stretching flame on the burning velocity (laminar and in some turbulence models, see also Section 2.7.3). The Markstein number, $Ma$, is a dimensionless number and is defined as the Markstein length, $L$, over the laminar flame thickness, $\delta_l$,

$$Ma = \frac{L}{\delta_l}$$

(3-8)

The flame thickness in this work is defined as,
\[ \delta_i = \frac{\nu}{u_i} \]  

(3-9)

where \( \nu \) is the kinematic viscosity (m\(^2\)/s), and \( u_i \) is the laminar burning velocity (m/s).

Liao et al. [2006] and Hu et al. [2009] report that for Methanol-air mixtures that the Markstein length varies little between different initial temperatures (300-480 K). Results presented by Gu et al. [2000] also show little change in the Markstein length for different temperatures between 300 and 400K. It is assumed in this work that Markstein length is independent of temperature.

Markstein numbers were derived in the Leeds experiments using the laminar burning velocity and flame thickness at 360K. The Markstein number associated with stretch is temperature corrected by using the temperature corrected values of laminar burning velocity at 298K and the calculated flame thickness at 298K (see later in Figure 3-8) including calculation of the kinematic viscosity at this temperature. The viscosity is proportional to the square root of the temperature and therefore increases with temperature, see APPENDIX C for a theoretical expression on how to calculate the viscosity.

### 3.4 Results of Temperature Correction

#### 3.4.1 Burning Velocity

In this section the results for the value of the exponent \( m \) obtained by applying Equation (3-6) to the predictions of both GRI and Konnov mechanisms are presented for 100% methane, 90% methane/10% hydrogen, 80% methane/20% hydrogen, and 50% methane/50% hydrogen.

The results of fitting Equation (3-6) to the predicted laminar burning velocity values from both GRI and Konnov mechanisms are shown in Appendix A.1 together with power law trend lines fitted to the data using Excel. The variation in the exponent \( m \), for different equivalence ratios, and different fuel compositions are shown in Figure 3-1 and Figure 3-2. The curves exhibit a
parabolic shape, with a minimum at an equivalence ratio of between 1.0 and 1.1. This is the region where the burning velocity (and flame temperature) is maximum. If the exponents are averaged at each equivalence ratio, a polynomial of degree two can be fitted to the averaged data, this is shown by the black line.

![Exponent m variation with ER - derived from GRI mechanism](image1)

![Exponent m variation with ER - derived from Konnov mechanism](image2)

Figure 3-1: Temperature exponent, $m$, variation with equivalence ratio, $\Phi$, using the GRI kinetic mechanism

Figure 3-2: Temperature exponent, $m$, variation with equivalence ratio, $\Phi$, using the Konnov kinetic mechanism

The formula for the average fit for the GRI mechanism is,

$$m = 2.369\Phi^2 - 5.0097\Phi + 4.2788 \quad (R^2 = 0.7675) \quad (3-10)$$

and for the Konnov mechanism,

$$m = 2.6357\Phi^2 - 5.9655\Phi + 5.0361 \quad (R^2 = 0.8157) \quad (3-11)$$

where $R^2$ is the square of the correlation coefficient.

Observations
The value of $m$ in Equations (3-10) and (3-11) is in general slightly higher for the lean fuel/air mixtures, the results of Liao et al. [2004], as seen later in Section 3.5.3, has the same trend.

It is interesting to consider why this may be the case physically. First the empirical effect of the exponent $m$ in Equation (3-6) is in the rate of change of the laminar burning velocity with initial temperature. That is, the sensitivity of the laminar burning velocity on the initial temperature for that mixture. Higher values indicate that the laminar burning velocity will increase faster with an increase in initial temperature. To explain why this effect may be stronger for lean fuel/air mixtures rather than rich fuel/air mixtures some general observations are made in Table 3-1,

<table>
<thead>
<tr>
<th></th>
<th>ER &lt; ER at $u_{l,max}$</th>
<th>ER at $u_{l,max}$</th>
<th>ER &gt; ER at $u_{l,max}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adiabatic flame</td>
<td>Decreases quicker than on rich side</td>
<td>Maximum</td>
<td>Decreases</td>
</tr>
<tr>
<td>temperature$^4$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Thermal Diffusivity</td>
<td>More air, which is heavier than methane/hydrogen</td>
<td>Increases, as more fuel lowers average molecular weight</td>
<td></td>
</tr>
<tr>
<td></td>
<td>mixtures thus lower thermal diffusivity</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Specific heat</td>
<td>Decreases quicker than on rich side</td>
<td>Maximum</td>
<td>Decreases</td>
</tr>
<tr>
<td>capacity at constant</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>pressure</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Reaction rate</td>
<td>Decreases quicker than on rich side since flame</td>
<td>Maximum, since maximum flame temperature</td>
<td></td>
</tr>
<tr>
<td></td>
<td>temperature also does</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Density</td>
<td>More dense as more air (assuming fuel lighter than</td>
<td>Density decreasing with increasing fuel</td>
<td></td>
</tr>
<tr>
<td></td>
<td>air)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3-1: Details of changing parameters of combustion has on the laminar burning velocity

$^4$ The calculated adiabatic temperature is the maximum theoretical temperature and is often higher than what is measured, due to the break down in the assumption of adiabatic conditions.
Figure 3-3 is a calculation of the adiabatic flame temperature for methane-air flames. It shows how the rate of increase in the flame temperature with equivalence ratio on the lean fuel side is greater than on the fuel rich side. The peak temperature generally occurs on the slightly rich side of stoichiometry. This mimics the change of the exponent, $m$, with equivalence ratio if Figure 3-1 and Figure 3-2 were inverted. That is, the minimum value of $m$ occurs at a similar equivalence ratio as that where the peak flame temperature occurs. The gradient of the line for $m$ is steeper on the lean side. Similarly, the rate of change in maximum temperature is highest on the lean side.

Looking at the work from Gu et al. [2000] we can see that the activation energy is constant for a methane-air mixture at a given equivalence ratio. In this case, the Arrhenius reaction rate, Equation (3-3), only changes with reaction (flame) temperature. Speculating as to why the lean mixtures are more sensitive to initial temperatures, may include the observation that the lower thermal diffusivity suggests that heat does not transfer as rapidly and so heat is kept more local, sustaining a higher reaction rate for longer.

![Adiabatic Flame Temperature of Methane](image)

*Figure 3-3: Graph showing how calculated adiabatic flame temperature, T, for methane varies with equivalence ratio, Φ*
The experimental measurements [Fairweather et al., 2006] of laminar burning velocity carried out by Leeds University were carried out at fuel compositions of 0, 10, 20 and 50% v/v hydrogen addition to pure methane. To temperature ‘correct’ the values at these compositions Equation (3-7) is used with the derived values for $m$ as shown above, with $T_b$ (the temperature of the measured value) set as 360K and $T_a$ (the temperature we would like values for) as 298K. $u_{ib}$ is the experimentally measured burning velocity at 360K.

Figure 3-4 to Figure 3-7 present the results from applying this procedure to experimental laminar burning velocity data. In the graphs the blue diamonds represent the experimentally determined laminar burning velocity data at the initial temperature of 360K. The green squares represent the application of the method to the experimental values for the Konnov mechanism derived values of $m$ (Equation (3-11)) and similarly the red triangles represent the corrections using the GRI mechanism derived values of $m$ (Equation (3-10)). The laminar burning velocity experiments were repeated twice, and some were repeated three times, and the methodology was applied to each repeated result. In general the application of both Konnov and GRI derived values of $m$ to the original data produce similar resulting laminar burning velocity values.
Figure 3-4: Graph showing the laminar burning velocity, $u_l$, as a function of equivalence ratio, $\Phi$, displaying experimental results at 360K and temperature correction applied using power laws derived from Konnov and GRI mechanisms- for methane.

Figure 3-5: Graph showing the laminar burning velocity, $u_l$, as a function of equivalence ratio, $\Phi$, displaying experimental results at 360K and temperature correction applied using power laws derived from Konnov and GRI mechanisms- for 90% methane 10% hydrogen.
Figure 3-6: Graph showing the laminar burning velocity, $u_l$, as a function of equivalence ratio, $\Phi$, displaying experimental results at 360K and temperature correction applied using power laws derived from Konnov and GRI mechanisms- for 80% methane 20% hydrogen.

Figure 3-7: Graph showing the laminar burning velocity, $u_l$, as a function of equivalence ratio, $\Phi$, displaying experimental results at 360K and temperature correction applied using power laws derived from Konnov and GRI mechanisms- for 50% methane 50% hydrogen.
A third degree polynomial was fitted to the resulting variation of burning velocity with equivalence ratio. The equations are presented in Table 3-2, along with associated \( R^2 \) values (the square of the correlation coefficient).

<table>
<thead>
<tr>
<th>%hydrogen</th>
<th>GRI derived m</th>
<th>( R^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>( u_l = -170.31\Phi^3 + 349.35\Phi^2 - 157.53\Phi + 14.3 )</td>
<td>0.9787</td>
</tr>
<tr>
<td>10</td>
<td>( u_l = 73.796\Phi^3 - 375.39\Phi^2 + 535.01\Phi - 193.69 )</td>
<td>0.9672</td>
</tr>
<tr>
<td>20</td>
<td>( u_l = -10.037\Phi^3 - 126.51\Phi^2 + 306.87\Phi - 127.71 )</td>
<td>0.9635</td>
</tr>
<tr>
<td>50</td>
<td>( u_l = -13.471\Phi^3 - 123.67\Phi^2 + 321.94\Phi - 130.06 )</td>
<td>0.9471</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>%hydrogen</th>
<th>Konnov derived m</th>
<th>( R^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>( u_l = -194.77\Phi^3 + 429.15\Phi^2 - 239.61\Phi + 40.077 )</td>
<td>0.9773</td>
</tr>
<tr>
<td>10</td>
<td>( u_l = 56.768\Phi^3 - 321.94\Phi^2 + 482.89\Phi - 178.35 )</td>
<td>0.9637</td>
</tr>
<tr>
<td>20</td>
<td>( u_l = -29.092\Phi^3 - 66.868\Phi^2 + 249.23\Phi - 111.06 )</td>
<td>0.9635</td>
</tr>
<tr>
<td>50</td>
<td>( u_l = -34.092\Phi^3 - 58.25\Phi^2 + 258.63\Phi - 112.23 )</td>
<td>0.9375</td>
</tr>
</tbody>
</table>

Table 3-2: Fitted correlations for the temperature corrected laminar burning velocity to 298K

### 3.4.2 Markstein Numbers

Markstein numbers (Equation (3-8)) were derived in the Leeds experiments using the laminar burning velocity and flame thickness at 360K.

Figure 3-8 illustrates how the flame thickness (Equation (3-9)) varies with equivalence ratio and temperature. At higher flame temperatures the flame thickness is smaller [Andrews and Bradley, 1972]. The flame thickness of a mixture at 298K is between 21-24% greater on average than a mixture at 360K.
Figure 3-8: Flame thickness variation with equivalence ratio, $\Phi$, in the laminar regime at 360K and 298K

Figure 3-9 shows Markstein numbers plotted against equivalence ratio at 360K and the new calculated values at 298K for the four fuel compositions in this study. Markstein numbers in the stable (positive y region) part of the graph indicate that the effect of stretch on the flame is to reduce the flame speed (see Equation (2-8) in Section 2.7.3) and Markstein numbers in the unstable (negative y region) indicate that the effect of stretch on the flame is to increase the flame speed. In general the new Markstein numbers are lower and at higher equivalence ratios the difference is greatest. A straight line fit is plotted and the associated equation displayed on the chart. For methane the fit of Tseng et al. [1993] is plotted also and shows good agreement with the current work.
3.5 Discussion

In this section the results obtained are discussed and compared with literature sources.

3.5.1 Sources of Correlations for Laminar Burning Velocity

The following are correlations found in the literature for laminar burning velocity and initial temperature effects for methane/natural gas, hydrogen and mixtures of methane and hydrogen.
3.5.1.1 Andrews and Bradley [1972] for methane

The authors experimentally studied the laminar burning velocity of methane and air mixtures over the equivalence range from 0.6 to 1.6, no correlation is presented for the laminar burning velocity at standard conditions. The laminar burning velocity with a dependence on the initial temperature, $T$ (K), is correlated as,

$$u_l = 10 + 0.000371T^2 \text{ (cm/s.)} \quad (3-12)$$

Therefore by comparison with the term $\left(\frac{T_b}{T_a}\right)^m$ in Equation (3-6) the exponent, $m$, is determined to be a constant 2. This relationship was derived from references in the literature over the general temperature range 298K to approximately 500K.

3.5.1.2 Sharma et al. [1981] for methane

The authors present a correlation for laminar burning velocity for methane at equivalence ratios, $\Phi$, between 0.8 and 1.2 at a temperature of 300K as,

$$u_i = A + \frac{B}{\Phi} + \frac{C}{\Phi^2} + \frac{D}{\Phi^3} \text{ (cm/s.)} \quad (3-13)$$

where the A, B, C and D are constants with the following values, A=-418, B=1287, C=-1196, and D=360. The effect of temperature on the laminar burning velocity is given by the following relationship,

$$u_{i,T_b} = u_{i,300} \left(\frac{T_b}{300}\right)^m$$

$$m = 1.68 \sqrt[3]{\Phi} \quad \Phi \leq 1.0$$

$$m = 1.68 \sqrt{\Phi} \quad \Phi > 1.0$$

(3-14)

where $T_b$ is in the range 300-600K and the exponent $m$ depends on the equivalence ratio. $u_{i,T_b}$ and $u_{i,300}$ are the burning velocities at $T_b$ and 300K respectively. The authors quote an error with respect of their experimental measurements of up to 9%, and for other work 4.5% to 34%.
3.5.1.3 **Lijima and Tadao [1986] for methane/hydrogen mixtures**

The authors present the following correlation for laminar burning velocity for methane/air mixtures between equivalence ratios of 0.8 and 1.3 at an initial temperature of 291K,

\[ u_l = 36.9 - 210(\Phi - 1.12)^2 - 335(\Phi - 1.12)^3 \text{ (m/s)} \]  

(3-15)

For the effect of initial temperature on the laminar burning velocity the exponent, \( m \), of Equation (3-6) is given as,

\[ m = 1.60 + 0.22(\Phi - 1) \]  

(3-16)

The authors state that the errors are lower than 10% for their experimental measurements.

3.5.1.4 **Stone et al. [1998] for methane**

The laminar burning velocity at an unburnt gas temperature of 298K for methane is correlated via the following fourth degree polynomial,

\[ u_l = u_{l0} + S_1(\Phi - 1) + S_2(\Phi - 1)^2 + S_3(\Phi - 1)^3 + S_4(\Phi - 1)^4 \text{ (m/s)} \]  

(3-17)

where \( u_{l0} \) is fitted as 0.376 and the constants \( S \) were fitted as, 0.15, -2.21,-0.458, and 3.58 respectively. For the effect of initial temperature on the laminar burning velocity the exponent, \( m \), of Equation (3-6) is given as,

\[ m = m_0 + (\Phi - 1)m_1 \]  

(3-18)

where the \( m_0 \) and \( m_1 \) are constants are 1.42 and -1.98 respectively.

The equivalence ratio was in the range between 0.6 and 1.4, and temperatures were in the range 293-454K. The standard deviation was 14.7%.

3.5.1.5 **Gu et al. [2000] for methane**

The authors develop a theoretical basis to take into account the initial conditions, but also present a power law correlation as per Equation (3-6). The following values for \( u_{la} \) and \( m \) for the equivalence ratios 0.8, 1.0 and 1.2 are given over the range of initial temperature of between 300K and 400K,

\[ u_{la} = 0.259, \ m = 2.105 \text{ for } ER = 0.8 \]  

(3-19)
\[ u_{la} = 0.360, m = 1.612 \quad \text{for } ER = 1.0 \]
\[ u_{la} = 0.314, m = 2.00 \quad \text{for } ER = 1.2 \]

### 3.5.1.6  
**Elia et al. [2001] for methane**

A second order polynomial is fitted to experimental laminar burning velocity values in the equivalence ratio range 0.8 to 1.2

\[ u_i = u_{i0}(a_0 + a_1\Phi + a_2\Phi^2) \text{ (cm/s)} \quad (3-20) \]

where \( a_1 \) to \( a_3 \) are constants with the values -5.883, 14.003 and -7.115 respectively and \( u_{i0} \) is 37.5. The temperature dependence of the laminar burning velocity over the range of initial unburnt gas temperatures of 298 to 550K is fitted to the Equation (3-6) power law with one value of \( m \) being 1.857. No error estimates are provided.

### 3.5.1.7  
**Yu et al. [1986] for methane (also propane) and hydrogen**

The authors carried out experiments to determine laminar burning velocity of methane with up to 50% hydrogen addition in 10% steps, for equivalence ratios between 0.5 and 1.4 (except for pure methane which started at 0.6 due to the lower flammability limit). The authors present a correlation based on an effective equivalence ratio and the relative amount of hydrogen; “because of the presence of three reactants in the mixtures, it is necessary to first decide on stoichiometric parameters for meaningful data reduction”. They assumed that since hydrogen is in small quantities that is should be completely oxidised, and then if the remaining air used to oxidise the methane then there exists an effective equivalence ratio,

\[ \phi_f = \frac{C_F}{C_A} - \frac{C_H}{(C_H/C_A)_{st.}} \quad (3-21) \]

where \( C_F \) is the mole fraction for the hydrocarbon fuel, \( C_H \) is the fuel fraction for the hydrogen in the mixture, and \( C_A \), is the mole fraction for the amount of
air. The subscript ‘st’ is for stoichiometric conditions. The relative amount of hydrogen addition is expressed as,

\[
R_H = \frac{C_H + \frac{C_H}{C_A}}{C_A + \left( \frac{C_H}{C_A} \right)_{st}}
\]

(3-22)

The authors suggest the following linear correlation with \( R_H \) for laminar burning velocity,

\[
u_t(\Phi_F, R_H) = \nu_{00}(\Phi_F, 0) + a_F(\Phi_F)R_H \text{ (cm/s)}
\]

(3-23)

where the first term is the laminar burning velocity for the pure fuel (methane) at an equivalence ratio given by the effective equivalence ratio, \( \Phi_F \), and \( a_F \) is a slowly varying function of the equivalence ratio with the same units as velocity. The value of \( a_F \) can be approximated by a constant for a methane and propane. The value of \( a_F \) is slightly different for methane and propane at 80 cm/s and 86 cm/s respectively, but an average gives little increase in error, and so 83 cm/s can be used.

3.5.1.8 **Laio et al. [2004] for natural gas**

At the initial temperature 300K a third degree polynomial is fitted to the laminar burning velocity, which has a 5% standard deviation, as,

\[
u_t = -177.43\Phi^3 + 340.77\Phi^2 - 123.66\Phi - 0.2297 \text{ (cm/s)}
\]

(3-24)

and for the initial temperature dependence (derived in temperature range 300K-400K),

\[m = 5.75\Phi^2 - 12.15\Phi + 7.98\]

(3-25)

The equivalence ratio range was 0.6 to 1.4.
3.5.1.9  *Huang et al. [2006] for natural gas, hydrogen and mixtures*

This correlation is based on experimental data using natural gas (96.16% methane) with hydrogen addition from 0% to 100%. The laminar burning velocity correlation for natural gas is as follows,

$$u_{l,CH_4} = -150.84\Phi^3 + 287.6\Phi^2 - 96.327\Phi - 1.2924 \text{ (cm/s)} \quad (3-26)$$

and the laminar burning velocity correlation for hydrogen is as follows,

$$u_{l,H_2} = 51.902\Phi^3 - 394.46\Phi^2 + 835.14\Phi - 267.07 \text{ (cm/s)} \quad (3-27)$$

For mixtures of natural gas and hydrogen there is a mixing correlation,

$$\frac{u_x - u_{CH_4}}{u_{H_2} - u_{CH_4}} = 0.00737e^{\frac{1.2}{20.38}} + 0.00334$$

where $u_x$ is the laminar burning velocity for a mixture with $x\%$ hydrogen addition. For the laminar burning velocity for pure fuels, the pure fuel correlation should be used as the above correlation does not asymptote to the pure fuel correlation laminar burning velocity value.

3.5.1.10  *Coppens et al. [2007] for methane/ hydrogen mixtures*

The author took an existing correlation by Gülder (1984) based on pure hydrocarbon fuels,

$$u_i = Z W \Phi^n e^{-\frac{\gamma}{2}(\Phi - \sigma)^\tau}$$

and extended it for hydrogen addition,

$$u_i = (1 + \gamma_\alpha^2) W \Phi^n e^{-\frac{\gamma}{2}(\Phi - \sigma + \Delta)^\tau}$$

where $\alpha$ is the volume fraction of hydrogen added and $\Phi$ is the equivalence ratio. Experiments were carried out with up to 35% hydrogen and the remaining symbols are constants and are as follows;

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Gülder</th>
<th>Coppens et al. [2007]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Z$</td>
<td>1</td>
<td>-</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>-</td>
<td>1.9153</td>
</tr>
<tr>
<td>$\tau$</td>
<td>-</td>
<td>1.533</td>
</tr>
<tr>
<td>$W$ (cm/s)</td>
<td>42.2</td>
<td>39.0542</td>
</tr>
</tbody>
</table>
3.5.2 Comparison of laminar burning velocity correlations at standard temperature and pressure

A summary of the surveyed correlations and their applicability from the literature is presented in Table 3-3.

<table>
<thead>
<tr>
<th>Ref</th>
<th>Fuels</th>
<th>Laminar Burning Velocity</th>
<th>Temperature correction correlation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Andrews and Bradley [1972]</td>
<td>methane</td>
<td>Experimental data, no correlation</td>
<td>Power law with constant exponent, 2</td>
</tr>
<tr>
<td>Lijima and Tadao, [1986]</td>
<td>methane, hydrogen (separate)</td>
<td>3rd Order Polynomial</td>
<td>Power Law with straight line fit for exponent</td>
</tr>
<tr>
<td>Stone et al. [1998]</td>
<td>methane</td>
<td>4th Order Polynomial</td>
<td>Power Law with straight line fit for exponent</td>
</tr>
</tbody>
</table>
Table 3-3: Comparison of correlations for laminar burning velocity and initial temperature changes (where available)

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>Correlation Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gu et al. [2000]</td>
<td>Power law</td>
<td>For 3 values of equivalence ratio</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Power law with 3 given value for selected equivalence ratios</td>
</tr>
<tr>
<td>Elia et al. [2001]</td>
<td>2nd order</td>
<td>2\textsuperscript{nd} order polynomial</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Power law with single value for exponent</td>
</tr>
<tr>
<td>Yu et al. [1986]</td>
<td>Straight line</td>
<td>Straight line fit of reduced parameters</td>
</tr>
<tr>
<td></td>
<td>fit</td>
<td></td>
</tr>
<tr>
<td>Laio et al. [2004]</td>
<td>3rd order</td>
<td>Power law with polynomial fit</td>
</tr>
<tr>
<td></td>
<td>polynomial</td>
<td></td>
</tr>
<tr>
<td>Huang et al. [2006]</td>
<td>3rd Order</td>
<td>3\textsuperscript{rd} Order Polynomial, and exponential function of mixing</td>
</tr>
<tr>
<td></td>
<td>Polynomial, and</td>
<td></td>
</tr>
<tr>
<td></td>
<td>exponential</td>
<td></td>
</tr>
<tr>
<td></td>
<td>function of mixing</td>
<td></td>
</tr>
<tr>
<td>Coppens et al. [2007]</td>
<td>Exponential</td>
<td>Exponential equation</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

3.5.2.1 Methane and natural gas

Figure 3-10 plots various correlations for methane and natural gas found in the surveyed literature (see previous section) and also the temperature corrected laminar burning velocity based on the Leeds data derived in this work. The correlations have been plotted over the equivalence ratio for which they were derived. They show a peak of the laminar burning velocity at around an ER of 1.1, which is known experimentally to have the fastest burning velocity. Over the correlations presented there is a maximum of the peak laminar burning velocity of about 0.4 ms\(^{-1}\) an increase of 18% on the minimum of 0.34 ms\(^{-1}\). As the equivalence ratio moves away from 1.1, the difference between minimum and maximum values of laminar burning velocity at a given
equivalence ratio is slightly less, except that at high ER (~1.4) the laminar burning velocity values (only 3 correlations in this range) have the maximum difference but there may be uncertainty at this extreme.

Figure 3-10: Comparison of laminar burning velocity at 298K for methane/natural gas

3.5.2.2  Methane/hydrogen mixtures

Figure 3-11 shows three correlations from the survey for the laminar burning velocity of methane with hydrogen addition. Only the Huang et al [2006] correlation has been tested over the range of 0-100% hydrogen addition to natural gas, though at 0 and 100% it is best to use the pure fuel correlations. The Yu et al. [1986] correlation was based on experiments of up to 50% hydrogen addition and the Coopens et al. [2007] up to 35% hydrogen addition.
However, the correlation has been extrapolated here to 100% to assess the performance outside their range by comparison against Huang et al. [2006] correlation. The correlation from Yu et al. [1986] after 50% hydrogen addition increasingly deviates from the Huang et al. correlation and predicts higher values than Huang et al. The Coopens et al. correlation looks more like a straight line and predicts lower values than Huang et al. after 60% hydrogen addition. The extrapolation exercise proves that the correlation should only be used for the range for which they were derived.

Figure 3-11: Comparison of correlations in the literature for laminar burning velocity of methane with %v/v hydrogen addition

Now, the correlations for laminar burning velocity for a range of methane/hydrogen mixtures are compared against the values derived by temperature correction of the Leeds data for an ER of 1.0, in Figure 3-12. The two curves showing the current work are very similar. The Coopens et al.
[2007] formula is close to the two curves of the current work up to 35% hydrogen addition. The Yu et al. [1986] formulation tends to under-predict the values in the current work for less than 40% hydrogen addition and crosses to over-prediction after 40% hydrogen addition. The most modern correlation Huang et al. [2006] compares well with the current work, until you get less than 20% hydrogen addition where the over-prediction has a maximum of nearly 29%.

![Natural Gas with Hydrogen addition Burning Velocity Correlation ER=1.0](image)

**Figure 3-12:** Comparison of correlations for laminar burning velocity at 298K with %v/v hydrogen addition from the literature and the work in this chapter

### 3.5.3 Comparison of temperature correction correlations

Figure 3-13 displays the exponent m from Equation (3-6) for the laminar burning velocity initial temperature relationship for surveyed literature sources and the values as determined from this work. Unfortunately there is no clear
agreement between the sources, there are: constant values, a polynomial function as a function of the equivalence ratio, a square and inverse square law as a function of equivalence ratio, and a straight line correlation with the independent parameter the equivalence ratio. The best fit for the current work is a polynomial which is plotted as the dashed curves on the figure. All of the values of $m$ are of the same order and lie in the general range of 1.5 to 2.5, however, the straight line fit from Stone et al. [1998] stands out and follows a markedly different path after an equivalence ratio of 0.9.

![Exponent m variation with ER](image)

**Figure 3-13: Comparison of the literature and current work of the temperature exponent, m, varying with equivalence ratio**

### 3.5.3.1 Burning velocity of methane at 360K

Plotted in Figure 3-14 are curves that have been calculated from using the surveyed correlations for temperature effect (Section 3.5.1) to derive laminar
burning velocities for methane at 360K. In each case, the temperature effect correlation was applied to the laminar burning velocity at normal conditions (298K and atmospheric pressure) from the same source reference. The Leeds laminar burning velocity experimental data are also plotted. The curves all follow the same trend and in general terms there is good agreement. However, the difference between the minimum and maximum predicted laminar burning velocity values are significant, for example at stoichiometric the difference from the lowest laminar burning velocity (0.45 ms$^{-1}$) to the highest (0.53 ms$^{-1}$) corresponds to an 18% increase.

![Correlation Comparision for the Laminar Burning Velocities of Methane at the Initial Temperatue of 360K](image)

Figure 3-14: Comparison of derived values for laminar burning velocity at 360K (by applying correlations found in the literature) and the Leeds laminar burning velocity data obtained at 360K.
3.6 **Conclusions**

In this chapter the dependences of laminar burning velocity and Markstein number on equivalence ratio and initial temperature have been explored. The following conclusions have been drawn:

- **Markstein number** increases with equivalence ratio approximately linearly. Markstein number decreases slightly with decreasing temperature with this effect being most marked at high equivalence ratios.

- **Laminar burning velocity** is a function of equivalence ratio. For methane and methane/hydrogen mixtures, burning velocity peaks at an equivalence ratio in the region 1.0 to 1.1.

- **Laminar burning velocity** increases with increasing initial temperature and correlations of the form $u_{lb} = u_{la} \left( \frac{T_b}{T_a} \right)^m$ are often used to relate a burning velocity $u_{lb}$ at $T_b$ to a burning velocity $u_{la}$ at $T_a$.

- Using the results of kinetic modelling, parabolic correlations for the exponent $m$ (as a function of equivalence ratio) were derived for use with methane and methane/hydrogen mixtures. The parabolic correlations for $m$ were compared with other approaches in the literature for temperature correction. Although the values of $m$ were generally in the same range, a diversity of relationships with equivalence ratio were found including linearly decreasing, constant and other parabolic shaped functions.

- The parabolic correlations for $m$ were used to temperature correct experimental data obtained at 360K to 298K. Polynomial functions were then fitted to provide expressions for the laminar burning velocity at 298K of methane/hydrogen mixtures as a function of equivalence ratio. These polynomial expressions can be used within explosion models.
• For methane, the temperature corrected burning velocities compared well with other literature data/correlations across a wide range of equivalence ratios.

• At an equivalence ratio of 1, the burning velocity of methane/hydrogen mixtures increases with increasing hydrogen content. The temperature corrected values derived in this work compare reasonably with correlations in the literature although no single correlation provided good agreement across the full range of hydrogen content.

In the next three chapters, the correlations for laminar burning velocity of methane/hydrogen mixtures at 298K are used to enable explosion models developed for methane (natural gas) to be applied to methane/hydrogen mixtures.
4.1 Introduction
This chapter is concerned with modelling the overpressures resulting from industrial scale explosions in confined, vented enclosures. The predictive modelling work was carried out with Shell’s SCOPE modelling software and modifications were made to the software in light of the work in Chapter 3 with respect to the burning velocity experiments on mixtures of methane and hydrogen. Model predictions are compared with experimental data generated within the NATURALHY project.

4.2 Experiments
Within the NATURALHY project, a series of large scale confined vented explosions were undertaken, representing explosions in an industrial building or housing. The experimental programme and results are detailed fully elsewhere [Lowesmith, 2007] and summarised (together with some predictions) in Lowesmith et al. [2010].

In summary, the experiments were carried out in an enclosure as shown in Figure 4-1 having dimensions of 8.25m by 3m by 2.8 m (length, width, height). On the smallest area face there was an opening of dimension 2.5m wide by 2.47m high, or 73.5% of the area of the face. The vent was covered by a polythene sheet serving to keep the gas contained prior to ignition and failing at a low pressure. As seen in the foreground of Figure 4-1 there was a pipe-work system that admitted the fuel/air mixtures and re-circulated it to achieve uniform gas/air mixtures throughout the enclosure prior to ignition.
Internally, there were seven sets of supports welded to the wall vertically, at regular intervals (1m apart), designed to hold up to 7 pipes horizontally forming obstacle arrays. Plastic pipes of 0.18m diameter were located on these supports in varying combinations to represent congestion within the enclosure as shown on Figure 4-2.

Figure 4-2: Schematic of test rig showing pipework congestion arrangement
[Lowesmith, 2007]
Pressure transducers were installed to measure the pressure development inside and outside the enclosure and ionisation probes (IPs) were installed to measure the flame time of arrival in the enclosure. Further, high speed video was used to obtain a visual record of the flame venting from the enclosure. Five pressure transducers were installed within the enclosure and four were installed externally extending up to a maximum distance of 32m directly away from the vent. Twenty ionisation probes were installed in the enclosure, eleven were placed at the vent and the remaining nine were distributed along the centre line of the enclosure. The ionisation probes near the vent were arranged in a grid like fashion around the centre of the vent. This was to determine whether or not the flame surface arrived at the vent as a planar flame surface (in which case the time of arrival of the flame registered by all the ionisation probes would be approximately the same) or if the flame surface was deformed. Figures 4-3 and 4-4 show the locations of the pressure transducers and IPs.

External transducers 1m above local ground level
Internal transducers at floor level

Figure 4-3: Plan view showing pressure transducer locations (squares) [Lowesmith, 2007]
The gas/air mixture was ignited by means of a spark located at either the centre of the enclosure or in the centre of the rear wall (furthest from the vent).

The experimental test conditions are detailed in Table 4-1 along with the maximum internal overpressure measured and the flame speed just outside the vent determined from analysis of video footage.


<table>
<thead>
<tr>
<th>Test</th>
<th>Gas Composition</th>
<th>ER</th>
<th>No. of Pipes</th>
<th>Ignition Location</th>
<th>Max Pressure* (mbar)</th>
<th>Flame Speed outside vent (m s⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>INDEXP04</td>
<td>80:20</td>
<td>1.10</td>
<td>0</td>
<td>Centre</td>
<td>63</td>
<td>41</td>
</tr>
<tr>
<td>INDEXP05</td>
<td>CH4</td>
<td>1.11</td>
<td>0</td>
<td>Centre</td>
<td>62</td>
<td>34</td>
</tr>
<tr>
<td>INDEXP06</td>
<td>80:20</td>
<td>1.10</td>
<td>0</td>
<td>Rear</td>
<td>432</td>
<td>168</td>
</tr>
<tr>
<td>INDEXP07</td>
<td>80:20</td>
<td>1.25</td>
<td>0</td>
<td>Rear</td>
<td>297</td>
<td>127</td>
</tr>
<tr>
<td>INDEXP08</td>
<td>80:20</td>
<td>0.80</td>
<td>0</td>
<td>Rear</td>
<td>129</td>
<td>99</td>
</tr>
<tr>
<td>INDEXP09</td>
<td>50:50</td>
<td>1.06</td>
<td>0</td>
<td>Centre</td>
<td>331</td>
<td>71</td>
</tr>
<tr>
<td>INDEXP10</td>
<td>50:50</td>
<td>1.05</td>
<td>0</td>
<td>Rear</td>
<td>950</td>
<td>191</td>
</tr>
<tr>
<td>INDEXP11</td>
<td>80:20</td>
<td>1.07</td>
<td>17</td>
<td>Rear</td>
<td>1338</td>
<td>263</td>
</tr>
<tr>
<td>INDEXP12</td>
<td>50:50</td>
<td>1.09</td>
<td>17</td>
<td>Centre</td>
<td>459</td>
<td>83</td>
</tr>
<tr>
<td>INDEXP13</td>
<td>NG</td>
<td>1.09</td>
<td>0</td>
<td>Rear</td>
<td>342</td>
<td>155</td>
</tr>
<tr>
<td>INDEXP14</td>
<td>50:50</td>
<td>1.09</td>
<td>17</td>
<td>Rear</td>
<td>2421</td>
<td>388</td>
</tr>
<tr>
<td>INDEXP15</td>
<td>80:20</td>
<td>1.06</td>
<td>17</td>
<td>Centre</td>
<td>258</td>
<td>69</td>
</tr>
</tbody>
</table>

Table 4-1 Confined vented explosion experimental parameters [Lowesmith, 2007]

* maximum pressure measured anywhere in enclosure after pressure traces subjected to 1.5ms rolling average

4.3 **Modelling Methodology**

Confined explosions may be completely enclosed but in practice there will generally be venting of gas either due to the presence of vents or because during the explosion process part of the enclosure fails, forming a vent. Venting can relieve the overpressure build up inside the enclosure and prevent catastrophic failure of the enclosure which could arise if the enclosure was built completely of the same strength material. The provision of panels placed on the walls or roof of an enclosure designed to fail if a certain overpressure is achieved is an effective and widely used way of providing relief in the event of an explosion.

Looking at the pressure-time relationship for a location within an enclosure that has some venting or relief panels can provide information about the different stages of an explosion. For this case there are four discernable stages that can be identified in the pressure time traces [Tite, 2001]:

1. Ignition – the pressure begins to rise as there is no venting
2. Vent opening – the initial pressure rises until such a point that the vent fails and opens allowing unburnt gas to vent.

3. Burnt gas venting and external combustion – as the flame arrives at the vent, hot burnt gas can start to vent which is followed by the combustion of previously vented unburnt gas/air mixture outside the vent.

4. Maximum flame area – the flame front has expanded to the walls of the enclosure

Tite [2001] describes some empirical methods from various authors that predict a particular stage of the pressure-time curve with varying degrees of applicability. There are two modes of this type of explosion, one where the vent is actually covered and then due to the pressure build up is removed, and secondly where there is no covering. The empirical methods presented by Tite [2001] may predict only the pressure associated with one of the above 4 phases. Also, the methods are only applicable to essentially empty and approximately cubical confined spaces. For this reason they are not applicable here.

Phenomenological models capable of modelling this scenario (Section 2.5.2) are GL’s CLICHÉ and Shell’s SCOPE model. The SCOPE software from Shell Global Solutions was chosen as the model in this work. It was made available by Shell to Loughborough University since Shell were also partners of the safety work package, whilst CLICHÉ was not available. However, it has one limitation limiting its predictive abilities for the current test program, it assumes the worse case scenario and that is for ignition at the rear of the enclosure. Therefore only tests 13, 6, 7, 8, 11, 10 and 14 can be modelled using SCOPE.

The model is an engineering type phenomenological model and predicts the pressure generated by a confined, vented explosion; it is an acronym for Shell Code for Overpressure Prediction in gas Explosions. The version used was 4.1. The latest publication describing SCOPE [Puttock et al., 2000] describes version 3 and its formulation is introduced in Section 2.5.2.1. Changes were
made to the code in collaboration with Jonathan Puttock of Shell Global Solutions.

Briefly, SCOPE contains a predictive flame speed model that predicts the speed of the flame as it progresses through arrays of obstacles. This is done by calculating the turbulence intensity generated by the flow passing through the obstacle grids (ahead of the flame) and then calculating the turbulent burning velocity using the turbulence intensity. The flame speed is then used to calculate the, uniform, pressure in the enclosure. Figure 4-5 shows the structure taken by SCOPE to determine the overpressure [Puttock et al. 2000].

![Figure 4-5: Flow chart describing the modelling steps undertaken within SCOPE [Puttock et al. 2000]](image)

### 4.3.1 Model Inputs

To use the SCOPE software input parameters regarding the fuel and geometry are entered, which can be saved to file to be recalled later. These are input in a graphical user interface with different tabs providing places to input the data. The relevant geometric parameters that are needed are: the enclosure dimensions; the position of obstacle grids and their blockage ratio
for both round and sharp blockage; the diameter of the obstacles on the grid; the complexity of the obstacles on that grid, that is, the range of obstacle diameters; and the area of the vent. For the fuel inputs, a fuel is selected from the fuel database and then the, uniform, concentration of the fuel in air is entered.

Defining the area blockage ratio (ABR) of each grid is straightforward but needs attention to detail. To get the area blockage for a grid the total area of all the pipes that face the oncoming flow is divided by the internal cross sectional area of the enclosure. The model can make allowances for different size obstacles within a grid and this term is called the complexity level, which has four levels. Increasing complexity increases the range of obstacle dimensions present in a grid and will act to increase the flame speed and hence the resulting overpressure. For our case all of the obstacle sizes in the grids are of the same size (round pipes) so this is simply set at level 1, though in most practical situations level 1 is not applicable due to a wide range of obstacle dimensions present.

However, it was found that this was not enough on its own to get satisfactory predictions and so other blockages to the flow need to be accounted for. In modelling these experiments, it was necessary to take into account the blockage arising from other items apart from the pipes. This included sensors, supporting metal work and perhaps even large bundles of wires. Within the experimental enclosure there were rectangular steel supports welded vertically to the walls in seven, 1m spaced positions starting from the rear wall. Additionally there was a steel central support column for sensors. Smaller obstacles include cables and wire supports and wires themselves, although most of these were run close to existing metal work. These were not explicitly included in the area blockage calculations. The support steel work holding the pipes had a depth of 7.5 cm and a width of 10 cm. The supports were of sufficient size to take into account when calculating the area blockage of a grid.
The area blockage ratio, ABR, is defined as the ratio of the area of blockage (the profile presented to the oncoming flow) over the cross-sectional area available for the flow,

\[
ABR = \frac{\text{Area of blockage}}{\text{Cross-sectional area}}
\]  

(4-1)

To calculate the area that the pipes in a grid present to the oncoming flow the diameter, \(d\), is multiplied by the pipe length, \(W\), and then by the number of pipes in the grid, \(n\). Then taking the ratio of the obstacle area over the cross sectional area of the enclosure (the product of the width of the enclosure, \(W\), and the height of the enclosure, \(H\)),

\[
ABR_o = \frac{n \times (d \times W)_{\text{pipe}}}{W \times H}
\]  

(4-2)

we arrive at the area blockage for round obstacles, represented by subscript \(o\). This is input as ‘round blockage’ in SCOPE.

To take into account the blockage from the pipe supports on the enclosure walls (subscript \(\#\)), we take the area given by the product of the depth of the support, \(s\), and height of the support (this is the full height of the enclosure), \(H\), and multiply it by two (for both walls), over the enclosure cross- sectional area (\(W \times H\)).

\[
ABR_{\#} = \frac{2 \times (s \times H)_{\text{sup port}}}{W \times H}
\]  

(4-3)

This blockage is represented as ‘sharp blockage’ in SCOPE.

Two pipe configurations were used in the enclosure for the experimental tests, one with no pipes added to the enclosure, and the other with seventeen pipes added, arranged in grids with alternating two pipes and three pipes, staggered so that the pipes of one grid were between the pipes of the next grid (see Figure 4-2). Seven grids were used which were 1m apart as shown on Figure 4-2. Table 4-2 summarises the results from the area blockage ratio calculations.
<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Enclosure Cross Sectional Area (m²)</td>
<td>8.4</td>
</tr>
<tr>
<td><strong>Pipe grid (Round Blockage)</strong></td>
<td></td>
</tr>
<tr>
<td>Pipe Diameter (m)</td>
<td>0.18</td>
</tr>
<tr>
<td>Pipe Area (m²)</td>
<td>0.54</td>
</tr>
<tr>
<td>ABR per pipe</td>
<td>0.0643</td>
</tr>
<tr>
<td>Pipe Number</td>
<td>2</td>
</tr>
<tr>
<td>ABR per grid</td>
<td>0.1286</td>
</tr>
<tr>
<td>Pipe Number</td>
<td>3</td>
</tr>
<tr>
<td>ABR per grid</td>
<td>0.1929</td>
</tr>
<tr>
<td><strong>Grid Supports (Sharp Blockage)</strong></td>
<td></td>
</tr>
<tr>
<td>Depth (m)</td>
<td>0.075</td>
</tr>
<tr>
<td>Length (m)</td>
<td>2.5</td>
</tr>
<tr>
<td>ABR per support</td>
<td>0.0223</td>
</tr>
<tr>
<td>ABR per grid</td>
<td>0.0446</td>
</tr>
</tbody>
</table>

Table 4-2: Summary of area blockage ratio (ABR) calculations

The next critical bit of the input is getting the correct fuel parameters. The fuel is selected from a list of fuels, in which the necessary parameters are stored as binary files on disk. There were fuel files for methane, and for hydrogen separately. Using the work within NATURALHY on burning velocity of methane/hydrogen mixtures, as discussed in Chapter 3, new fuel files for 2 different methane/hydrogen mixtures were developed in collaboration with Shell Global Solutions. The mixtures considered contained 20% and 50% hydrogen in methane.

In particular, the laminar burning velocity for these mixtures as derived in Chapter 3 were implemented for 20% and 50% hydrogen addition to methane, for equivalence ratios of between 0.8 and 1.1.

The stretch Markstein number is also needed for the turbulent burning model of SCOPE and these were taken from the Leeds report [Fairweather et al., 2006] and implemented within the new fuel files.
The model for turbulent burning velocity in SCOPE assumes that the turbulent burning velocity is proportional to one over the cube root of the Markstein number (Puttock et al. [2000] eq 16). Hence, fuels with a larger Markstein number have a reduced turbulent burning velocity. Turbulent burning velocity correlations were also derived by Leeds University [Fairweather et al, 2006] and these suggested that the turbulence intensity affects the burning velocity of 50:50 methane:hydrogen mixtures more than 80:20 mixtures. Figure 4-6 shows the data and correlations for the 50:50 mixture and mixtures with 20% or less hydrogen added to methane. \( u_B \) is the turbulent burning velocity, \( u'k \) is the effective r.m.s (root mean square) turbulent velocity, \( K \) is the Karlovitz stretch factor. The correlation for the turbulent burning velocity for methane and mixtures containing up to 20% hydrogen was,

\[
\frac{u_B}{u'k} = 0.37K^{-0.49} \tag{4-4}
\]

and for 50:50 mixture was,

\[
\frac{u_B}{u'k} = 0.54K^{-0.47} \tag{4-5}
\]

The data and correlations indicate that for a given turbulence level the 50:50 mixture will exhibit a faster turbulent burning velocity. It is also noted that, the exponents in Equations (4-4) and (4-5) are very similar and if taken to be the same the turbulent burning velocity for the 50:50 mixture would be 1.46 times greater than for mixtures containing 20% or less hydrogen.
Restricting the discussion to approximately stoichiometric mixtures, the Markstein number for methane, as used in SCOPE, is 3.76. The average Markstein number derived from the Leeds burning velocity experiments for methane and for 80:20 mixture is 3.75 and for the 50:50 mixture is 1.6. As the turbulent burning velocity correlation in SCOPE is inversely proportional to the cube root of the Markstein number, by using the Markstein number for a 50:50 mixture and for mixtures with less than 20% hydrogen, we can deduce that the increase in the turbulent burning velocity for a 50:50 mixture predicted by SCOPE would be \((1.6/3.75)^{1/3} = 1.33\). This value is only slightly smaller than the 1.46 increase suggested by the Leeds work. Hence it was decided to retain the existing correlation within SCOPE to derive the turbulent burning velocity.
4.4 Results – Comparison of predictions with data

SCOPE provides a summary of the explosions including, the maximum internal overpressure, the flame exit speed, an account of the flow history through the girds and vent, details on the external explosion and the pressure decay in the free field for any receivers specified resulting from the external explosion. SCOPE also produces graphs for how the pressure varies in time (the model assumes uniform pressure internally) and the pressure in the enclosure relative to the location of the flame front. There is a correspondence between the time at which the enclosure is at a certain pressure and the position of the flame front at that pressure. Therefore it is possible to determine the time that the flame is at a particular position and thus calculate the flame speed.

From the experimental data, the maximum pressure was determined by studying the pressure traces from each experiment, which are a reliable source of information. The flame speed at the vent is more difficult to determine accurately. Up to three methods (and at least two) have been applied to determine this value: (1) ionisation probe (IP) flame time of arrival data; (2) greyscale (b&w) 1000 frames per second (fps) high speed video; and (3) normal colour video footage. Ionisation probes were located internally up to the vent and also within the vent itself. The two cameras were aimed at the vent to capture the flame exiting. The flame speed outside the vent was calculated from analysis of the video footage by determining the position of the flame and the time of the frame it appears, this enables the flame speed to be deduced. However, this method is subjective as the flame front can be hard to determine accurately and depends on the light conditions in each experiment and the person carrying out the analysis. The vent flame speed could be determined from the video analysis by taking a best line fit through the calculated flame speed outside the vent and extrapolating back towards the vent.

Only tests 6, 7, 8, 10, 11, 13, and 14 involved rear ignition and could be appropriately modelled using SCOPE. The fuel file revision allowed a range of
equivalence ratios from 0.8 to 1.1 to be modelled, and therefore, test 7 could not be effectively modelled as the equivalence ratio was 1.25. (Trying to model test 7 at a lean gas concentration to try and obtain the same laminar burning velocity is not a sensible option as properties such as the density and Markstein number are different).

### 4.4.1 Predictions of flame exit speed and maximum internal overpressure

The predicted flame exit speed and maximum internal overpressure are plotted and compared with experimental observations (these can be found in Table 4-1).

In Figure 4-7 the flame exit speed at the vent as predicted by SCOPE is plotted against the experimental flame exit speed, for 0%, 20% and 50% hydrogen added to methane and for no pipes and 17 pipes inside the enclosure. In general the predictions are very good lying on the right side of conservatism. For methane (test 13) the prediction is close to the experimental value, being over-predicted by only 7.8%. This is to be expected as the model has been validated extensively against methane and natural gas explosions. For 20% hydrogen addition, (tests 6 and 11), the results are also good, the error being less than 16%. When 50% hydrogen is added the model performs well when there is pipe congestion (9% over-prediction) although when there are no pipes the over-prediction is greatest (31% over-prediction).

Overall, the agreement is satisfactory given the difficulty of modelling explosions and the variability which occurs from one explosion to another under apparently identical conditions (see Section 2.6).
In Figure 4-8 the predicted maximum internal pressure is plotted against the experimental data, for 0%, 20% and 50% hydrogen added to methane and for no pipes and 17 pipes inside the enclosure. The experimental maximum internal overpressure is plotted as the average peak overpressure\(^5\) experienced and the horizontal bars represent the range of peak overpressure experienced. In general the predicted values are conservative but within a factor of two of the observed value. (During the validation program of SCOPE the range of predictions for the maximum internal overpressure reached a maximum of a factor of 2 and thus these results are within the errors already documented for the model [SCOPE, v4.1, help file].) The maximum overpressure for the methane test is over-predicted by 44%. For 20% hydrogen addition and for no pipes the error is similar, however for 17 pipes

---

\(^5\) The average peak overpressure was determined by averaging the peak overpressure observed at each pressure transducer and not just the absolute maximum observed
with this fuel the error is reduced to 12%. Adding more round blockage into SCOPE to represent pipes results in reduced rate of the increase of the overpressure. For 50% hydrogen addition the results are again generally conservative except that the absolute maximum overpressure is underpredicted for the test involving 17 pipes. However, this magnitude of pressure would be a short duration event.

![Diagram of Maximum Internal Overpressure: Experimental and SCOPE](image)

Figure 4-8: Comparison of maximum internal overpressure from SCOPE predictions and experiments (data from [Lowesmith, 2007])

Nevertheless, the agreement overall is good and provides confidence in the model's capability for methane/hydrogen explosions.

### 4.4.2 Flame Speed and Blast Decay

SCOPE has the ability to provide predictions of the external explosion caused by the flame pushing gas out the vent, which is then ignited when the flame exits the enclosure. This also has an effect on the internal overpressure predicted by SCOPE. For the external blast decay the external explosion is
the source region for the model. The external explosion is assumed to be a hemisphere, the radius and the overpressure of this source region are calculated.

As mentioned at the beginning of Section 4.4, SCOPE also provides flame speed predictions within the enclosure. The following figures show further, detailed, predictions from SCOPE for the flame speed development with time inside the enclosure and also for the blast decay away from the vent.

The predictions are presented alongside the experimental data. The flame speed data presented is calculated from 2 or 3 of the following, ‘IP’ derived data, high speed ‘B&W video’ or normal ‘colour video’. The overpressure away from the vent is calculated at 0, 8, 16 and 32 m, as these correspond to the locations of instruments. The source region of the blast is from the external explosion and thus the prediction at 0 m away from the source is in fact the pressure generated by the external explosion. For the experimental data [Lowesmith, 2007], the overpressure at the vent presented is using the data from 2 instruments located just inside the enclosure close to the vent, one under the centre of the vent and one in the corner of the test rig (see Figure 4-3). A higher pressure was recorded for the transducer in the corner of the rig, probably due to the proximity of boundaries on 3 sides. As these transducers are just inside the vent there are not directly comparable with the blast decay predictions at the vent (particularly the corner transducer), but the result from the centre transducer is used. The instruments outside the vent, also shown on Figure 4-3, were 8 m away in 2 (perpendicular) directions, and lastly at 16 and 32 m away from the vent.
4.4.2.1 **INDEXP 13**

(Test 13 - Pure methane, ER=1.1, no pipes)

The predicted flame speed (Figure 4-9 (a)) development follows the observed trend up to 5m from the rear wall, then the flame speed is predicted to accelerate towards the vent emerging at a speed similar to the deduced flame speed outside the vent.

The blast decay (Figure 4-9 (b)) is conservatively predicted, with the location 8m away from the vent seeing the greatest overprediction.

![INDEXP 13: Flame Speed](image1)
![INDEXP13: Maximum Overpressure Outside Chamber](image2)

Figure 4-9: (a) INDEXP13: Flame Speed; (b) INDEXP13: Maximum overpressure outside chamber (data from [Lowesmith, 2007])
4.4.2.2  \textit{INDEXP 6}

(Test 6 - 80\% methane/20\% hydrogen, ER=1.1, no pipes)

The predicted flame speed (Figure 4-10 (a)) development follows the observed trend up to 5m from the rear wall, then the flame speed is predicted to accelerate towards the vent emerging at a speed similar to the deduced flame speed outside the vent.

The blast decay (Figure 4-10 (b)) is conservatively predicted, with the location 8m away from the vent seeing the greatest overprediction.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4_10.png}
\caption{Figure 4-10: (a) INDEXP06: Flame Speed; (b) INDEXP06: Maximum overpressure outside chamber (data from [Lowesmith, 2007])}
\end{figure}
4.4.2.3  INDEXP 8

(Test 8 - 80% methane/20% hydrogen, ER=0.8, 0 pipes)
The predicted flame speed (Figure 4-11 (a)) development follows the observed trend up to 4 or 5m when the flame speed is predicted to accelerate faster than observed towards the vent emerging at a speed similar to the deduced flame speed outside the vent.

The blast decay (Figure 4-11 (a)) is greatly overpredicted, with the location 8m away from the vent seeing the greatest overprediction.

Figure 4-11: (a) INDEXP08: Flame Speed; (b) INDEXP08: Maximum overpressure outside chamber (data from [Lowesmith, 2007])
4.4.2.4  **INDEXP 11**

(Test 11 - 80% methane/20% hydrogen, ER=1.1, 17 pipes)

The predicted flame speed (Figure 4-12 (a)) development follows the observed trend up to 6m when the flame speed is predicted to accelerate faster than observed towards the vent emerging at a speed similar to the deduced flame speed outside the vent.

The blast decay (Figure 4-12 (b)) is conservatively predicted but markedly less so then the previous tests. The source overpressure is being underpredicted and at the flame speeds predicted the assumption of no compression of the gas in the external cloud no longer holds [Puttock et al., 2000]. The pressure at the vent in this experiment is seen to be under predicted in this simulation.

![INDEXP 11: Flame Speed](image1)

![INDEXP11: Maximum Overpressure Outside Chamber](image2)

**Figure 4-12:** (a) INDEXP11: Flame Speed; (b) INDEXP11: Maximum overpressure outside chamber (data from [Lowesmith, 2007])
4.4.2.5 **INDEXP 10**

(50% methane/50% hydrogen, ER=1.1, no pipes)

The predicted flame speed (Figure 4-13 (a)) development follows the observed trend up to 5m when the flame speed is predicted to accelerate faster than observed towards the vent emerging at a speed similar to the deduced flame speed outside the vent.

Some of the blast decay (Figure 4-13 (b)) predictions show a reasonable fit in the far field but the (source) pressure at the vent is underpredicted in this simulation. Once again, at the high flame speeds predicted the assumption of no compression of the gas in the external cloud no longer holds.

![INDEXP 10: Flame Speed](image1)

![INDEXP 10: Maximum Overpressure Outside Chamber](image2)

Figure 4-13: (a) INDEXP10: Flame Speed; (b) INDEXP10: Maximum overpressure outside chamber (data from [Lowesmith, 2007])
4.4.2.6  **INDEXP 14**

(50% methane/50% hydrogen, ER=1.1, 17 pipes)

The predicted flame speed (Figure 4-14 (a)) development follows the observed trend closely up to 6m when the flame speed is predicted to accelerate slightly faster than observed towards the vent emerging at a speed similar to the deduced flame speed outside the vent. Interestingly the flame is predicted to slow down by a small amount before it reaches the vent.

The blast decay (Figure 4-14 (b)) is mostly underpredicted. This may be due to the high flame speed and the assumption of no compression of the gas in the external cloud.

![INDEXP 14: Flame Speed](image1)

![INDEXP14: Maximum Overpressure Outside Chamber](image2)

**Figure 4-14:** (a) INDEXP14: Flame Speed; (b) INDEXP14: Maximum overpressure outside chamber (data from [Lowesmith, 2007])
4.4.2.7 Overall Comments

The results for flame speed show how the flame speed increases as it passes through obstacle grids (dashed vertical lines in the graphs). In general there is very good agreement across all the tests.

The blast decay predictions for tests 13, 6, and 8 (Figure 4-9 (a), Figure 4-10 (a) and Figure 4-11 (a) respectively) are mostly reasonable and are on the conservative side. The source pressure is similar to the range seen in the experiments and the decay is of the right general form. For tests 11, 10 and 14 (Figure 4-12 (a), Figure 4-13 (a) and Figure 4-14 (a) respectively) the initial source pressure is underpredicted but the pressure decay becomes reasonable after 16m. These tests are for 17 pipes with 20% hydrogen, and 50% hydrogen with 0 and 17 pipes, and are the tests with the highest vent flame speeds and pressures.

The predicted overpressure is compared with the measured overpressures from transducers just inside the enclosure and on the floor, a fairer comparison would be with an overpressure measurement in the centre of the vent where the effect of the floor and vent lip would not be present. Further, it is noted that the model does not include any terms to allow for the compression of the gas in the external cloud [Puttock et al., 2000] which may also explain the underpredictions for the faster flame speeds.

4.5 Conclusion

New fuel files have been created for SCOPE, for fuel mixtures of 20% and 50% hydrogen addition to methane, using the burning velocity work studied in Chapter 3 and from the Leeds turbulent burning velocity experiments. Comparisons have been made of predictions by the modified SCOPE model against experimental data with favourable results for both vent flame speed and overpressure in the enclosure, for methane, 80:20 and 50:50 methane:hydrogen mixtures in cases where no pipework and for 17 pipes.
were included inside the enclosure. Further, SCOPE predicts well the flame speed development inside the enclosure and the free field decay away from the vent, although the external explosion was sometimes under-predicted in cases where the flame speed was high.

The importance of representing the roughness, or blockage, of metal work on the enclosure walls has been emphasized for good predictions, and should be included in the guidance of preparing the input data for the model.

The way in which SCOPE is able to model different fuels means that to model other fuel mixtures of varying amounts of hydrogen new fuel files are needed to be created. Although work on the laminar burning velocity for a complete range of hydrogen addition to natural gas has been done, the variation of the Markstein number and turbulent response over the full range has not been studied. This may present implementation problems, and while it may be possible to hypothesize the effects, any validation will need to wait until such information is available.
5 Compact Cubic Explosion

5.1 Introduction

An explosion occurring from the central ignition of a uniform mixture of gas and air in a compact congested region, that is, where the length of each side of the rig is approximately the same as each other, is studied in this chapter. This geometry has been extensively studied as part of the MERGE European project comprising of experiments and modelling [Mercx, 1994]. In this chapter the Shell CAM2 model [Puttock, 1999] (see Section 2.5.1.4) is used and a model from GL Industrial Services (see Section 2.5.2.3) is modified to enable explosions involving methane/hydrogen mixtures to be simulated. The predictions from both models are compared with the results of experiments conducted within the NATURALHY project.

5.2 Experiments

The compact congested region used for this work consisted of a three dimensional region of obstacles where the length of each dimension of the rig was approximately the same. The rig had dimensions of 3m by 3m and was 2m high and thus was approximately cubic. As part of the NATURALHY project experiments were performed in this geometry in which explosions involving the ignition of mixtures of methane and hydrogen were studied. Shell Global Solutions performed the experiments at the HSL test site, Buxton, UK, and is reported by [Roberts et al., 2006]. A similar geometry has been studied previously as part of the European Commission funded MERGE project. The experimental rig is shown in Figure 5-1. It can be seen from the photograph that the rig is placed in front of a concrete wall.
The rig consisted of a metal framework structure based upon 1m cubes. Inside the rig there was a series of metal grids, in the lower half of the rig the grids were vertical and in the upper half they were horizontal. The grids were arranged to form 9 concentric squares (squares within squares), where 2 started in the centre cube of the rig. The bars on the grids were in line with other grids and measured 26mm±1mm, spaced 125mm apart and this provided a 20% area blockage ratio (ABR). The volume blockage ratio (VBR), which is the obstacle volume divided by the volume of the rig, was 4.4%. Important geometric parameters are listed in the Table 5-1.
Five experiments were undertaken in the rig in which stoichiometric mixtures of fuel and air were ignited. The fuel was initially held back by polythene sheeting. The fuel compositions used were approximately at an equivalence ratio (ER) of 1.1 which gives the worse case as the flame speeds will be the highest. During the tests the overpressure was measured inside and outside the congested region. Outside the congested region were three sets of pressure transducers, one set in a direction away from the wall, one set in a direction parallel to the wall and one set in a line vertically up the wall. It was thought that the presence of the wall would have negligible impact on the pressures measured, although this is discussed later. No direct measurement was taken of the flame speed and, although normal speed video footage was taken, this is not fast enough to resolve the flame speed with any accuracy. The test conditions are listed in Table 5-2 along with a summary of the maximum overpressures observed at selected locations which give an indication of the effect on the overpressure by the presence of hydrogen in methane.

<table>
<thead>
<tr>
<th>Rig Properties</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Overall dimensions (w x l x h)</td>
<td>3m x 3m x 2m</td>
</tr>
<tr>
<td>Grids</td>
<td></td>
</tr>
<tr>
<td>Bar size</td>
<td>26 mm ±1mm</td>
</tr>
<tr>
<td>Grid ABR</td>
<td>20%</td>
</tr>
<tr>
<td>Bar spacing</td>
<td>125 mm</td>
</tr>
<tr>
<td>Grid Spacing</td>
<td>150 mm</td>
</tr>
<tr>
<td>Number of concentric square grids</td>
<td>9</td>
</tr>
<tr>
<td>Grid starts (from centre ignition)</td>
<td>0.27m</td>
</tr>
<tr>
<td>Grid ends (from centre ignition)</td>
<td>1.43m</td>
</tr>
<tr>
<td>Number of layers of grids (upper)</td>
<td>7</td>
</tr>
<tr>
<td>Rig Volume</td>
<td>18 m$^3$</td>
</tr>
<tr>
<td>Obstacle Volume</td>
<td>0.793 m$^3$</td>
</tr>
<tr>
<td>Gas Volume</td>
<td>17.207 m$^3$</td>
</tr>
<tr>
<td>Volume Blockage Ratio (VBR)</td>
<td>4.4056%</td>
</tr>
</tbody>
</table>

Table 5-1: Compact congested rig parameters [Roberts et al., 2006]
### Table 5-2: Compact congest experimental programme of different fuel compositions

<table>
<thead>
<tr>
<th>Test</th>
<th>Fuel Composition (CH₄:H₂)</th>
<th>ER</th>
<th>Maximum Overpressures (mbar)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NatHy_02</td>
<td>CH₄</td>
<td>1.06</td>
<td>118</td>
</tr>
<tr>
<td>NatHy_04</td>
<td>75:25</td>
<td>1.09</td>
<td>137</td>
</tr>
<tr>
<td>NatHy_03</td>
<td>50:50</td>
<td>1.06</td>
<td>440</td>
</tr>
<tr>
<td>NatHy_05</td>
<td>25:75</td>
<td>1.08</td>
<td>793</td>
</tr>
<tr>
<td>NatHy_01</td>
<td>H₂</td>
<td>1.20</td>
<td>3032</td>
</tr>
</tbody>
</table>

Table 5-2: Compact congest experimental programme of different fuel compositions [Roberts et al., 2006]

In test NatHy_01 with 100% hydrogen a transition to detonation (DDT) is believed to have occurred close to the corners of the test rig. This is not reflected in the maximum pressures recorded as no instruments were positioned at the corners of the rig. However, the polythene sheeting was shredded into very small pieces, which is a characteristic of detonations, and this observation would be difficult to explain otherwise.

### 5.3 Modelling Methodology

Two modelling approaches have been used. The first was the Shell model CAM2 (see Section 2.5.1.4) and the second was a model called CCEM (Compact Congested Explosion Model) developed by the author, which is a modified version of a model developed by GL Industrial Services compact explosion model (see Section 2.5.2.3). These models where chosen as the most sophisticated models available of both empirical and phenomenological model types respectively.

#### 5.3.1 CAM2

An overview of this model was given in 2.5.1.4. The model was developed using a body of experimental work, from the E.U. project MERGE [Mercx, 1994] and experiments conducted by Shell in rigs of regular and symmetrical congestion. Briefly, the model includes a correlation for the maximum source overpressure and a pressure decay correlation. The derivation and application
of the model is discussed in the paper and will be presented here for an understanding of the model and any changes necessary for application to methane/hydrogen mixtures.

5.3.1.1 Source Pressure Model

The source overpressure correlation includes terms for fuel scaling, number of rows and their spacing, the blockage ratio, and size scaling [Puttock 1999].

Fuel Scaling

The overpressure is dependent on the rate of propagation of the flame which is a function of laminar burning velocity (amongst others). The CAM2 model used results from the MERGE experiments, which were carried out at small, medium and large scale, and then compared with several scaling theories. The author found that the overpressure should be proportional to the expression,

\[(u_l (E-1))^{2.712}\]

where \(u_l\) is the laminar burning velocity (m/s) and \(E\) is the expansion ratio (ratio of unburned to burned gas densities). When the expansion ratio drops to one there is no expansion driving flow ahead of the flame and there would be no overpressure generated, so this expression tends to zero as the expansion ratio drops to one.

Number and spacing of rows

It is found that the overpressure generation is dependent on the number of rows of obstacles passed by the flame. The row spacing is also importance, this effects how much turbulence is generated. As the flow passes an obstacle, turbulence is generated downstream, however this turbulence will decay and eventually dissipate (due to viscous forces) if no other obstacles are met. Thus for sufficiently large gaps the turbulence field may completely decay and the burning velocity will become small (and laminar). The question has been asked, and stated by Puttock as “When are two regions of congested plant sufficiently far apart that they can be considered as a separate area for the purposes of assessing explosions hazard?”.
The model takes into account the number of rows of obstacles, \( n \), by the power law \( n^{a_1} \) and their spacing, \( r \) (m), by \( r^{a_3} \), where \( a_1 \) and \( a_3 \) are constants.

**Blockage Ratio**

The expression used here is \( e^{a_2 b} \), where \( a_2 \) is a constant and \( b \) is the area blockage ratio which is a number between 0 and 1.

**Size Scaling**

The effect of the size of the obstacles, \( d \) (m), on the overpressure is to increase it. Fractal theory used for fuel scaling predicts that the overpressure will rise proportional to a representative obstacle diameter raised to the power of 0.71. Analysis of the MERGE experiments and other experiments showed this power to be closer to 0.55, hence \( d^{0.55} \) is used.

**Source Overpressure**

The final expression for pressure, \( P \) (bar), obtained is,

\[
P = a_0 \left( u_c (E - 1) \right)^{2.71} d^{0.55} n^{a_1} e^{a_2 b} r^{a_3},
\]

where the four ‘\( a \)’s are constants to be determined from fitting the expression to experimental data.

**Severity Index**

Puttock [1999] points out that there is no limit to the overpressure predicted by Equation (5-1). It is seen in experiments that if for one fuel the overpressure is low, say 40 mbar, doubling the fuel reactivity (that is, a fuel with double the laminar burning velocity) you are likely to get double the pressure. However, if for the first fuel the overpressure was 4 bar, the double reactivity fuel would not give 8 bar. For hydrocarbons, overpressures of about 8 bar (due to the expansion of the hot combustion products) are reached when burned at constant volume (confined explosion), that is, with no flow at all. If the gas in an unconfined explosion were being compressed to nearly 8 bar then there would be no flow and no turbulence to create the high overpressures. This is a negative feedback effect which reduces the flow and limits the increase of
pressure. If the fuel laminar burning velocity is increased, the overpressure does not necessarily increase by a proportional amount, the increase in overpressure rise with fuel reactivity becomes increasingly smaller with increasing overpressure.

To deal with this issue, Puttock introduces an easy to use correction factor termed the ‘severity index’ which is directly related to the overpressure. At low overpressures, the severity index is approximately the same as the pressure but for higher overpressures the severity index rises steeply and at around 8 bar the severity tends to infinity. The expression for the severity index is expressed as,

\[ S = P \exp\left( \frac{0.4 P}{E^{0.08} - 1 - P} \right) \]  \hspace{1cm} (5-2)

where \( P \) is the overpressure (bar) and \( E \) is the expansion ratio. This equation needs to be solved for \( P \) by iteration.

**Fitted model**

The final fitted expression is expressed as the following,

\[ S = a_0 \left( u_1 (E - 1) \right)^{2.71} l^{0.55} n^{a'_{1.1} e^a_{1.1}} \]  \hspace{1cm} (5-3)

where the fitted constants have the values, \( a_0 = 3.9 \times 10^{-5}, \ a_1 = 1.99 \ (a_1 = a_1 - 0.55), \ a_2 = 6.44 \) and \( l \equiv nrd \) which represents the distance of congestion the flame has to travel (m). Equation (5-3) is then equated with Equation (5-2) and solved, by iteration, for \( P \), the overpressure.

**Other Parameters**

There are other parameters that the author presents guidance for,

- Obstacle complexity
- Sharp edged obstacle
- Non-symmetrical congestion
- Plant with a roof
- One wall
- Long Narrow areas of plant
- Partial fill
Some of the guidance is applicable to calculating predictions but some is to seek further advice.

### 5.3.1.2 *Blast Decay Model*

The free field pressure decay model was introduced in Section 2.5.1.4 and is described by Puttock [1995]. To define a realistic and accurate pressure decay (blast decay) curve it is necessary to use numerical modelling to fill the gaps. This enables an accurate determination of the overpressure pressure field and discovers how it behaves in-between experimental measurements, which are often sparse and far apart. The calculations were performed in one dimension and with spherical symmetry and driven by a piston. The velocity-time history of the piston was chosen so that the pressure pulse measured just outside the source region was fitted. This method is similar to the method of TNO used for the multi energy method but in that methodology a constant velocity piston was assumed due to the absence of pressure-time data.

It is seen in experiments that after a certain distance the rate of pressure decay becomes faster. This is because the pressure wave has ‘shocked up’ to become a shock wave which dissipates faster. When the calculations of the pressure decay for different source pressures were plotted they could be made to coincide, apart from in the near field. This suggested that the same curve could represent the rapid part of the decay if shifted laterally on the distance axis. Data from the MERGE experiments were used to determine the appropriate lateral shift for the universal curve. The initial decay (near field) is still represented by acoustic decay, that is, the inverse of the distance.

The source radius, $R_0$ (m), is calculated as,

$$R_0 = \sqrt{\frac{3V_0}{2\pi}}$$  \hspace{1cm} (5-4)

where $V_0$ is the source volume (m$^3$) that is the volume of the gas compressed by the explosion.
Now we define, \( r \) (m), as the source radius plus the real target receiver distance, \( r' \) (m), from the edge of the congested region,

\[
r = R_0 + r'
\] (5-5)

The expression used to determine the pressure decay, \( P_1 \) (bar), with distance for the shocked up decay is,

\[
\log P_1 = 0.08 l^4 - 0.592 l^3 + 1.63 l^2 - 3.28 l + 1.39
\] (5-6)

where \( l \) is as follows,

\[
l = \log \frac{r}{R_0} + 0.2 - 0.02P_0
\] (5-7)

where \( P_0 \) is the source pressure (bar). Finally, to determine the pressure, \( P \) (bar), at a target receiver at a distance \( r \) from the centre of source explosion, the following expression is used,

\[
P = \min \left( \frac{R_0}{r} P_0, P_1 \right)
\] (5-8)

where the first term is the acoustic pressure decay law (inverse distance), and the second term is calculated as above in Equation 5-7.

Puttock presents sample curves calculated as above. They can be seen to be similar to the multi-energy curves but the faster decay starts later due to the more realistic accelerating piston. This method is also easy to use for different and arbitrary source pressures, whereas for the multi-energy method, it is necessary to read values off a graph which presents ten different source pressures.

**Pulse duration and shape**

Puttock also presents an expression for the duration of the pressure pulse and the pressure rise time (time from start of pressure increase to its peak). This allows structural response calculations. Although the TNO multi-energy method includes curves for duration there is none for its rise time. Puttock goes on to show how data from the MERGE experiments can be used to derive adequate expressions for both.
Puttock fits a triangle to each positive part of the pressure trace outside the source region. Three times are defined, $t_1$ is the first time (s) at which the best fit triangle crosses the x-axis, $t_2$ (s) is the time of the peak (of the triangle), and $t_3$ (s) is the last time the triangle crosses the axis. The duration is then defined as $t_3-t_1$ (s) and the author introduces $\frac{t_2-t_1}{t_3-t_1}$ (dimensionless) as the shape factor, or the ratio of the rise time to duration. The shape factor tends to zero for shocked waves.

The change of shape of the pressure wave is much higher for greater pressures. The author found that the duration and shape factor correlated very well when plotted against the distance scaled by the square of the source pressure, as follows,

$$d_f = \frac{t'}{R_0} \left( \frac{P_0}{P_a} \right)^2$$  \hspace{1cm} (5-9)

where $P_a$ is the ambient/atmospheric pressure (bar). For the duration time, $t_3-t_1$, the author presents,

$$t_3 - t_1 = C \frac{R_0}{\sqrt{\frac{P_0}{\rho_a}}}$$  \hspace{1cm} (5-10)

where $\rho_a$ is the ambient density and $C$ is a constant and has values as follows,

$$C = 0.65 \text{ for } d_f < 5$$

$$C = 0.65 \left( \frac{d_f + 10}{15} \right) \text{ for } 5 < d_f < 20$$  \hspace{1cm} (5-11)

$$C = 1.3 \text{ for } 20 < d_f$$

The shape factor is represented by taking a linear decay with $d_f$ and is as follows,

$$\frac{t_2-t_1}{t_3-t_1} = \max(0.65(1 - 1.25d_f),0)$$  \hspace{1cm} (5-12)
5.3.1.3 **Model Implementation and Usage**

To use this model for the current application, it is necessary to consider how it may handle methane and hydrogen mixtures of varying combinations. The model has two parameters that take into account the effect of the fuel, these are the laminar burning velocity $u_l$, and the expansion ratio $E$. These parameters need to be known for a fuel to be able to evaluate a prediction. The other parameters are known or can be calculated from the geometry of the situation. It was found that by inputting the laminar burning velocity and the expansion ratio for methane/hydrogen mixtures, that the model gave good results and so no fundamental modifications were needed.

To run predictions the model was implemented in a spreadsheet (Microsoft Excel). Some special functions were implemented in Excel macros to find the roots of an equation (using the False Position Method), specifically to solve for $P$ in Equation (5-2). The laminar burning velocity was determined from Chapter 3, and the expansion ratio was determined from Gaseq 0.79 [www.arcl02.dsl.pipex.com].

Once developed, a set of spreadsheets corresponding to each of the five tests was created and developed to perform the model calculations. These were appropriately populated with the geometry parameters and the corresponding change in fuel parameters. The spreadsheet program then evaluated the (maximum) source overpressure. This source overpressure value then linked through to the pressure decay model and pulse shape model.

5.3.2 **Compact Congested Explosion Model (CCEM)**

The GL Services model for compact congested regions was introduced in Section 2.5.2.3 and can be found in the papers by Cleaver and Robinson [1996] and Cleaver et al. [1997]. It consists of three parts that link together:

- First there is a flame speed model which produces the flame speed profile (flame speed with distance);
• second there is an overpressure model which uses the flame speed profile to produce predictions of the overpressure at the flame front through the source congested region;
• finally the source overpressure profile is taken in by the blast decay model that advects the overpressure points with time to produce pressure-time curves at transducer locations.

The following is list of assumptions stated by Cleaver and Robinson [1996],
• complete combustion as the flame passes into the mixture ahead of it,
• uniform conditions behind the flame,
• instantaneously there is an incompressible flow field ahead of the flame,
• adiabatic compression of the fluid ahead of the flame,
• the total drag of one obstacle can be represented by the sum of its inertial and form drag,
• the total drag of the obstacles can be represented by the sum of the drag of each obstacle,
• the half-cube-shaped region can be mapped onto a hemisphere of equal volume.

5.3.2.1 Flame Speed Model

It was found from the MERGE experiments that for all but the most explosive experiments the flame speed profile over the congestion could be made to collapse onto a single curve if made dimensionless. To do this, the flame speed was normalised using the maximum flame speed and a length scale was used to normalise the distance. A correlation was then fitted to this curve. Correlations were then produced for the maximum flame speed and the distance length scale which are valid only for methane.

Cleaver et al. [1997] present the general equation of this model giving the flame speed, \( S_f \) (m/s), as a function of the (average) flame radius, \( R_f \) (m), from the centre spark as a prescribed shape as follows,
Chapter 5

\[ S_f(R_f) = S_{f_{\text{max}}} \exp\left(0.5 \left(\frac{R_f - L}{\alpha L}\right)^2\right) \]  
(5-13)

where, \( L (\text{m}) \) is a length scale (see equation (5-17)), \( S_{f_{\text{max}}} \) is the maximum flame speed (m/s) and \( \alpha \) is a dimensionless constant as follows,

\[ \alpha = 0.3 \text{ for } \frac{R_f}{L} \leq 1 \]  
(5-14)

when the flame is inside the congested region and

\[ \alpha = 0.4 \text{ for } \frac{R_f}{L} > 1 \]  
(5-15)

when the flame is outside the congested region. This controls the acceleration of the flame.

The maximum flame speed, \( S_{f_{\text{max}}} \), can be found by the following correlation [GL code, 2006],

\[ S_{f_{\text{max}}} = S_0 K (\text{ABR})^A (\text{Pitch})^B (\text{Scale})^C \]  
(5-16)

where \( S_0, K, A, B, C \) are constants and ABR is the area blockage ratio (a number between 0 and 1), Pitch is the representative distance between congestion grids/arrays (m), and Scale is a representative length scale that turbulence occurs over which is represented by the diameter of the obstacles in the congestion (m).

The length scale is the acceleration distance to the maximum speed, and is calculated as follows [GL Code, 2006],

\[ L = \left(\frac{S_{f_{\text{max}}}}{S_{f_{\text{rep}}}}\right)^E \]  
(5-17)

where \( E \) is a constant, and \( S_{f_{\text{rep}}} \) is a representative flame speed.

### 5.3.2.2 Flame Speed Model Modifications for CCEM

In the GL model there are various parts:
(1) there is the non-dimensional flame speed correlation which gives the expected shape of the flame speed profile for a cubical geometry (Equation (5-13))

(2) the maximum flame speed obtained ($S_{f_{max}}$ given by Equation (5-16))

(3) the distance it takes to get to $S_{f_{max}}$ ($L$, given in Equation (5-17))

Parts (2) and (3) give dimension to part (1), controlling how the prescribed shape expands in both the distance and speed axes. The maximum flame speed is calculated through a correlation that is a function of ABR, Pitch and a length scale. The correlation has been fitted and constants derived for natural gas at nominally stoichiometric concentrations. The acceleration distance is a function of the maximum flame speed and has two constants.

The question is, how will adding hydrogen affect the flame speed and how can this can be implemented into the correlations of this model? Adding hydrogen to methane is known to increase the laminar burning velocity (Chapter 3), at an increasing rate with hydrogen addition by volume. Therefore, it follows that the burning velocity in a flame will also increase with hydrogen addition. This will change the maximum flame speed attained and how fast it accelerates.

It is assumed that the geometry parameters in the correlation for the maximum flame speed apply no matter what the fuel is. However, the fuel type will affect the maximum flame speed and hence the acceleration distance. As the correlations were derived for natural gas there is no explicit dependence on the fuel. The aim in this work was to introduce an explicit dependence on fuel properties to generalise the applicability of the model to other fuels.

If one assumes that the geometric considerations apply to the current situation (that is, application to a similar geometry) then the only other term in the maximum flame speed expression (Equation (5-16)) related to flame speed is the constant $S_{00}$ (m/s), which is some reference speed calibrated to natural gas. Since the acceleration distance is a function of the maximum flame speed...
speed the acceleration distance will change if the maximum flame speed changes.

It is known that different fuels and mixtures burn differently. The (unstretched) laminar burning velocity of a fuel gives an indication of the reactivity of the fuel and can be easily compared to other laminar burning velocities of other fuels to gauge reactivity. It is reasonable to assume that given a different fuel with a different laminar burning velocity that the flame speed will be different, due to, in particular, the change in mass burning rate, area generation rate, expansion rate, acceleration of the flame, and turbulence intensity, all of which may affect each other. Furthermore, at the same scale (predictions for flame speeds are difficult to scale [Mercx et al., 1995]) it seems reasonable to suggest that, if a particular fuel burns a proportion faster than another, then the maximum flame speed (at the same scale) may also be that same proportion faster. Hence,

\[
\frac{S_{\text{new}}}{S_{\text{reference}}} \propto \frac{u}{u_{\text{reference}}}
\]

(5-18)

The GL model does not include a dependence on the fuel and its concentration and is only applicable for nominally stoichiometric natural gas mixtures.

Different fuels and fuel/air mixtures have different expansion ratios. The expansion ratio defines how much more volume the hot combustion products occupy than when at the initial conditions. The expansion of the hot combustion products helps push the flame outwards and this affects the flame speed. In this geometry the hot combustion products are trapped behind the flame front and the expansion pushes the flame outwards. The lower the expansion ratio the less the push on the flame front and thus a lower flame speed and vice versa. So the difference in the expansion ratio of a selected fuel compared to the fuel used to generate the original correlation needs to be taken into account. The effect on the maximum flame speed achieved is taken to be the ratio of the expansion ratio for the selected fuel over the expansion ratio for the reference fuel (natural gas at an equivalence ratio of 1) as follows,
The turbulent burning velocity data of Leeds University [Fairweather et al., 2006] suggests that mixtures containing 50% methane and 50% hydrogen exhibit an enhanced response to the turbulence level (see Section 4.3.1 for a discussion). The turbulent burning velocity for a 50:50 CH\textsubscript{4}:H\textsubscript{2} mixture was found to be 1.46 times greater (for the same turbulence intensity level) than the turbulent burning velocity for a methane/hydrogen mixture containing 20% or less hydrogen.

As a flame develops it may develop a cellular structure on its surface as a consequence of diffusion-thermal instability which results from the competing effects of heat conduction from the flame and reactant diffusion towards the flame [Hu et al., 2009]. The Lewis number ($Le$) can be used to represent this instability, it is calculated as the ratio of heat diffusivity of the mixture to mass diffusivity of the limiting reactant (the reactant in the reaction that limits the amount of product that can be formed). When the Lewis number is below a critical value (slightly lower than one) the flame develops a cellular structure on its surface and when the Lewis number is above one the flame is said to be stable. Adding hydrogen to methane decreases the Lewis number and the flame becomes more unstable [Hu et al., 2009].

Defining $F_{td}$ as the thermal diffusive factor that takes into account the enhanced turbulent burning velocity at 50% hydrogen addition, then, the maximum flame speed is proposed to be affected as follows,

$$\frac{(S_{f_{new}})_{new}}{(S_{f_{new}})_{reference}} \propto \frac{(E)_{new}}{(E)_{reference}} \cdot F_{td} \quad (5-20)$$

Putting all this together, the maximum flame speed is now an explicit function of laminar burning velocity, expansion ratio and a factor to take into changes in the turbulent burning velocity for 50:50 mixtures, as follows,
where $u_{gas}$ and $u_{NG}$ are the laminar burning velocities of the fuel concerned and natural gas and similarly for $E$. $F_{td}$ equals 1 for methane and concentrations up to 20% hydrogen and equals 1.46 for 50:50 mixtures. By introducing the dependence on burning velocity, this means that different equivalence ratios and different fuels can also be simulated by using an appropriate burning velocity and expansion ratio.

To use this formulation parameters for the reference fuel, natural gas at stoichiometric concentrations, are needed. Laminar burning velocity data and correlations for various fuels can be found in the literature. The expansion ratio can be calculated from the density of the fuel mixture at ambient conditions and the density of the fuel mixture at the adiabatic flame temperature.

The overpressure predictions are not as sensitive to the flame acceleration distance as they are for the maximum flame speed. Therefore, as the flame acceleration distance (Equation (5-17)) already depends on the maximum flame speed, this equation was unmodified.

### 5.3.2.3 Source Overpressure Model

The overpressure model used by GL Services is described by Cleaver and Robinson [1996]. The resulting equations are “used to relate the value of the overpressure at the flame front to the flame position as a function of time”. The derivation can be found in the appendix of Cleaver and Robinson [1996], and are introduced here.

The conservation of mass is written, in spherical coordinates, as,

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial \rho ur^2}{\partial r} = 0$$  \hspace{1cm} (5-22)

where $r$ is the radius, $u$ is the fluid velocity, $t$ is the time and $\rho$ is the fluid density. The conservation of momentum is written as,
\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial r} = \frac{-1}{\rho} \frac{\partial p}{\partial r} - f
\]  \hspace{1cm} (5-23)

where \( p \) is the pressure and \( f \) is the force drag term, given by:

\[
f = k_1 \frac{\partial u}{\partial t} + k_2 \frac{1}{2} u^2
\]  \hspace{1cm} (5-24)

when the flame is in the congested region, and \( f = 0 \) when the flame is outside the congestion.

For the flame inside the congested region of radius, \( R_c \), then,

\[
(1 + k_1) \frac{\partial u}{\partial t} + k_2 \frac{1}{2} u^2 + \frac{\partial}{\partial r} \frac{1}{2} u^2 = \frac{-1}{\rho} \frac{\partial p}{\partial r}
\]  \hspace{1cm} (5-25)

and for \( r > R_c \),

\[
\frac{\partial u}{\partial t} + \frac{\partial}{\partial r} \frac{1}{2} u^2 = \frac{-1}{\rho} \frac{\partial p}{\partial r}
\]  \hspace{1cm} (5-26)

To include compressibility in a simple fashion, \( \rho \), has been expressed, assuming adiabatic compression, in terms of pressure as

\[
\frac{-1}{\rho} \frac{\partial p}{\partial r} = \frac{p_0^{\gamma/\gamma}}{\rho_0} \frac{\gamma}{(\gamma - 1)} \frac{\partial p}{\partial r}^{(\gamma - 1)/\gamma}
\]  \hspace{1cm} (5-27)

where \( \gamma \) is the ratio of specific heats, and the subscript \( 0 \) represents a reference condition.

Substituting equation (5-27) into the sum of Equations (5-25) and (5-26) and integrating the resulting equation from flame front radius, \( R_f \), to the outer boundary at infinity gives

\[
k_1 \int_{R_f}^{R} \frac{\partial u}{\partial t} dr + \int_{R_f}^{\infty} \frac{\partial u}{\partial t} dr + \int_{R_f}^{\infty} \frac{\partial}{\partial t} \frac{1}{2} u^2 dr + k_2 \int_{R_f}^{R} \frac{1}{2} u^2 dr
\]

\[
= \frac{-p_0^{\gamma/\gamma}}{\rho_0} \frac{\gamma}{(\gamma - 1)} \int_{R_f}^{\infty} \frac{\partial p}{\partial r}^{(\gamma - 1)/\gamma}
\]  \hspace{1cm} (5-28)

In this equation the density of the air and the fuel/air mixture ahead of the flame have both been put equal to \( \rho_0 \) as the difference for most fuels of interest within the flammable limits is small.
To evaluate the first, second and fourth integrals in Equation (5-28) a velocity field must be specified. This has been done by treating the equation of conservation of mass as incompressible. Integrating Equation (5-22) using this assumption gives

\[ u(r) = u(R_f) \frac{R_f^2}{r^2} \quad (5-29) \]

where \( u(R_f) \) is the value of the velocity as the flame front is approached from the unburnt gas. This is a simplification which will become less valid for higher flame speeds.

Substituting Equation (5-28) into Equation (5-27) and integrating gives,

\[ \frac{p(R_f)}{p(\infty)} = \left[ \frac{\gamma - 1}{a^2} \left\{ 2u(R_f) \frac{dR_f}{dt} + R_f \frac{du}{dt} (R_f) \left( 1 + k_f \left( 1 - \frac{R_f}{R_c} \right) \right) \right\} \right]^{\gamma/(\gamma-1)} \quad (5-30) \]

where the reference pressure \( p_o \), and density \( \rho_0 \) have been set to \( p(\infty) \) and \( \rho(\infty) \), respectively, which represent the ambient atmospheric pressure and density, and \( a \) is the speed of sound in the ambient fluid.

Introducing \( u(R_f) = S_f - u_i \) and \( u(R_f) = S_f \left( \frac{E - 1}{E} \right) \), where \( u_i \) is the laminar burning velocity, \( S_f \) is the flame speed and \( E \) is the expansion ratio of the fuel. The expansion ratio is chosen to be constant inferring uniform conditions behind the flame. Using this relationship and noting that \( \frac{dR_f}{dt} = S_f \) the following, analytical, equation is obtained,

\[ \frac{p(R_f)}{p(\infty)} = \left[ \frac{\gamma - 1}{a^2} \left( A + B - C + D \right) + 1 \right]^{\gamma/(\gamma-1)} \quad (5-31) \]

where \( A, B, C, \) and \( D \) are,
\[ A = \frac{(E - 1)}{E} \left( 2S_f^2 + R_f \frac{dS_f}{dt} \right) \]

\[ B = k_1 \left( 1 - \frac{R_f}{R_c} \right) A \]

\[ C = 1/2 \left( S_f \frac{(E - 1)}{E} \right)^2 \]

\[ D = k_2 \frac{R_f}{3} \left( 1 - \left( \frac{R_f}{R_c} \right)^3 \right) C \]

The use of a single value of the expansion ratio infers that conditions behind the flame are uniform and the validity of this assumption is discussed in the paper.

5.3.2.4 Drag

Drag is the force that resists the movement of a solid object through a fluid. ‘Form’ drag arises due to the shape of the solid body and can be easily modified by changing the shape. Inertial drag arises due to the body pushing the fluid out of the way.

The inertial drag experienced by an obstacle is written as

\[ F_i = C_m V_0 \rho \frac{\partial u_g}{\partial t} \]

where \( F_i \) is the force on the body, \( V_0 \) is the volume of the obstacle, \( \rho \) is the density, \( u_g \) is the velocity of the incoming gas flow and \( C_m \) is a constant that depends on the shape of the obstacle.

To find the value of the constant \( k_1 \) in Equation (5-24), the form inertial term of \( f \) (first term in Equation (5-24) is integrated over a volume \( V \), multiplied by the density, and setting this equal to Equation (5-33) and rearranging we arrive at,

\[ k_1 = C_m V_b \]
used for grids of obstacles. \( C_m \) has been taken to be 1.5 for spherical bodies and 2.0 for cylindrical bodies.

The force due to form (in uniform flow) is written as,

\[
F_d = \frac{1}{2} \rho u_g^2 C_d A_0
\]  

(5-35)

where \( F_d \) is the force due to drag, \( \rho \) is the density, \( A_0 \) is the profile area of the object normal to the flow, \( u_g \) is the incoming gas velocity, and \( C_d \) is the coefficient of drag which is a number that depends on the shape of the object and the Reynolds number of the flow.

To find the value of the constant \( k_2 \) in Equation (5-24), the form drag term of \( f \) (second term in Equation (5-24) is integrated over a volume \( V \), multiplied by the density, setting this equal to the Equation (5-35) and rearranging we arrive at,

\[
k_2 = C_d \frac{A_0}{V}
\]  

(5-36)

Moreover, if it is assumed that for an array of obstacles that there is no interaction of the flow between them (true in the limit of small \( A_0d/V \) or \( V_{\text{obstacle_extent}}/V \), where \( d \) is the obstacle diameter),

\[
k_2 = C_d \frac{A_t}{V}
\]  

(5-37)

where \( A_t \) is the total obstacle area normal to the flow in volume \( V \) of the congested region. The authors suggest modifying \( C_d \) to take into account of interaction of the wakes downstream of obstacle arrays. The value of \( C_d \) used in the model is 1.0. This seems reasonable looking at how the coefficient changes with Reynolds number in the Reynolds number range of 20 to about 10x10^5 for a circular cylinder [Blevins, 1984, pp338].

### 5.3.2.5 Blast Model

The overpressure model predicts the overpressure at the flame front when given the flame speed-distance profile. This implicitly associates the predicted
pressure with the input value of the flame speed and position, and thus this value is also associated with the time the flame was at this position. This information is used by the blast model to predict how the pressure wave propagates into free space.

This model, unlike correlation based approaches (such as the TNO multi-energy curves and Puttock's [1995] correlations), uses a series of approximate equations to predict the general advancement of a waveform. It does this by assuming that the propagation of a general pressure wave can be "determined from the relationships used to describe the propagation of a shock wave in still air" [Cleaver et al., 1996].

The speed of propagation of a point on the wave-form describing overpressure is defined by the following relationship [Whitham, 1974, pp174],

\[
\frac{d\Delta P}{dr} = -\frac{\Delta P}{r} \tag{5-39}
\]

where \( r \) is the distance from the source and \( \Delta P \) is the overpressure.

Eventually parts of the waveform may steepen and without any intervention would become 'triple valued', which in gas-dynamics is not physically possible (unlike for water waves). This can be seen in Figure 5-3 where the value of \( P \)
(pressure) has three values for a specific value of x (distance) shown as the vertical dashed line. Thus a correction thus needs to be applied. The following sketch also shows the method used to fit a discontinuity into the wave-form. The dashed line defines the new wave-form which is determined by conserving mass (density) between the two areas of the initial curve that it intersects.

Figure 5-2: Diagram of a ‘breaking’ pressure wave

The authors state that using this technique the velocity of the shock front, \( w_s \), can be calculated via,

\[
ws = \frac{\int \rho(P)w(P)dP}{\int \rho(P)dP}
\]  

(5-40)

Where \( \rho \) is the density of air, \( P \) is the pressure and \( w \) is the speed of propagation of a point on the wave (Equation (5-38). The result is that the speed of the shock front is actually less than that of the maximum part of the pressure wave, and thus once a shock has formed the decay rate is faster than the acoustic rate. For small pressure disturbances, that is, acoustic waves (linear waves) this methodology correctly predicts propagation without change of shape, and for stronger waves correctly predicts the formation of a shock discontinuity in the wave-form.
The authors present an application of this model and compare it to the waveforms from the TNT equivalence method and show good agreement.

### 5.3.2.6 CCEM Model Implementation and Usage

The CCEM model described above was implemented in a computer program in a manner that allowed various modifications to be trialled and different ways of data input to be used. Experimental input conditions come from a series of electronic files, combustion data for the various fuel compositions come from a electronic file, and appropriate thermodynamic properties come from an electronic file [McBride and Gordon, 1996] (see APPENDIX C).

There are three parts of the model that need to be run, the flame speed model, the source overpressure model, and the blast decay model. Results from the previous part are needed to run the next part along the chain.

#### Flame Speed Model of CCEM

The flame model was implemented as a loop over the distance from the spark as the flame propagates with distance the flame speed is calculated by the model. Geometric parameters that are needed are the dimensions of the rig, a representative obstacle diameter, the pitch or the distance between obstacle array. These parameters are readily evaluated from the specification of the experimental rig and can be found in Roberts et al. [2006].

Care should be applied when calculating the representative diameter of the obstacles. When a range of obstacles with differing diameters or lengths are present then it is not enough to take just the diameter of the majority of the obstacles. The flame speed increases with increasing obstacle diameter and even when there is only a relatively small amount of obstacles with a larger diameter this can act to increase the flame speed. Therefore, in this analysis, (where the majority of the obstacles had a diameter of 26mm) the diameter used as input was increased to 34mm because of the larger diameter steel support framework.
The laminar burning velocity for the various fuel compositions was taken from the correlation in Huang et al. [2006] for convenience (this was compared against the experimental work from Leeds University and other correlations in Section 3.5.2). The expansion ratio was calculated using the heat of combustion of the specific mixture (specific for the equivalences ratio) and finding the temperature that the enthalpy of the mixture equals the heat of combustion [Kuo, 2005]. The value of $F_{td}$ (Equation (5-20) in Section 5.3.2.2) is taken to be 1 for hydrogen additions up to 50% and 1.46 for 50% H$_2$ addition to methane and above (Note that no specific data is available for higher hydrogen concentrations).

**Source Overpressure and Blast Decay Model**

The density expansion ratio and ratio of specific heats were calculated from the mixture properties and thermodynamic data from an electric source. The reference density and pressure was taken to be ambient air at standard conditions (1 atm and 25°C).

The overpressure model predicts the overpressure at the flame front, so that each value is provided at a given (advancing) location and a specific time. The blast model needs the wave form, that is, the pressure with distance at a specific time, to be able to propagate the pressure wave away from the flame. This is done by iterating with time (through the source region) and using the blast model (the model assumes free space, although in this region there is congestion which would provide reflection and distortion of the wave-form) to advect each point to determine the pressure wave-form at the current time step. Each point given by the source overpressure model is at a different time. Therefore the waveform at the edge of the congested region, at the time the flame exits, (the starting point for the blast model as pressure generation is developing inside the congested region but decays outside) is needed. This is done by iterating over the points in the source overpressure model and advecting them by the time it takes for the flame front at that location to exit the congestion. The closer the flame gets to the edge of the congestion the shorter the time to advect the source overpressure at that location.
5.4 Results – Comparison of predictions with data

To assess the performance of the models it is necessary to run predictions for the experiments described in Section 5.2 and then compare the predictions with the experimental results [Roberts et al., 2006]. The overpressures were recorded in this set of experiments, and although the explosion was filmed, this was done at normal speed, 25fps (frames per second), and not fast enough to successfully determine how the flame speed develops in any resolution. Hence, the success of the flame speed modelling can only be judged by considering the resulting pressure predictions. If the overpressure is predicted accurately, it suggests that the flame speed model must have provided sensible predictions.

5.4.1 Comparison of predicted explosion overpressure against experimental data

A summary of the source overpressure for the 5 experiments as predicted by the Shell CAM2 (a) and CCEM model (b) is compared against the experimental observations [Roberts et al., 2006] in Figure 5-3. The Shell CAM2 model (Figure 5-3 a) predicts the source overpressure very well, within 45% of the experimental measurement. However, for 50% hydrogen test there is a 25% underprediction. The prediction for the 100% hydrogen test is the largest overpredictions at 44% over the measured value, but this is discussed further in the following paragraph. The CCEM model (Figure 5-3 b) also predicts the maximum overpressure well up to 50% hydrogen addition, having a maximum overprediction of 32% more than observed. For 75% hydrogen addition the maximum overpressure is overpredicted, by 166. For 100% there is a very large over-prediction compared to the measured value.
As the experimental rig is cubical in shape the distance from the centre of the rig to the corner is larger than from the centre of the rig to the edge. The pressure transducers in the experiments were placed on the axis from the centre of the rig to the middle of the edge of the rig and not in the corners. The consequence of this is that the pressures in the corners are not measured and in this location higher overpressures are experienced due to the flame having to travel through a greater distance of congestion, plus the flame approaches the 3 sides of the congestion support framework at the corners. The consequence of this, is that the maximum overpressure measured in the experiment may not be the actual highest generated. This may be evident in the experiments with more hydrogen content in the mixture as the flame is moving much faster and the acceleration is faster so the pressure increase is occurring over a small length scale. As noted under Table 5-1, it is thought that the overpressures generated in the 100% hydrogen test were higher than actually measured and that a transition to detonation occurred at the corners of the test rig. Consequently, the model predictions for the 100% hydrogen cases may not be an overprediction. However, these models were not designed to simulate detonations nor the transition for deflagration to detonation. It is sufficient that the models predict a high and generally unacceptable pressure.
An alternative and interesting view of the data is presented in Figure 5-4. This graph plots the source overpressure against the percentage of hydrogen added to methane. This shows the increasing rate at which the source overpressure rises with hydrogen addition.

![Graph showing source overpressure increase with hydrogen addition](image)

**Figure 5-4: Source overpressure increase with hydrogen addition**

### 5.4.2 CAM2 – Detailed Results

Predictions have been obtained for tests NatHy_01 to NatHy_05. The following table summarises the source overpressures predicted and the experimental results, including the factor difference to the experimental values.
Table 5-3: Summary of explosion overpressures from CAM2 predictions and experiments (data from [Roberts et al., 2006])

<table>
<thead>
<tr>
<th>Test</th>
<th>%v/v hydrogen</th>
<th>Overpressure (bar) Result</th>
<th>Factor Increase</th>
</tr>
</thead>
<tbody>
<tr>
<td>NatHy_02</td>
<td>0</td>
<td>0.118</td>
<td>1.039</td>
</tr>
<tr>
<td>NatHy_04</td>
<td>25</td>
<td>0.137</td>
<td>1.170</td>
</tr>
<tr>
<td>NatHy_03</td>
<td>51</td>
<td>0.44</td>
<td>0.731</td>
</tr>
<tr>
<td>NatHy_05</td>
<td>75</td>
<td>0.793</td>
<td>1.448</td>
</tr>
<tr>
<td>NatHy_01</td>
<td>100</td>
<td>4.58</td>
<td>1.387</td>
</tr>
</tbody>
</table>

The following five graphs plot the pressure decay away from the source region predicted in two ways; firstly using the predicted source overpressure and secondly using the experimentally determined source overpressure. This allows one to see how the pressure decay model compares with the experimentally measured decay given the same source pressure. There are two sets of experimental data shown on the plots from the transducers in two different directions relative to the wall located by the test rig (Section 5.2).

As can be seen from Figure 5-5 to Figure 5-9, the predictions of pressure decay with distance (noted as free field on the figures) generally good in the near field (to about 4 or 5m) but in the far field the predictions are lower than the data.

It was noted in Section 5.2 that there was a concrete wall located near the test rig, which was thought to have no effect on the pressures measured [Roberts et al., 2006]. However it is known that if a pressure wave hits a flat wall then part of it is reflected back, therefore it could be expected that the large concrete wall behind the test rig may be reflecting pressure waves and resulting in slightly higher pressures being measured during the tests. To model this situation, the source volume, $V_0$, is doubled to take into account the concrete wall as a reflecting surface and the effective source radius, $R_0$, in Equation (5-4) is recalculated which increases by $2^{(1/3)}$. In reality it takes time...
for the reflected wave to travel to the wall to reflect off the wall and travel
towards a transducer by which time the main blast has propagated away so
there is no direct combination of the maximum of the main blast wave and
maximum of the reflected wave. The graphs below (Figure 5-5 to Figure 5-9)
include additional predictions which account for the reflected wave and are
labelled ‘with reflection’. The free field predictions are labelled ‘free field’. As
can be seen, the predictions ‘with reflection’ are mostly conservative
compared to the data.

![NatHy_02: Methane - Maximum Overpressure with Distance](image)

Figure 5-5: NatHy_02 – 100% methane - CAM2 and experimental (data from [Roberts et
al., 2006]) overpressure-distance graph
Figure 5-6: NatHy_04 - 75:25 CH₄:H₂ - CAM2 and experimental (data from [Roberts et al., 2006]) overpressure-distance graph
Figure 5.7: NatHy_03 – 50:50 CH₄:H₂ - CAM2 and experimental (data from [Roberts et al., 2006]) overpressure-distance graph
Figure 5-8: NatHy_05 - 25:75 CH₄:H₂ - CAM2 and experimental (data from [Roberts et al., 2006]) overpressure-distance graph
5.4.3 CCEM – Detailed Results

Five files were created and populated with the correct parameters required by the model. These were then loaded by the program and the model run. Output files were generated by each part of the model (flame, overpressure and blast) in a text delimited format which were then imported into spreadsheets (Microsoft Excel) which provided the results in graphical form.

The flame speed profile and maximum overpressures with distance can also be plotted to compare with the experimental values.

Figure 5-10 shows the predicted flame speed profiles for all 5 experiments. The methane flame was the slowest and took the longest to accelerate.
Adding hydrogen to the fuel mixture resulted in an increase in the flame speed and the acceleration distance decreased. As stated before the flame speed was not determined during the experiments, although we could infer, from the validation of the original model, that the methane predictions are satisfactory. Validation of the predicted flame speeds can be inferred providing the explosion overpressures compare favourably with the experimentally measured overpressures.

![Flame Speed Chart](image.png)

**Figure 5-10: CCEM flame speed profile results for all tests**

Figure 5-11 to Figure 5-15 show the predicted overpressure with distance plotted with the experimental observations, for the 5 experiments in order of increasing hydrogen content. In general the source overpressure is predicted well for up to 50% hydrogen, but for test NatHy_05 and NatHy_01 (with 75% and 100% hydrogen), the source overpressures are significantly overpredicted. This information is summarised in Table 5-4. This can be explained by the fact that at large flame speeds (approaching and passing the speed of sound) compressibility effects become important. This model assumes incompressibility to simplify the problem, for predictions of compressible flow use of a CFD model is advisable.
<table>
<thead>
<tr>
<th>Test</th>
<th>%v/v hydrogen</th>
<th>Overpressure (bar)</th>
<th>Factor Increase</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Result</td>
<td>Prediction</td>
</tr>
<tr>
<td>NatHy_02</td>
<td>0</td>
<td>0.118</td>
<td>0.118</td>
</tr>
<tr>
<td>NatHy_04</td>
<td>25</td>
<td>0.137</td>
<td>0.158</td>
</tr>
<tr>
<td>NatHy_03</td>
<td>51</td>
<td>0.44</td>
<td>0.579</td>
</tr>
<tr>
<td>NatHy_05</td>
<td>75</td>
<td>0.793</td>
<td>2.109</td>
</tr>
<tr>
<td>NatHy_01</td>
<td>100</td>
<td>4.58</td>
<td>54.765</td>
</tr>
</tbody>
</table>

Table 5-4: Summary of explosion overpressures from CCEM predictions and experiments (data from [Roberts et al., 2006])

As can be seen from Figure 5-11 to Figure 5-13, with up to 50% hydrogen, the predicted pressure decay with distance is satisfactory in the near field but under-predicts the experimental results in the far field. For the 75% hydrogen and 100% hydrogen cases (Figure 5-14 and Figure 5-15) the predictions of pressure decay with distance are unsatisfactory due to significant overpredictions of the source overpressure. As noted in Section 5.4.2, it is possible that the experimental measurements were affected by reflections of the pressure waves off the wall located by the test rig.
Figure 5-11: NatHy_02 - 100% methane – CCEM and experimental (data from [Roberts et al., 2006]) maximum overpressure with distance

Figure 5-12: NatHy_04 - 75:25 CH₄:H₂– CCEM and experimental (data from [Roberts et al., 2006]) maximum overpressure with distance
Figure 5-13: NatHy_03 - 50:50 CH$_4$:H$_2$ – CCEM and experimental (data from [Roberts et al., 2006]) maximum overpressure with distance

Figure 5-14: Test NatHy_05 - 25:75 CH$_4$:H$_2$ – CCEM and experimental (data from [Roberts et al., 2006]) maximum overpressure with distance
5.5 **Conclusions**

The Shell CAM2 has been applied (unmodified) to model the experimental programme and for the full range of methane and hydrogen fuel compositions. New laminar burning velocities (studied in Chapter 3) for the various fuel compositions, and expansion ratios were calculated and used as input to the model which was produced in spreadsheet format. The predicted source overpressure was found to be within a factor of 2 (see Section 2.6.2) across the full range of methane and hydrogen compositions. Further, the blast decay was also found to be mostly satisfactory, although appeared to be slightly underpredicted in the far field but this may be due to the presence of the concrete wall near the rig. Therefore, CAM2 is suitable for predicting the consequences of explosions following the release of a methane/hydrogen mixture into a compact congested region of pipework, providing a transition to detonation does not occur.
A phenomenological called CCEM (Compact Congested Explosion Model) has been developed based on a GL model. It includes a modified expression for flame speed which enables the model to be used for fuels other than methane and at a range of equivalence ratios. Predictions compared favourably with the results of the tests with up to 50% hydrogen. Hence, it is concluded that CCEM can be used to predict the consequences of explosions following the release of a methane/hydrogen mixture containing up to 50% hydrogen into a compact congested region of pipework. For concentrations above 75% hydrogen the model overpredicts the overpressure. Indeed for the 100% hydrogen case a overpressure of 55bar was predicted. During the experiment a transition to detonation occurred, so whilst the overpressure prediction may not be accurate, it did correctly identify an extreme event.

Because the predictions for 100% hydrogen are so significantly overpredicted it is useful to explore how the model behaves between 75% hydrogen in the fuel mixture up to pure hydrogen, and particularly if the pressure predicted may indicate the possibility of detonation. Figure 5-16 shows the predicted flame speed for 2 other methane/hydrogen ratios inbetween the experimentally studied compositions. The three flame speed plots are for 10% methane 90% hydrogen, 5% methane 95% hydrogen and pure hydrogen. It can be seen that even for a small increase in the hydrogen content of the fuel mixture the significant difference in the flame speed predicted. This is due to the increasing rate at which the laminar burning velocity increases; for 10% methane 90% hydrogen the laminar burning velocity is 1.62 m/s, for 5% methane 95% hydrogen the laminar burning velocity is 1.97 m/s and for pure hydrogen is the laminar burning velocity is 2.65 m/s.
Figure 5-16: Predicted flame speed for 90% and 95% hydrogen added to methane

Figure 5-17 shows the predicted free field pressure decay for 10% methane 90% hydrogen. The source pressure (~10bar) is over double what is measured in the pure hydrogen test. Figure 5-18 shows the predicted free field pressure decay for 5% methane 95% hydrogen. The source pressure (~24bar) is nearly 5 times what is measured in the experiment with pure hydrogen. At these predicted overpressure levels catastrophic damage to life and property will result and, although may not be representative of the actual event, the predictions indicate that the consequences are devastating which for risk assessment purposes may be sufficient. These predictions also suggest that a transition to detonation would probably occur for the case with 90% and 95% hydrogen in the mixture.
Figure 5-17: 90% hydrogen 10% methane – maximum overpressure with distance and data for 100% hydrogen

Figure 5-18: 95% hydrogen 5% methane – maximum overpressure with distance and data for 100% hydrogen
6 Pipe Rack with Initial Confinement

6.1 Introduction

In this chapter an explosion resulting from the ignition of a uniform gas-air mixture in an unconfined long congested region (typical of an industrial piperack) is studied. This type of geometry has been studied before by GL Industrial Services and a model had been developed for application to natural gas. In this chapter, this model is extended to take into account hydrogen addition to the fuel and the inclusion of a confined vented region prior to the pipework congestion.

6.2 Experiments

The NATURALHY project experiments were undertaken in a region of congestion much longer than it was wide or high, that is the aspect ratio, length of the dimension in the other orthogonal direction, is high (over 3:1) [Lowesmith, 2008]. Photographs of the high aspect ratio vapour cloud explosion rig are shown in Figure 6-1 and Figure 6-2. The region contained a series of regular pipe grids representing idealised congestion. Additionally there was a confined region which was located at one end of the congested region. This enclosure was confined on all faces except the face to which the congested region was attached. Pipes forming congestion could also be installed in the confined enclosure in a series of rows or racks. The whole of the rig consisting of the confined and congested regions was filled with a uniform fuel/air mixture. Ignition for most of the experiments took place at the wall at the back of the confined enclosure creating a flame which vented out of the enclosure into the congested region where it interacted with the pipework.
obstacles. (Polythene sheet was wrapped around the sides of the congested region to prevent the fuel/air mixture escaping prior to ignition).

Figure 6-1: Photograph of external congested region and initial confined enclosure [Lowesmith, 2008]

Figure 6-2: Photograph of the rig for the high aspect ratio vapour cloud explosion experiments [Lowesmith, 2008]
The experimental setup for the ionisation probes (IP), used to detect the flame position with time, is presented in Figure 6-3 and the experimental setup for the pressure transducers is presented in Figure 6-4 [Lowesmith, 2008]. The labels with prefix ‘IP’ are the locations of the ionisation probes and the labels with prefix ‘R’ identify the name of the row or rack of pipes.

![Diagram of experimental setup](image_url)

**Figure 6-3: Plan and elevation view of ionisation probes [Lowesmith, 2008] (‘IP’: ionisation probe, ‘R’: pipe rack)**

**Figure 6-4: Plan view of pressure transducers [Lowesmith, 2008] (‘T’: pressure transducer, ‘R’: pipe rack)**
Fourteen experiments were undertaken by Loughborough University at the GL Industrial Services test site at Spadeadam, UK. The experiments were designed with a region of confinement before the congested region so that the speed of the flame entering the congested region could be varied. The purpose of this arrangement was to facilitate studying the effect of the initial flame speed and subsequent flame acceleration in the congested region with methane/hydrogen mixtures.

It was known from previous work in a similar test configuration that methane reaches a limiting flame speed. However, hydrogen would be expected to accelerate and undergo a transition to detonation (based on the findings of Chapter 5). Hence, it is important to assess the behaviour of methane/hydrogen mixtures with different levels of hydrogen.

The confined enclosure located at the beginning of the congested region was the same enclosure as that used for the confined vented explosion (as studied in Chapter 4) and could also include pipework congestion inside. The number of pipes in the confined enclosure was varied to alter the flame speed exiting into the congested region. The congested region was 18m long, 3m wide and 3m high, and consisted of twelve racks holding up to seven pipes each and placed 1.5m apart along the length of the rig. The number of pipes in the congested region was also varied during the test programme. Ignition was initiated by means of a spark which was located within the enclosure for most of the tests. The spark could be located on the rear wall of the enclosure opposite the vent, the centre of the enclosure, or in the vent opening of the enclosure. The ignition location also affected the flame speed entering the congested region. The test conditions are given in Table 6-1 identifying the nominal flame speed which entered the congested region and the methane/hydrogen mixture used.
### Table 6-1: Test condition matrix

* shaded cells indicate the test conditions that lead to, and are expected to lead to (for blank cells), a flame that continues to accelerate - see Section 6.4.2.1 for a discussion.

(a) VCE06 was a repeat of VCE05 as no IP data was collected during VCE05.
(b) VCE09 was a repeat of VCE07 as a non-uniform gas mixture was thought to be produced during VCE07.
(c) VCE10 was ignited at the end of the congestion. It is considered that the flame acceleration was adversely affected by the proximity of the chamber ahead of the flame.
(d) VCE13 was ignited at the beginning of the congested region, at the vent of the chamber.

Data was recorded from ionisation probes (IP’s), high speed video cameras, and pressure transducers [Lowesmith, 2008]. The ionisation probes detected when the flame arrived at each probe location, and from the distance-time data the average speed between probes was calculated. The flame speed was also determined from analysis of the high speed video records. Table 6-2 also presents the experimental test conditions in test order with more details of the test arrangement and also as summary of the results in terms of flame speed and overpressure development through the congested region.

<table>
<thead>
<tr>
<th>Gas Composition</th>
<th>Standard Congestion Arrangement</th>
<th>Reduced Congestion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>VCE01, VCE04</td>
<td></td>
</tr>
<tr>
<td>80:20</td>
<td>VCE02, VCE05, VCE06\textsuperscript{a}</td>
<td>VCE14</td>
</tr>
<tr>
<td>70:30</td>
<td>VCE12</td>
<td></td>
</tr>
<tr>
<td>60:40</td>
<td>VCE08</td>
<td></td>
</tr>
<tr>
<td>50:50</td>
<td>VCE10\textsuperscript{c}, VCE13\textsuperscript{d}</td>
<td>VCE03, VCE11, VCE07, VCE09\textsuperscript{b}</td>
</tr>
<tr>
<td>Test</td>
<td>Gas</td>
<td>Ignition Location</td>
</tr>
<tr>
<td>--------</td>
<td>-----</td>
<td>-------------------</td>
</tr>
<tr>
<td>VCE 01</td>
<td>CH4</td>
<td>Centre of box</td>
</tr>
<tr>
<td>VCE 02</td>
<td>81:19</td>
<td>Centre of box</td>
</tr>
<tr>
<td>VCE 03</td>
<td>51:49</td>
<td>Centre of box</td>
</tr>
<tr>
<td>Test</td>
<td>Gas</td>
<td>Ignition Location</td>
</tr>
<tr>
<td>-------</td>
<td>-----</td>
<td>-------------------</td>
</tr>
<tr>
<td>VCE 04</td>
<td>CH4</td>
<td>Rear of box</td>
</tr>
<tr>
<td>VCE 05</td>
<td>79:21</td>
<td>Rear of box</td>
</tr>
<tr>
<td>VCE 06</td>
<td>79:21</td>
<td>Rear of box</td>
</tr>
<tr>
<td>Test</td>
<td>Gas</td>
<td>Ignition Location</td>
</tr>
<tr>
<td>-------</td>
<td>-------</td>
<td>-------------------</td>
</tr>
<tr>
<td>VCE 07</td>
<td>51:49</td>
<td>Centre of box</td>
</tr>
<tr>
<td>VCE 08</td>
<td>58:42</td>
<td>Centre of box</td>
</tr>
<tr>
<td>VCE 09</td>
<td>51:49</td>
<td>Centre of box</td>
</tr>
<tr>
<td>VCE 10</td>
<td>48:52</td>
<td>East end of congestion</td>
</tr>
</tbody>
</table>

**Notes:**
- ER: Expansion Ratio
- Overpressure values are in mbar.
<table>
<thead>
<tr>
<th>Test</th>
<th>Gas</th>
<th>Ignition Location</th>
<th>Pipes in Box</th>
<th>Congestion</th>
<th>Actual ER</th>
<th>Vent Speed m/s</th>
<th>Flame Speed in Congestion</th>
<th>Overpressure in congestion (based on 0.1ms rolling average data)</th>
<th>Other Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>VCE 11</td>
<td>51:49</td>
<td>Rear of box</td>
<td>0</td>
<td>Standard</td>
<td>1.07</td>
<td>150</td>
<td>Accelerated to about 750m/s by Rack 10 then DDT after Rack 11</td>
<td>Pressures over 2 bar throughout and peaks about 12bar. Many transducers lost due to blast</td>
<td></td>
</tr>
<tr>
<td>VCE 12</td>
<td>71:29</td>
<td>Centre of box</td>
<td>5</td>
<td>Standard</td>
<td>1.09</td>
<td>~60</td>
<td>Accelerated to about 200-250m/s for mid section of congestion. Steadied to about 180-200m/s</td>
<td>Pressures highest in the central region of the congestion at up to 560mbar.</td>
<td></td>
</tr>
<tr>
<td>VCE 13</td>
<td>49:51</td>
<td>At Vent</td>
<td>0</td>
<td>Standard</td>
<td>1.05</td>
<td>0</td>
<td>Accelerated to about 140 m/s by end of congestion</td>
<td>Pressures increased throughout congestion reaching about 570mbar by end of congestion</td>
<td></td>
</tr>
<tr>
<td>VCE 14</td>
<td>79:21</td>
<td>Rear of box</td>
<td>21</td>
<td>Standard</td>
<td>1.03</td>
<td>~340</td>
<td>Accelerated to 600-650m/s and remained at that level to end</td>
<td>Very high pressures produced. Generally 3-7bar in congestion. Increased and then remained fairly steady.</td>
<td></td>
</tr>
</tbody>
</table>

Table 6-2: Test conditions and summary of observations
6.3 **Modelling Methodology**

The GL Services model for high aspect ratio congested regions for natural gas VCEs was provided in source code format and is called HAREM (High Aspect Ratio Explosion Model). HAREM predicts the flame speed, source overpressure and blast decay for natural gas explosions. Similar to the model for compact regions (Section 5.3.2), it consists of three parts that link together.

- First, a flame speed model which produces the flame speed profile (flame speed with distance);
- Second, an overpressure model which uses the flame speed profile to produce predictions of the overpressure at the flame front through the source congested region;
- Finally, the source overpressure profile is taken in by the blast decay model that advects the overpressure points with time to produce pressure-time curves at transducer locations.

### 6.3.1 Flame Speed within HAREM

For natural gas in this type of geometry, when ignited from a spark, the resulting flame accelerates until it reaches a terminal speed which (in uniform congestion) will be sustained until the end of the congestion before decelerating. However, in some of the NATURALHY experiments mixtures of natural gas and hydrogen produced flames which continued to accelerate until the end of the region. It is not known, if the flame would have achieved a terminal speed if the congested region had been longer.

The flame speed model assumes that a maximum flame speed is achieved. The flame speed correlation has multiple parts to it. The non dimensional profile is divided into 3 stages, representing a phase where the flame accelerates; a terminal velocity phase; and a deceleration phase after the flame exits the congested region. The maximum speed and distance over which the flame achieves this speed is given by correlations.
For a distance less than the distance over which the flame accelerates, $X_{S_{f_{\text{max}}}}$, [Humphreys, 1999], the flame speed, $S_f$, at a distance from ignition, $x$, is given by,

$$S_f(x) = \max\left(S_{f_{\text{min}}}, S_{f_{\text{max}}} \sin^2\left(\frac{\pi x}{2X_{S_{f_{\text{max}}}}}\right)\right) \quad \text{for} \quad x < X_{S_{f_{\text{max}}}}$$ \hspace{1cm} (6-1)

where $S_{f_{\text{min}}}$ is the minimum flame speed allowed, $S_{f_{\text{max}}}$ is the maximum flame speed achieved. After $X_{S_{f_{\text{max}}}}$, the flame is assumed to travel at the terminal velocity until the end of the congested region,

$$S_f(x) = S_{f_{\text{max}}} \quad \text{for} \quad X_{S_{f_{\text{max}}}} \leq x \leq L$$ \hspace{1cm} (6-2)

where $L$ is the length of the congested region. After the flame exits the congested region, the deceleration of the flame is described by the following

$$S_f(x) = S_{f_{\text{max}}} \exp\left(-3.125 \frac{(x-L)}{X_{S_{f_{\text{max}}}}}^2\right) \quad \text{for} \quad x > L$$ \hspace{1cm} (6-3)

The maximum flame speed, $S_{f_{\text{max}}}$, [Fortran code, 2006], is determined as,

$$S_{f_{\text{max}}} = 60.0(VBR)^{1.73} \frac{D_{\text{min}}^{2.23}}{d^{1.73}}$$ \hspace{1cm} (6-4)

and the acceleration distance, $X_{S_{f_{\text{max}}}}$,

$$X_{S_{f_{\text{max}}}} = 1.3 \left(8.0(VBR)^{1.5} \frac{D_{\text{min}}^{2.19}}{d^{1.19}}\right)$$ \hspace{1cm} (6-5)

where $VBR$ is the volume blockage ratio of the congestion (a number between 0 and 1), $D$ is the minimum dimension of the congested region (m) and $d$ is a representative diameter of the congestion (m).

### 6.3.2 Modification to the Flame Speed Model

In the GL model there are various parts:

1. there is the non-dimensional flame speed correlation which gives the expected shape of the flame speed profile (Equations (6-1) to (6-3))
2. the maximum flame speed obtained (Equation (6-4))
(3) the distance it takes to get there (Equation (6-5))

Parts (2) and (3) give dimension to part (1), controlling how the prescribed shape expands in both the distance and speed axes. The maximum flame speed and the acceleration distance are calculated through correlations that are functions of the VBR, obstacle diameter and the minimum dimension of the congested region. These have been fitted to natural gas experiments at nominally stoichiometric concentrations.

To enable the model to be applied to the VCEs involving methane/hydrogen mixtures in the geometry described in Section 6.2, it was necessary to make modifications to accommodate a flame which already has some velocity as it enters the congestion. Additionally, the flame acceleration and maximum speeds will differ for methane/hydrogen mixtures compared to methane due to the increased burning velocity of these fuels. Finally, the flame speed model was also modified to allow for non-stoichiometric mixtures to be simulated.

### 6.3.2.1 Comments on Ignition Conditions

In the NATURALHY test programme (see Section 6.2) the ignition of the VCE in the unconfined region was provided by an explosion venting from an enclosure. Therefore, when looking at the flame speed in the unconfined region, the flame speed starts at some value and not from rest. As the HAREM flame speed model is for spark ignition of a gas-air mixture in an unconfined region the model needs to be modified to account for an incoming flame that is already moving at some speed and with some incoming turbulence.

The flame exiting the enclosure already has some speed and overpressure has already been generated. The pressure wave travels ahead of the flame into the unconfined region. The flame then, when it enters the unconfined region, experiences a turbulent flow field which acts to increase the flame speed. As the flame speed is increased this itself generates more turbulence ahead of the flame which acts to further increase the flame speed. For some
fuels there is a limit to the flame speed that can be achieved but for other fuels the turbulence acts to keep increasing the flame speed. Therefore the acceleration of the flame and maximum flame speed achieved may be affected by the incoming conditions from the confined enclosure.

As the HAREM model is in the form of a correlation which has been fitted to experimental observations where the natural gas-air was spark ignited, the model embodies the effect of turbulence within the congested region. For low incoming flame speeds it may be possibly to start the flame profile at the exit flame speed from the enclosure by ‘shifting’ the flame profile along the distance axis. However, for faster flames, the turbulent flow field may be significantly different to that embodied in the correlations of the flame speed model as the flame is already turbulent as it vents from the enclosure.

The flow conditions at the vent of the enclosure can be determined from another model such as Shell’s SCOPE model, as used in Chapter 4. Therefore, the approach taken here was to use SCOPE to model the explosion in the enclosure and the results in terms of flame speed, pressure, and turbulence at the vent of the enclosure was used as input conditions for the flame model of the unconfined region.

### 6.3.2.2 Maximum Flame Speed

Neglecting, for the moment, the confined explosion ignition of the VCE in the unconfined region, it is also necessary to consider the effect of the fuel itself on the flame speed achieved. Similar arguments to those used for the CCEM model in Section 5.3.2 are applied.

The question is, how will adding hydrogen affect the flame speed and how can this be implemented by modifying the correlations of this model? Adding hydrogen to methane is known to increase the laminar burning velocity (Chapter 3), at an increasing rate with hydrogen addition by volume. Therefore, it follows that the burning velocity of the flame will also increase
with hydrogen addition. This will change the maximum flame speed attained and its rate of acceleration.

It is assumed that the geometry parameters in the correlation for the maximum flame speed apply no matter what fuel is used. However, the fuel type will affect the maximum flame speed and the acceleration distance. As the correlations were derived for natural gas there is no explicit dependence on the fuel properties. The aim in this work was to introduce an explicit dependence on fuel properties to generalise the applicability of the model to other fuels.

It is known that different fuels and mixtures burn differently. The (unstretched) laminar burning velocity of a fuel gives an indication of the reactivity of the fuel and can be easily compared to the laminar burning velocities of other fuels to gauge reactivity. It is reasonable to assume that given a different fuel with a different laminar burning velocity that the flame speed will be different, due to, in particular, the change in mass burning rate, area generation rate, expansion rate, acceleration of the flame, and turbulence intensity, all of which may affect each other. Furthermore, at the same scale (predictions for flame speeds are difficult to scale [Mercx et al., 1995]) it seems reasonable to suggest that, if a particular fuel burns proportionally faster than another, then the maximum flame speed (at the same scale) may also be that same proportion faster. Hence,

\[
\frac{\left( S_{f,\text{new}} \right)_{\text{new}}}{\left( S_{f,\text{new}} \right)_{\text{reference}}} \propto \frac{(u_f)_{\text{new}}}{(u_f)_{\text{reference}}} \tag{6-6}
\]

The original GL model does not include a dependence on the fuel concentrations and is only applicable for nominally stoichiometric mixtures. Equation (6-6) allows the model to accommodate changes in equivalence ratio as well as changes in the fuel type thereby broadening the applicability of the model.

The turbulent burning velocity data of Leeds University [Fairweather et al., 2006] suggest that mixtures containing 50% methane and 50% hydrogen
exhibit an enhanced response to the turbulence level (see Section 4.3.1 for a discussion). The turbulent burning velocity for a 50:50 CH$_4$:H$_2$ mixture was found to be 1.46 times greater (for the same turbulence intensity level) than the turbulent burning velocity for a methane/hydrogen mixture containing 20% or less hydrogen.

As a flame develops it may develop a cellular structure on its surface as a consequence of diffusion-thermal instability which results from the competing effects of heat conduction from the flame and reactant diffusion towards the flame [Hu et al., 2009]. The Lewis number ($Le$) can be used to represent this instability, it is calculated as the ratio of the heat diffusivity of the mixture to mass diffusivity of the limiting reactant (the reactant in the reaction that limits the amount of product that can be formed). When the Lewis number is below a critical value (slightly lower than one) the flame develops a cellular structure on its surface and when the Lewis number is above one the flame is said to be stable. Adding hydrogen to methane decreases the Lewis number and the flame becomes more unstable [Hu et al., 2009].

Defining $F_{td}$ as the thermal diffusive factor that takes into account the enhanced turbulent burning velocity at 50% hydrogen addition, then, the maximum flame speed is proposed to be affected as follows,

$$\left(\frac{S_{f_{new}}}{S_{f_{new}}}_{\text{reference}}\right) \propto F_{td}$$

(6-7)

### 6.3.2.3 Maximum Flame Speed with Incoming Explosion Ignition

As stated previously in Section 6.3.2.1, the maximum flame speed achieved in the unconfined piperack is affected by the incoming explosion venting from the enclosure. To take this into account a correlation for the effect on the maximum flame speed has been developed,

$$\left(\frac{S_{f_{new}}}{S_{f_{new}}}_{\text{reference}}\right) \propto 1.2 \left(\frac{u}{u_1}\right)^{0.75} + 1$$

(6-8)
where $u'$ is the turbulent fluctuation value (m/s). This equation does not modify the maximum flame speed if there is no incoming turbulence and the influence on the maximum flame speed slowly decreases with increasing turbulent fluctuation levels.

The correlation for the flame acceleration, Equation (6-1), is used with $x$ set as $x_r$, the real distance to the ignition, for a flame that begins at a zero speed. For an incoming flame with a speed (predicted from another model) the value of $x$ is set as $x'$ which is a ‘virtual’ distance from the flame to the ignition to shift the correlation laterally. $x'$ is set at a value that gives $S_f(x')$ as the incoming flame speed and can be defined as $x' = x_r + x_{in}$, where $x_{in}$ is the distance in which the correlation gives the incoming flame speed.

Therefore, the flame speed and turbulent fluctuations at the vent are needed as input to the model of the VCE in the congested region. In this work, the model SCOPE from Shell Global Solutions is used for this purpose as described in Chapter 4.

### 6.3.2.4 Flame Acceleration

For flames that do no continue to accelerate, it is seen in the experiments that the distance that the flame travels before it reaches its maximum speed varies.

As a flame propagates it is subject to stretching effects due to surface curvature and strain. The flame speed is affected by the stretching process (as introduced in Section 2.7.3). The Markstein number represents the sensitivity of the flame speed to stretch effects (Equation (2-8)). A fuel mixture with a positive Markstein number has its flame speed reduced by stretch effects (stable flames) and for negative Markstein numbers the flame speed increases with flame stretch (unstable flames). Therefore, the flame speed for a fuel with a smaller Markstein (positive) number is faster given the same stretch rate. The acceleration is modified simply as follows,
Note that in the limit of the assumptions made in the source overpressure model, in the next section, the acceleration distance is less important than the maximum flame speed. There is also some evidence in the tests where the flame speed reached a terminal speed that the flame starts to decelerate at the very end of the congested region. However, within the limit of accuracy of the source overpressure model, considering this aspect does not improve the predictions.

\[
\frac{X_{S_{\text{new}}}^{\text{new}}}{X_{S_{\text{new}}}^{\text{ref}}} \propto \frac{(Ma)_{\text{new}}}{(Ma)_{\text{ref}}}
\]  

(6-9)

6.3.3 Source Overpressure Model within HAREM

Assuming an infinitely wide congested region the flow can be considered as a one dimensional problem. For the case of a piperack the gas flow is neither planar or spherical, however, it is assumed that the pressure drop will be of similar form. Approximating the flame front as a planar surface, an equation was derived for the pressure drop in a similar manner as that for the compact cubic explosion [Cleaver and Robinson, 1996], see Section 5.3.2, and can be solved “pseudo” analytically. The flow behind the flame is no longer stationary as in the compact cubic explosion scenario hence an expression for the velocity of the gas behind the flame is also needed. The resulting, analytical, expression is as follows [Humphreys, 2000],
\[
\begin{align*}
P(R_f) &= \frac{\rho_0}{P_0^{1/\gamma}} + P_0^{1/\gamma} \left[ \frac{D}{2C-1} \frac{dS_f}{dt} + DS_f^2 \left( \frac{1}{2C-1} \right) + 0.5D^2E_i^2S_f^2 \\
& \quad + K_1 \left( \frac{D}{2C-1} - \frac{1}{2C-1} \right) \left( 1 - \left( \frac{R_f}{R_c^*} \right)^{2C-1} \right) \right] \\
& \quad + 0.5K_2 \frac{D^2}{4C^2-1} \frac{S_f^2}{E_i} \frac{R_f}{1 - \left( \frac{R_f}{R_c^*} \right)^{4C^2-1}} \right]^{\gamma-1} \\
&\quad \left[ + P_0^{1/\gamma} \right] \\
&\quad \left[ + P_0^{1/\gamma} \right]
\end{align*}
\]

(6-10)

\(R_f\) is the distance of the flame front from the ignition (m)
\(S_f\) is the flame speed at \(R_f\) (m/s)
\(P_0\) is the ambient pressure (Pa)
\(E\) is the expansion ratio
\(E_i = \frac{E-1}{E}\)
\(\gamma\) is the ratio of specific heats
\(\rho_0\) is the density (kg/m\(^3\))
\(R_c^* = L-x\)
\(x\) is the distance from the ignition point (m)
\(L\) is length of the congested region (m)
\(D\) is a constant with value of \(\min(Y,Z)\)/\((Y+Z)\)
\(Y\) is the \(y\) dimension of the congested region (m)
\(Z\) is the \(y\) dimension of the congested region (m)
\(C\) is a constant with value of 1 for this case where there are no walls or ceilings
\(K_1\) and \(K_2\) are constants derived in Section 5.3.2.4 and repeated here
\(K_1\) is a constant with value \(K_1 = C_mV_c\)
\(K_2\) is a constant with value \(K_2 = C_dV_c \frac{4\pi}{d}\)
\(C_m\) is the coefficient of inertia constant
\(C_d\) is the coefficient of drag constant

\(V_e\) is the effective volume blockage (0 to 1)

\(d\) is a representative pipe diameter (m)

The source overpressure model was not changed for the application to methane/hydrogen expressions except that, for high speed flames, that is flames over 350 m/s, Equation (5-2) [Puttock, 1999] was used to limit the overpressure.

### 6.3.4 Blast Decay Model within HAREM

This is the same model as for CCEM in Section 5.3.2.5. As the model is designed to predict the propagation of a general pressure wave, there are no assumptions about its shape and hence it is applicable to this model.

### 6.3.5 Model Implementation and Usage

The HAREM model described above including the modifications proposed was implemented in a computer program in a manner that allowed various modifications to be tested and different ways of data input to be used. Experimental input conditions come from a series of electronic files, combustion data for the various fuel compositions come from an electronic file, and appropriate thermodynamic properties also come from an electronic file [McBride and Gordon, 1996] (see APPENDIX C).

There are three parts of the model that need to be run, the flame speed model, the source overpressure model, and the blast decay model. Results from the previous part are needed to run the next part along the chain.

**Flame Speed Model**

The flame model was implemented as a loop over the distance from the spark as the flame propagates with distance the flame speed is calculated by the model. Geometric parameters that are needed are the dimensions of the rig, a
Chapter 6

representative obstacle diameter, the pitch or the distance between obstacle arrays. These parameters are readily evaluated from the specification of the experimental rig.

The laminar burning velocity for the various fuel compositions was taken from the correlation in Huang et al. [2006] for convenience (this was compared against the experimental work from Leeds University and other correlations in Section 3.5.2). The expansion ratio was calculated using the heat of combustion of the specific mixture (specific for the equivalences ratio) and finding the temperature that the enthalpy of the mixture equals the heat of combustion [Kuo, 2005].

Source Overpressure and Blast Decay Model
The expansion ratio and ratio of specific heats were calculated from the mixture properties and thermodynamic data from an electric source. The reference density and pressure was taken to be ambient air at standard conditions (1 atm and 25°C).

The overpressure model predicts the overpressure at the flame front, so that each value is provided at a given (advancing) location and a specific time. The blast model needs the wave form, that is, the pressure with distance at a specific time, to be able to propagate the pressure wave away from the flame. This is done by iterating with time (through the source region) and using the blast model (the model assumes free space, although in this region there is congestion which would provide reflection and distortion of the wave-form) to advect each point to determine the pressure wave-form at the current time step. Each point given by the source overpressure model is at a different time. Therefore the waveform at the edge of the congested region, at the time the flame exits the congestion, (the starting point for the blast model as pressure generation is developing inside the congested region but decays outside) is needed. This is done by iterating over the points in the source overpressure model and advecting them by the time it takes for the flame front at that location to exit the congestion. The closer the flame gets to the edge of the
congestion the shorter the time to advect the source overpressure at that location.

6.4 Results – Comparison with experimental data

Predictions of flame speed with distance and maximum overpressure with distance are now compared against experimental measurements [Lowesmith, 2008].

In the sections that follow two graphs are presented, the first shows the flame speed observed, using ionisation probes (IP) and high speed video analysis, compared against the model predictions. The second graph shows with the maximum overpressure observed and predicted at locations along the rig. The experimental data shown presents the maximum overpressure measured at each transducers location and also the maximum overpressure after the pressure traces have been subject to a rolling average of 0.1ms (see Section 2.6.1). This relatively short time period for the rolling average was selected to retain the structure of the pressure profile in some detail. However, it should be noted that short duration peaks do not contribute to structural response (see also Section 2.6.1).

The pressure traces generated by flame propagation through repeated obstacles have multiple peaks associated with pressure increase as the flame accelerate and passes through each obstacle array (piperack). Usually, the highest of these multiple peaks is associated with passage of the flame through the nearest piperack to the transducer location. Figure 6-5 shows an example pressure trace from transducer 8 (refer to Figure 6-4) for test 2. Also, the flame speed varies locally even if the overall speed is approximately steady, as it will accelerate as it passes through the obstacles on the piperack and decelerate in between the piperacks.
Figure 6-5: Pressure trace from a transducer within the congested region showing multiple pressure peaks produced by interaction of the flame with successive piperacks (R#) [Lowesmith, 2008]

The overpressure at the vent is taken as the predicted pressure at the vent as predicted by SCOPE. Table 6-3 lists the model predictions obtained from SCOPE at the vent of the enclosure and used as input into the flame speed model for the congested region for all the tests.

The presentation of results are split into two parts, the experiments where the flame speed reached a terminal speed and experiments where the flame continued to accelerate through the rig.
<table>
<thead>
<tr>
<th>Test</th>
<th>% CH₄</th>
<th>Ign. Loc</th>
<th>Pipes in Box</th>
<th>Unconfined Region Congestion</th>
<th>Vent Speed m/s</th>
<th>Ign. Pos. from the vent m</th>
<th>Turb. Int. m/s</th>
<th>Burn Rate m/s</th>
<th>Flow Speed m/s</th>
<th>Flame Speed m/s</th>
<th>Press mbar</th>
<th>Gas/Air Consumed m³</th>
</tr>
</thead>
<tbody>
<tr>
<td>vce01</td>
<td>100</td>
<td>C</td>
<td>17</td>
<td>S</td>
<td>45</td>
<td>4.1*</td>
<td>0.4</td>
<td>1.5</td>
<td>48.1</td>
<td>56.9</td>
<td>85</td>
<td>4</td>
</tr>
<tr>
<td>vce02</td>
<td>80</td>
<td>C</td>
<td>12</td>
<td>S</td>
<td>57</td>
<td>4.1*</td>
<td>0.7</td>
<td>2.5</td>
<td>63.5</td>
<td>78.1</td>
<td>145</td>
<td>5</td>
</tr>
<tr>
<td>vce03</td>
<td>50</td>
<td>C</td>
<td>0</td>
<td>S</td>
<td>70</td>
<td>4.1*</td>
<td>0.3</td>
<td>1.8</td>
<td>44.6</td>
<td>52.4</td>
<td>51</td>
<td>4</td>
</tr>
<tr>
<td>vce04</td>
<td>100</td>
<td>R</td>
<td>10</td>
<td>S</td>
<td>156</td>
<td>8.3</td>
<td>2.2</td>
<td>5</td>
<td>143.2</td>
<td>206.3</td>
<td>749</td>
<td>13</td>
</tr>
<tr>
<td>vce05</td>
<td>80</td>
<td>R</td>
<td>5</td>
<td>S</td>
<td>200</td>
<td>8.3</td>
<td>1.8</td>
<td>5</td>
<td>136</td>
<td>199</td>
<td>664</td>
<td>13</td>
</tr>
<tr>
<td>vce06</td>
<td>80</td>
<td>R</td>
<td>5</td>
<td>S</td>
<td>200</td>
<td>8.3</td>
<td>1.6</td>
<td>4.6</td>
<td>129</td>
<td>186.7</td>
<td>596</td>
<td>13</td>
</tr>
<tr>
<td>vce07</td>
<td>50</td>
<td>C</td>
<td>0</td>
<td>R</td>
<td>60</td>
<td>4.1*</td>
<td>0.3</td>
<td>1.8</td>
<td>44.6</td>
<td>52.4</td>
<td>51</td>
<td>4</td>
</tr>
<tr>
<td>vce08</td>
<td>60</td>
<td>C</td>
<td>5</td>
<td>S</td>
<td>75</td>
<td>4.1*</td>
<td>0.6</td>
<td>2.6</td>
<td>68.2</td>
<td>82.5</td>
<td>152</td>
<td>5</td>
</tr>
<tr>
<td>vce09</td>
<td>50</td>
<td>C</td>
<td>0</td>
<td>R</td>
<td>65</td>
<td>4.1*</td>
<td>0.3</td>
<td>1.8</td>
<td>44.6</td>
<td>52.4</td>
<td>51</td>
<td>4</td>
</tr>
<tr>
<td>vce10</td>
<td>50</td>
<td>E</td>
<td>0</td>
<td>S</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>vce11</td>
<td>50</td>
<td>R</td>
<td>0</td>
<td>S</td>
<td>150</td>
<td>8.3</td>
<td>1.1</td>
<td>4.3</td>
<td>128.5</td>
<td>180.1</td>
<td>562</td>
<td>13</td>
</tr>
<tr>
<td>vce12</td>
<td>70</td>
<td>C</td>
<td>5</td>
<td>S</td>
<td>60</td>
<td>4.1*</td>
<td>0.5</td>
<td>2.1</td>
<td>60.4</td>
<td>72</td>
<td>119</td>
<td>4</td>
</tr>
<tr>
<td>vce13</td>
<td>50</td>
<td>V</td>
<td>0</td>
<td>S</td>
<td>0</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>vce14</td>
<td>80</td>
<td>R</td>
<td>21</td>
<td>S</td>
<td>340</td>
<td>8.3</td>
<td>4.9</td>
<td>9.2</td>
<td>167.2</td>
<td>282.5</td>
<td>1173</td>
<td>17</td>
</tr>
</tbody>
</table>

Table 6-3: SCOPE predictions at enclosure vent

* modelled as half the enclosure length with ignition on rear wall of shortened enclosure

1 S for standard congestion (7 pipes and 6 pipes in arrays), R for reduced congestion (4 pipes and 3 pipes in arrays)
6.4.1 Predictions for explosions where the flame reaches a stable speed (non-accelerating flames)

The explosion experiments where an approximately stable flame speed was achieved were VCE01, 02, 04, 07, 09, 10 and 12 (VCE09 was a repeat of VCE07 as it was thought that the mixture during VCE07 was non-uniform. Hence only VCE09 is considered here).

As noted above the flames within congested regions of this type accelerate as they pass through each piperack and then decelerate again in-between (to a greater or less extent depending on whether the flame is overall accelerating, decelerating or reaching an approximately steady speed). Similarly, the overpressures vary locally. This makes comparison with single experimental values difficult even for these cases where an approximately steady flame speed was achieved. A better approach is to compare predictions with measurements along the length of congested region with measurements along the length of congested region, particularly within the region where the flame has achieved an approximately stable speed. Hence, Figures 6-6, 6-8, 6-10, 6-12, 6-14 and 6-16 present a comparison of predictions with data for the flame speed with distance through the congestion for tests VCE01, 02, 04, 09, 10 and 12 respectively. Figures 6-7, 6-9, 6-11, 6-13, 6-15 and 6-17 present a comparison of predictions with data for the overpressure with distance for tests VCE01, 02, 04, 09, 10 and 12 respectively.
Figure 6-6: VCE 01: predicted and experimental [Lowesmith, 2008] flame speed with distance

Figure 6-7: VCE 01: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance
Figure 6-8: VCE 02: predicted and experimental [Lowesmith, 2008] flame speed with distance

Figure 6-9: VCE 02: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance
Figure 6-10: VCE 04: predicted and experimental [Lowesmith, 2008] flame speed with distance

Figure 6-11: VCE 04: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance
Figure 6-12: VCE 09: predicted and experimental [Lowesmith, 2008] flame speed with distance

Figure 6-13: VCE 09: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance
Figure 6-14: VCE 10: predicted and experimental [Lowesmith, 2008] flame speed with distance

Figure 6-15: VCE 10: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance
6.4.1.1 **Discussion of flame speed predictions**

As can be seen by visual inspection of Figures 6-6, 6-8, 6-10, 6-12, 6-14 and 6-16 the flame speed is generally predicted well (mostly conservative compared to the locally measured maximum speed) across the experiments.
However, this is not a quantitative measure. To compare the predicted flame speed with experimental data quantitatively is difficult since speed fluctuates locally and hence any comparison will depend upon the location where the speed is measured. Additionally, video analysis to determine flame speed is difficult and sometimes subjective as it depends on the lighting conditions and visibility of the flame. Nevertheless, to provide a more quantitative assessment two approaches are attempted as summaries in Table 6-4. The first is to compare the predicted maximum flame speed with the maximum measured at any location (and by either video or IP data) and the second comparison was determined by further analysis of the video and IP time of arrival data to determine the average speed over the section of the congested region where the flame speed is approximately stable.

<table>
<thead>
<tr>
<th>Test</th>
<th>Maximum Flame Speed (ms⁻¹)</th>
<th>Flame Speed over Stable Region</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Measured</td>
<td>Predicted</td>
</tr>
<tr>
<td>01</td>
<td>159</td>
<td>158</td>
</tr>
<tr>
<td>02</td>
<td>181</td>
<td>219</td>
</tr>
<tr>
<td>04</td>
<td>383</td>
<td>390</td>
</tr>
<tr>
<td>09</td>
<td>130</td>
<td>122</td>
</tr>
<tr>
<td>10</td>
<td>82</td>
<td>103</td>
</tr>
<tr>
<td>12</td>
<td>232</td>
<td>194</td>
</tr>
</tbody>
</table>

1: Predicted value/measured value
2: Determined from either video analysis or IP data as the average speed over a region extending from approximately R4 to R10 (see Figure 6-3) except test 10 where the region was R8 to R3.

Table 6-4: Comparison of predicted and measured maximum flame speeds for tests with non-accelerating flames (data from [Lowesmith, 2008])
As can be seen from Table 6-4 the maximum flame speed is within a factor of 0.84 to 1.26 of the maximum flame speed as determined at all locations. When compared with an average flame speed determined over the region of stable speed, the predictions are with a factor 1.18 to 1.6. This comparison is probably a more representative assessment of model capability.

Overall, the predictions of flame speed are satisfactory (see Section 2.6.2), indicating the modifications to the model for the influence of the explosion venting from the enclosure into the congestion and the change in fuel has been accounted for satisfactorily.

6.4.1.2 Discussion of overpressure predictions

Inspection of Figures 6-7, 6-9, 6-11, 6-13, 6-15 and 6-17 show that the prediction of overpressure is generally conservative overpredicted. A summary of the maximum predicted and measured overpressure is given in Table 6-5.

<table>
<thead>
<tr>
<th>Test</th>
<th>Maximum Overpressure (mbar)</th>
<th>Observed</th>
<th>Predicted</th>
<th>Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>01</td>
<td></td>
<td>343</td>
<td>567</td>
<td>1.65</td>
</tr>
<tr>
<td>02</td>
<td></td>
<td>812</td>
<td>1233</td>
<td>1.52</td>
</tr>
<tr>
<td>04</td>
<td></td>
<td>2821</td>
<td>7485</td>
<td>2.65</td>
</tr>
<tr>
<td>09</td>
<td></td>
<td>276</td>
<td>252</td>
<td>0.91</td>
</tr>
<tr>
<td>10</td>
<td></td>
<td>141</td>
<td>186</td>
<td>1.32</td>
</tr>
<tr>
<td>12</td>
<td></td>
<td>557</td>
<td>930</td>
<td>1.67</td>
</tr>
</tbody>
</table>

1: Measured value is based on a 0.1 ms rolling average
2: Predicted value/measure value

Table 6-5: Comparison of predicted and measured maximum overpressure for tests with non-accelerating flames (data from [Lowesmith, 2008])

As can be seen, with the exception of VCE04, the predicted overpressure is within a factor of 2 of the measured overpressure (factor range 0.91 – 1.65) which is considered satisfactory for explosion modelling and within the
accuracy expected when modelling this type of complex event (see Section 2.6.2).

With regard to VCE04, the assumption of incompressibility in the source overpressure model is known to become less valid for faster fluid flows, particularly when the fluid flow approaches the speed of sound in the fluid. In this modified model a 'severity index' was incorporated (similar to Shell CAM2, equation (5-2)) to help to limit the overprediction in cases with high flame speeds, but the pressure was still significantly overpredicted in this case.

6.4.2 Predictions for explosions where the flame continues to increases its speed (accelerating flames)

The explosion experiments where an accelerating flame was observed were VCE03, 05, 06, 08, 11, 13 and 14. The predicted and measure flame speeds through the congested region are shown in Figures 6-18, 6-20, 6-22, 6-24, 6-26, 6-28 and 6-30 for these tests respectively. Similarly the predicted and measured overpressures are shown in Figures 6-19, 6-21, 6-23, 6-25, 6-27, 6-29 and 6-31.
Figure 6-18: VCE 03: predicted and experimental [Lowesmith, 2008] flame speed with distance

Figure 6-19: VCE 03: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance
Figure 6-20: VCE 05: predicted and experimental [Lowesmith, 2008] flame speed with distance

Figure 6-21: VCE 05: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance
Figure 6-22: VCE 06: predicted and experimental [Lowesmith, 2008] flame speed with distance

Figure 6-23: VCE 06: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance
Figure 6-24: VCE 08: predicted and experimental [Lowesmith, 2008] flame speed with distance

Figure 6-25: VCE 08: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance

*the predictions use a $F_{\text{td}}$ value (Equation (6-7)) that is equal to the value for a 50:50 CH$_4$:H$_2$ mixture, 1.46, to improve the predictions. Please see Section 6.4.2.1 for justification.
Figure 6-26: VCE 11: predicted and experimental [Lowesmith, 2008] flame speed with distance

Figure 6-27: VCE 11: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance

*Note many of the transducers were destroyed during this test, so the measured values do not necessarily represent the true overpressure achieved. A DDT occurred at the end of the congested region.*
Figure 6-28: VCE 13: predicted and experimental [Lowesmith, 2008] flame speed with distance

Figure 6-29: VCE 13: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance
Figure 6-30: VCE 14: predicted and experimental [Lowesmith, 2008] flame speed with distance

Figure 6-31: VCE 14: predicted and experimental [Lowesmith, 2008] maximum overpressure with distance
6.4.2.1 Discussion of flame speed predictions

As can be seen from the figures of flame speed, for flames which are observed to accelerate throughout the congested region, there is a fundamental problem when using the model developed here, since it inherently assumes that a limiting flame speed is achieved. So the predicted profile of accelerating, steady and decelerating is fundamentally incorrect and will not match the continuously accelerating profile observed experimentally. Furthermore, it can be seen from the predictions that the maximum flame speed predicted is lower than that achieved by the end of the congestion. This suggests that the correlations in the model are not modelling some aspect of the expected flame acceleration. On a more positive note the model does appear to predict flame speeds which are similar those observed about halfway through the congestion.

The experiments which result in an accelerating flame involve either or both of the following:

a) A methane/hydrogen mixture with 40\% of more hydrogen;

b) A high speed highly turbulent flame venting into the congestion (>150 m/s) and at least 20\% hydrogen in the fuel.

It is also necessary for a certain level of congestion to prevail. This is demonstrated by Tests 07 and 09 (Figure 6-12 and Figure 6-13) which also involved a 50:50 CH\textsubscript{4}:H\textsubscript{2} mixture but the reduced density of the congested region prevented continued flame acceleration and a limiting flame speed was achieved. This is illustrated by the shaded cells in Table 6-1; cells in the test condition table that have been shaded indicate the test conditions that lead to, and are expected to lead to (for blank cells), a flame that will continue to accelerate.

It is clear that the addition of hydrogen is having an effect such that the response of the flame to turbulence is increased. It is probable that the accelerating flames in these cases are creating turbulence which feeds back to increase the flame speed further. One possible way to examine this theory would be through the use of a CFD code to examine the turbulence.
generation. Although some work using a CFD code has been undertaken within the NATURALHY project [Fairweather and Woolley, 2009] it was also found difficult to predict the behaviour of these complex vapour cloud explosions and it was not possible to progress this aspect further.

The case of test 08 is interesting as it involved a 60:40 CH₄:H₂ mixture. Two predictions were done. The first prediction (Figure 6-24) used the original assumption that the additional factor for an increase in the flame speed due to turbulence effects (given lack of data), given by Equation (6-7), would not apply (it is only for \( \geq 50\% \) H₂ addition). However, in the second prediction (Figure 6-24), applying this modification for levels of hydrogen for 40\% H₂ and rerunning test 08 proved very successful in increasing the flame speed such that the speed about half way along the congestion is satisfactorily predicted. This is supported by CFD work [Fairweather and Woolley, 2009] that suggests a change in the flame behaviour after 40\% hydrogen is added.

### 6.4.2.2 Discussion of overpressure predictions

It is interesting to note that in most cases (except test 13 in which a flame starting with zero speed in the congestion) the overpressures predicted were high – at a level typically considered unacceptable and likely to cause structural collapse. This means from a purely practical point of view the model is correctly identifying severe explosions, which may be sufficient in practical applications within industry and at least identifies a scenario which requires further study.

Finally the case of test 13 (Figure 6-28 and Figure 6-29) is also interesting as this test concerned ignition within the congested region itself by a spark, with no initial turbulence, and yet the flame continued to accelerate. This supports the proposition that for mixtures containing 50\% hydrogen there is some additional turbulence generated by the flame itself which acts as a positive feedback mechanism on the flame speed.
6.5 Conclusions

In this chapter an existing explosion models for explosions in long congested regions were modified to allow for:

- Non-stoichiometric mixtures
- Fuels other than natural gas to be involved (in particular methane/hydrogen mixtures)
- An initially moving flame with associated turbulence to enter the congest region
- Sensitivity of the flame to stretch effects
- Limiting overpressure for high speed flames

The modified model was then used to predict flame speed and overpressure for a series of explosions and compared with experimental data.

The fundamental basis of the model was that a limiting flame speed would be achieved in the congested region. For experiments which also exhibited a stable flame speed, the model successfully predict the maximum flame speed and the predictions of maximum overpressure were also generally satisfactory (within a factor of 2 and generally conservative, see Section 2.6.2). This indicates that the modifications to the model correctly accounted for the change in fuel and the initial flame velocity and turbulence.

However, for explosion experiments which exhibited a continuously accelerating flame, the fundamental profile within the model prevented replication of the observed trend. Furthermore, the maximum flame speeds and overpressures achieved by the end of the congested region were significantly underpredicted. These cases of accelerating flames involved either more than 40% hydrogen or a high speed highly turbulent flame venting into the congestion with at least 20% hydrogen. Therefore it appears that there is some feedback mechanism associated with the response to turbulence un these cases which results in increased flame acceleration/ This aspect is suggested as an area for further study perhaps through the use of CFD models to examine turbulence generation. Nevertheless, despite not predicting the true flame speed of overpressure profile, the model did correctly
identify situations where damaging levels of overpressure would be experienced and hence would have some value in identifying scenarios for more detailed examination.
References to electronically available articles are provided with their DOI reference (document object identifier), please visit http://www.doi.org/ and enter the DOI reference to find the corresponding article online.

3894(97)81620-2, also

mixtures”, Int. J. of hydrogen Energy 32(13),


Manual and Program Description”, NASA Glenn Research Center, 

- Mercx W.P.M, 1994, “Modelling and experimental research into gas 
explosions, Overall final report of the project MERGE”, CEC Contract 
STEP-CT-0111 (SSMA), European Commission, Directorate General XII, 
Brussels, Belgium.

gas explosions. Final report of the EMERGE project”, CEC contract 
EV5VCT930274.

Techniques for Experimental Vapor Cloud Explosion Investigations”, 

- Mercx, W.P.M., van den Berg, A.C., Hayhurst, C.J., Robertson, N.J., 
modelling”, J. of Hazardous Materials 71, doi:10.1016/S0304-
3894(99)00085-0.

- Metghalchi, Mohamad, Keck, James C., 1982, “Burning velocities of 
mixtures of air with methanol, isoctane, and indolene at high pressure and 
temperature”, Combustion and Flame 48, doi:10.1016/0010-
2180(82)90127-4, pp191-210.

Acceleration Due to Turbulence Produced by Obstacles”, Combustion and 

- Molkov, V.V., Makarov, D.V., Schneider, H., 2005, “Hydrogen-Air 
Deflagration in Open Atmosphere: Large Eddy Simulation Analysis of 
Experimental Data”, International Conference on Hydrogen Safety, Pisa, 
Italy.


Ltd.


Assessment Method”, Second European Conference on Major Hazards 
On- and Off-shore, Manchester 1995, IChemE.


PART B

Fires

In this part of the thesis the topic of fires is studied.
Symbols used in this part of the thesis:

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
<td>Surface emissive power (SEP)</td>
<td>W/m$^2$</td>
</tr>
<tr>
<td>$F$</td>
<td>Fraction of heat radiated</td>
<td>-</td>
</tr>
<tr>
<td>$H$</td>
<td>Calorific value</td>
<td>J/kg</td>
</tr>
<tr>
<td>$I$</td>
<td>Incident thermal radiation</td>
<td>W/m$^2$</td>
</tr>
<tr>
<td>$L$</td>
<td>Length of flame (visible)</td>
<td>M</td>
</tr>
<tr>
<td>$m$</td>
<td>Mass flow rate</td>
<td>kg/s</td>
</tr>
<tr>
<td>$n$</td>
<td>Number of point sources in MPS model</td>
<td>-</td>
</tr>
<tr>
<td>$Q$</td>
<td>Total heat release</td>
<td>W</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature of the flame</td>
<td></td>
</tr>
<tr>
<td>$x$</td>
<td>Mass fraction</td>
<td>-</td>
</tr>
<tr>
<td>$V$</td>
<td>View factor</td>
<td></td>
</tr>
</tbody>
</table>

Greek symbols used in this part of the thesis:

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon$</td>
<td>Stefan-Boltzmann law emissivity</td>
<td>-</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Stefan Boltzmann constant</td>
<td>$5.6704\times10^{-8}$ W/m$^2$/K$^4$</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Atmospheric transmissivity</td>
<td></td>
</tr>
</tbody>
</table>
8 Predicting Large Scale Gas Fires

8.1 Introduction

In Part A the subject of explosions following releases from the natural gas infrastructure was addressed. Explosions occur when a flammable gas is released into a confined and/or congested space, and ignition occurs after sufficient time has elapsed for the vapour to have mixed with air to form a flammable cloud. If the flammable gas cloud is formed in an unconfined and/or uncongested region or ignition occurs before a flammable cloud can be formed, then, an explosion does not occur and significant overpressure is not generated. The event that results is known as a fire. In this chapter the basics for modelling fires are addressed an introduction into empirical and phenomenological modelling techniques it presented, which are the models most widely used by industry for risk assessment purposes.

8.2 Fire

Fire is a major hazard in the process industries. Fire causes more serious accidents than explosion and toxic release [Lees, 2005a, pp16/2], but is regarded as “having a potential disaster less than explosion or toxic release”. Fires come in many forms and are classified by how they are formed and the resulting shape of the flames. For example, the non-explosive burning of a flammable cloud formed in an unconfined and uncongested region is known as a flash fire and is characterised by the shape of the flammable cloud. The ignition of a continuous release of flammable gas from a small hole in the wall of a pipe or a vessel forms a jet-fire and produces a flame shaped like a
feather. In all cases large fires resulting from releases of flammable gas radiate intense heat which can be harmful to both life and structures.

Fire is a combustion process, and three essential ingredients are required: fuel; oxygen (usually in the form of air); and an ignition source. All three ingredients must be present for a fire to occur.

Unlike explosions, which require the fuel gas and oxidiser to be mixed prior to ignition, fires of the type considered in this work do not involve the combustion of premixed fuel and air. That is, fuel is released into the atmosphere where mixing of the fuel and air takes place through the process of diffusion. The mixing process is considerably enhanced by turbulence within the released gas, turbulence present within the air and turbulence generated by the interaction of the released gas with the air. Combustion can only occur where the fuel/air mixture is within the flammability range. Since the rate of reaction of the fuel/air mixture is much greater than the rate at which a mixture within the flammable range can be formed, the size and shape of the fire is determined, primarily, by the nature of the release and the subsequent rate of mixing. Of secondary importance with regard to the size and shape of the fire are the effects of air movement (wind) and buoyancy.

### 8.3 Fire Types

As mentioned in Section 8.2, fires are classified by the way in which they are formed and the resulting shape of their flames.

The types of fires of greatest interest with regard to accidental releases from the natural gas infrastructure [Cowley and Johnson, 1992] are:

1. Pool fires
   These types of fires occur when a flammable liquid such as liquefied natural gas (LNG) is released, forms a pool and the vapours from the pool mix with the surrounding air and are ignited. The heat transfer from the flame to the pool surface controls the rate of evaporation which then determines the rate of combustion and ultimately the size of
the fire. Larger pools also produce larger flames although a limit is reached. Due to the low momentum of the flame, it can be affected by the prevailing wind conditions resulting in significant flame tilt [Cowley and Johnson, 1992].

2. Vapour cloud fires
A vapour cloud fire (sometimes called a flash fire) occurs when a flammable cloud (fuel/air mixture) is formed in an unconfined and uncongested region and is then ignited. In the absence of congestion, the vapour cloud burns without the generation of overpressure and hence is called a fire rather than an explosion.

3. Fireball
A fireball is formed when a large inventory of flammable gas is released instantaneously and is ignited immediately. The flammable vapours mix with the air and a spherical flame develops which grows in size as the fuel is consumed and rises as a result of the initial momentum of the release and the effects of buoyancy. For example, fireballs can occur following the catastrophic failure of a pressure vessel containing a flammable liquid or gas, such as during the rupture of a liquid petroleum gas (LPG) storage tank or a high-pressure gas pipeline.

4. Jet fires
A jet-fire occurs if high pressure gas is released from containment through a small hole in the wall of a vessel or pipe. If ignition occurs immediately then a jet fire is produced. A jet fire is an example of a turbulent diffusion flame where the gas release is sonic. The rate of release determines the rate of combustion and the resulting fire size. Jet fires are highly directional and, due to the initial high momentum, are not greatly affected by the wind or buoyancy forces until towards the end of the flame where the velocity of the gases has decayed. Depending on the fuel, the flame may not stabilise on the release point, but start at some point downstream, this is usually called flame lift-off [Lowesmith et al 2007]. A jet fire may also be seen during routine oil and gas operations as a flame on a flare stack and is an important hazard scenario in industry.
5. Pipeline fires

In this scenario pressurised gas in a pipe is released when the pipe fails catastrophically (such as the rupture of a natural gas transmission pipeline). On rupture of the pipeline, a crater is formed from which gas escapes into the atmosphere from both of the severed ends of the pipeline. If ignition occurs immediately, a fireball, or mushroom shaped fire, is formed initially followed by a large gradually decaying fire. Due to the loss of momentum in the crater and the gas/air mixing process in the crater, there is generally less lift-off height for these fires compared to jet fires and, as the pressure drops, the fire may be increasingly tilted by the wind.
8.4 The Effect of Fire

From the aspect of safety, the most significant effect of fire is the transfer of heat to objects and people engulfed by the fire and at locations outside of the fire. Heat is transferred to anything engulfed by the fire through the mechanisms of convection and radiation, and any object engulfed by a fire can, in general be considered to be destroyed and any person engulfed by a fire can be considered to become a casualty. When assessing the impact of operating the natural gas infrastructure on the safety of the general public, the transfer of heat to objects (such as buildings) and people that are remote from the fire through the mechanism of radiation is the most important effect of fire.

The work described in this thesis is concerned with determining the consequences of explosions and fires following the ignition of releases from the natural gas infrastructure, in particular, the underground pipeline system.
This information will then be used to evaluate the change in risk presented to the general public as a result of transporting a mixture of natural gas and hydrogen rather than only natural gas, so that the feasibility of adding an increasing proportion of hydrogen can be assessed. Consequently, the work has concentrated on those fire types associated with releases from natural gas pipeline networks, since they can occur outside of operational site boundaries and are events with which the general public can come into direct contact. Hence, the fire types studied in this work are jet fires and pipeline fires and the heat transfer mechanism studied is radiation to objects and people remote from the fire since it is this mechanism that determines safety distances.

8.5 **Emission of Thermal Radiation**

In a fire, radiative energy is emitted. The total amount of radiative energy emitted from a surface diffusely is termed emissive power. The magnitude of the emissive power depends on the wave-length, temperature, and a surface property, called emissivity, which relates the ability of a surface to emit radiative energy to that of an ideal surface, which emits the maximum possible energy. Such an ideal surface is known as a ‘blackbody’.

Radiation emitted from a fire comes from two sources, emission from soot particles (that is carbon particles) and molecular radiation predominately from carbon dioxide and water molecules [Mannan, 2005]. The respective emissivities have been studied, and standard graphs have been produced for the emissivities of carbon dioxide and hydrogen, while for soot the theory is more complex [Mannan, 2005]. Carbon dioxide and water vapour molecules are strong emitters but the emissions are restricted to discrete wavelength bands, whereas soot emits continuously over the visible and infra-red spectrum, and contributes greatly to the luminosity of the flames [Venetsanos et al., 2007].

Attenuation of radiation occurs when radiation is transmitted through the Earth’s atmosphere due to absorption and scattering, particularly from water
vapour and carbon dioxide [Mannan, 2005]. The amount of attenuation is a function of the number of absorbing molecules in the path and the size of any droplets. The atmospheric transmissivity is the measure of the amount of attenuation thermal radiation experiences through its path from the surface it was emitted from and the target. Further, it is a function of distance.

8.5.1 Modelling Radiant Transfer

The governing equation for radiant heat transfer is the radiant transfer equation (RTE) [Novozhilov, 2001]. Venetsanos et al., [2007] introduce some of the commonly used radiant transfer models to solve the RTE:

- Zonal Method
  This method is useful for estimating the radiative transfer in the absence of detailed information of the participating media. The method is applicable to enclosures which are divided into a series of zones. View factors are then defined between pairs of zones resulting in a series of simultaneous equations for each zone [Venetsanos et al., 2007].

- Statistical or Monte-Carlo Method
  Purely statistical methods, such as the Monte-Carlo method, usually yield radiation heat transfer predictions as accurate as the exact method [Venetsanos et al., 2007]. The main principle is that a finite number of photons are tracked using a random number generator to sample a probability distribution for scattering angles and path length between collisions. As the number of photons emitted from each volume element increase this method converges on the exact solution of the problem.

- The Flux or Multi Flux Method
  The angular dependence of radiation complicates radiant transfer calculations since all possible directions must be taken into account. Assuming that the intensity is uniform over given intervals of the solid angle, then the radiation transfer equation (RTE) can be simplified to a series of linear differential equations in terms of average radiative intensities. By changing the number of solid angles where the radiative
intensity is assumed constant a number of different flux methods can be derived; increasing the number increases the accuracy of the solution. The six-flux (3 dimensional) method has been applied with reasonably success for fire spread and smoke movement inside compartments. However, the method is not suitable for flame spread over surfaces or flames exiting outside through openings where finer discretization of the solid angle is required.

- The Discrete Ordinate Method
  This method applies a discrete-ordinate approximation to the radiation transfer equation (RTE) through discretising the entire solid angle [Venetsanos et al., 2007]. A simpler version of this method is called the $S_N$-approximation where spherical space is divided into $N$ equal solid angles. The $S_N$-approximation has been used successfully in comparison with full numerical solutions [Venetsanos et al., 2007]. However, the method suffers from “ray effects” which cause anomalies in the flux distribution but as the scattering increases and the radiation field is more isotropic (does not vary with direction) the problem becomes less noticeable. The convergence rate may also take longer in these situations.

- The Discrete Transfer Method
  This method is a mixture of the Monte-Carlo, zone and flux methods [Venetsanos et al., 2007]. The method is much faster but to obtain ray insensitive solutions the method may require more rays than is economic for practical problems.

In addition to the above, models for the radiative properties, such as the absorption and scattering coefficients of the combustion products, are required for the modelling purposes [Venetsanos et al., 2007]. Examples of these include [Venetsanos et al., 2007]: narrow band model; wide band model; Grosshandler’s total transmittance, non-homogeneous (TTNH) model; mixed grey gas model; and the banded mixed grey gas model.
However, for engineering calculations an alternative approach, to the models above, exists. There are two predictive approaches for use in empirical and phenomenological models [Cowley and Johnson, 1992]. The first is the more fundamental approach and uses values for the surface emissive power of a flame with a solid geometry, and the second is to use a point source approach and a fraction of heat radiated to calculate the amount of radiation leaving the flame. These are described in more detail in the following sections.

8.5.2 Surface Emitter Models

Heat is transferred from the flame to a remote target by radiation. The Stefan-Boltzmann law [Sparrow and Cess, 1978] represents the rate at which thermal energy is emitted per unit surface area by a grey body, known as the flame surface emissive power, \( E \) (W/m\(^2\)/s),

\[
E = \varepsilon\sigma T^4
\]

(8-1)

where \( \varepsilon \) is the emissivity and is 1 for black bodies and lower for grey bodies, \( \sigma \) is the Stefan-Boltzmann constant (5.6704x10\(^{-8}\) W/m\(^2\)/K\(^4\)), and \( T \) is the temperature of the flame (K).

As the energy is supplied via the heat release during the combustion process, the emissive power of the flame (Equation (8-1)) is equal to the thermal radiation emitted by the flame per unit area of the flame surface,

\[
E = \varepsilon\sigma T^4 = \frac{FQ}{A}
\]

(8-2)

where \( Q \) is the total rate of heat release via combustion (W), that is the product of mass flow rate and the heat of combustion (calorific value) of the fuel, \( A \) is the surface area (m\(^2\)) of the flame and \( F \) is the fraction of the heat release that is radiated. The fraction of heat radiated is important; it determines the proportion of the energy released by combustion that is radiated as heat. The fraction of heat radiated is determined from experiments.

To determine the incident radiation, \( I \) (W/m\(^2\)), on a target in space the following formula holds,
\[ I = \tau VE \quad (8-3) \]

where $\tau$ is atmospheric transmissivity, $V$ is the view factor and $E$ is given by Equation (8-2). The atmospheric transmissivity accounts for the fact that the thermal radiation may be attenuated by the medium through which it passes, by means of absorption and scattering. A transmissivity of unity represents no participating medium, but, for example, high levels of humidity in the air will cause the transmissivity to be less than unity because water droplets in the air can absorb thermal energy from thermal radiation passing through it. The view factor\(^6\) is a function of the geometry of the flame position and orientation of the target, and describes the fraction of diffuse (uniform over all directions) of radiant energy leaving one surface and arriving at another infinitesimal surface. In simple geometries the view factor can be calculated by analytical methods such as found in [Sparrow and Cess, 1978] but for general geometries a numerical method can be used [Hankinson, 1984] (see Section 9.3.2.3 for a numerical methodology).

There are three ways in which to use to Equation (8-3). One is to work in terms of the flame temperature and emissivity, second is to use an empirical value for the flame surface emissive power. Third, is to calculate the total heat generated and apply the fraction of heat radiated. In addition, the determination of the flame surface is required.

### 8.5.3 Point Source Approach

If the flame is represented as a point source emitting thermal radiation, then the incident radiation at a target is given by [Coley and Johnson 1992],

\[ I = \frac{\pi FQ}{4\pi S^2} \quad (8-4) \]

where $S$ is the distance from the point source to the receiving target, $Q$ is the power of the flame, and $F$ is the fraction of heat radiated. The advantage here is that there is no need to define the flame surface or calculate the view factor as in the surface emitter type model. However, since $I$ is inversely

\(^6\) Also known as configuration factor, angle factor
proportional to $S^2$, as $S$ tends to zero, $I$ tends to infinity, so the approach is only suitable for locations more remote from the fire. To some extent this difficulty can be mitigated by taking a number of point sources rather than one point source (multi-point source model which is described further in Section 9.3.1.1).

For this approach, the determination of the fraction of heat radiated is crucial. The fraction of heat radiated depends on various factors including the species composition within the flame, the amount of soot formation, heat lost by convection to the entrained air, and the flame size [Mannan, 2005]. Fraction of heat values are generally derived experimentally and are sometimes presented as a correlation. The fraction of heat radiated values are used in point source type models [Cowley and Johnson, 1992]. In a point source type model radiation is assumed to be emitted from a number of point sources that emit in all directions.

Chamberlain [1987] reports that the fraction of heat radiated decreases as jet velocity increases. Chamberlain suggests “that an increasingly greater fraction of the heat of combustion is lost by convection to the entrained air”. Other factors may also contribute to this observation such as the change of sooting propensity (tendency), and the amount of radiating molecules such as carbon dioxide and H$_2$O present (as well as intermediate species).

Markstein [1984] found that for turbulent and laminar buoyant diffusion flames, the radiated heat fraction can be linearly correlated with the flame smoke point. The author defines smoke point as the height that soot just begins to be released at the tip of the flame. This has been confirmed by the work of Orloff et al. [1992].

Another technique to study the parameters affecting the radiant fraction is found in the scaling studies of Turns and Myhr [1991]. They deduce that the fraction of heat radiated is proportional to the Planck-mean absorption coefficient, the temperature of the flame to the power of four and the exit diameter all over the exit velocity. It expresses the dependency of the fraction
of heat radiated on the “time available for radiant energy to be lost from the
flame” [Turns, 2000, p502].

Another method of correlating the fraction of heat radiated is with use of the
global flame residence time \( T_G \) [Choudhuri and Gollahalli, 2003]. This
parameter represents the “time required for a stoichiometric mixture of hot
products to pass through a volume equal to that occupied by the visible flame”
[Turns and Myhr, 1991]. For a momentum dominated flame it is found that it is
directly proportional to the convective time scale which is the exit diameter \( d \)
over the exit velocity \( u \), \( d/u \). For buoyancy dominated flames the global
residence time changes more slowly with increases in the convective time
scale, \( d/u \). Choudhuri and Gollahli [2003] produced a correlation for the
radiative heat fraction as a linear fit with the global residence time. This
method however requires more information about the flame and thus is not as
simple to use as the other methods presented, and requires a correlation for
each fuel.

In practice most fraction of heat radiated values come from experimental
studies and correlations of data.

8.6 Approaches to Modelling Fires

The three essential features of a fire model for hazard assessment are: a
prediction of the size, shape, and location in space of the flame; an
assessment of the amount of radiation emitted by the flame; and, finally, a
method of calculating the radiation incident upon a target that is remote from
the fire (see previous Section).

Fire models can be divided into three groups: empirical models;
phenomenological models and computational fluid dynamics (CFD) models.
Again, the purpose of this work is to investigate models that are suitable for
carrying out quantitative risk assessments for the production of safety cases.
The type of model suitable for such a task must have a short run time since
many different scenarios need to be considered, hence empirical or phenomenological models are generally used.

Although more widely applicable than the other types of models, a CFD model is usually complex to apply, often requires a specialised user, very large computational power and an extremely long run time to obtain a prediction for a single scenario. Although outside the scope of this thesis, it should be noted that there are a number of CFD models which have been developed for predicting fires.

## 8.6.1 Empirical Models

Empirical models, as their name suggests, are derived entirely from experimental data. Experiments are performed, if possible covering the entire range of scenarios for which predictions are required.

Examples of models which use a simple length or trajectory to represent the flame include those of Lowesmith et al. [2007], Cook et al. [1987] and Studer et al. [2009]. Examples of models that predict the dimensions of a solid geometry to represent the flame include Johnson et al. [1994] and Chamberlain [1987] which both use a conical frustum as the flame shape.

Predictions from empirical models of the dimensions of a solid geometric shape or the flame length are used as input to the radiation transfer models described in Section 8.5.2 (solid geometry model) and 8.5.3 (point source model) respectively.

Generally, point source models and solid flame models employ uniform values of fraction of heat radiated and flame surface emissive power, respectively, which facilitates quick calculations but this can be varied. For example, when an array of point sources is used their strengths can vary, as in the model given by Cook et al., [1987]. Also, the flame surface emissive power can vary over the flame surface to account for such factors as obscuration of the flame by smoke, etc. For example, the Johnson et al. [1994] is a solid geometry
model that uses different values of the surface emissive power for the ends and sides of the flame.

Empirical models can provide very good predictions that are sufficiently accurate for risk assessment purposes, provided the predictions are within the range of the experimental data upon which the model is based. Unfortunately, many of the safety scenarios of interest, such as the rupture of a large diameter, high pressure natural gas pipeline, are beyond the scale (both geometrically and financially) of what can be undertaken as a programme of experiments. Consequently experiments as large as possible must be undertaken, a model developed, and then the results of the model extrapolated to full scale events.

8.6.2 Phenomenological Models

In an attempt to develop models that are more widely applicable than empirical models, phenomenological models have been developed based upon simplified forms of the full conservation equations that are used in CFD models. Examples of this type of model are given in references [Caulfield et al., 1993a, 1993b; Fairweather et al., 1992]. Solution of these simplified equations provides predictions of the flame size, shape and location in space and predictions of the spatial variations of composition and temperature within the flame from which the radiative output of the flame over its surface can be derived. The radiation incident at a location remote from the flame can then be calculated in a manner identical to that described in Section 8.5.2 or 8.5.3 using a surface emitter or multi-point source approach.

As a consequence of the simplification of the conservation equations, phenomenological models are not as general as CFD models. However, since they are based on the physical processes that take place within a particular class of fires, they are more widely applicable than empirical models. However, all models, including CFD models require considerable input from experiments to provide closure for the solution process.
8.6.3 Note on CFD models

Although outside the scope of this thesis, it should be noted that there are a number of CFD models which have been developed for predicting high pressure fires.

A CFD model for fire modelling consists of the fluid flow equations, a turbulence model and a combustion model. As was seen for the introduction to CFD models in Section 2.5.4, that for each of the constituent components, that is the fluid flow equations, turbulence model and combustion models, there is a choice between various models to complete the solution. As with all CFD solutions, the definition of the grid is an important part of the definition of a model.

CFD has been applied widely to compartment or enclosures fires probably as fires tend to impinge on the walls of the enclosure or can suffer from under ventilation, both of which lead to complex fire behaviour which CFD codes are able to resolve. No CFD modelling of fire was undertaken as part of the NATURALHY project, primarily due to the simpler nature of free, well ventilated, jet fires. Examples of commercially available CFD codes that are capable of predicting this type of event include FDS (http://fire.nist.gov/fds/), SMARTFIRE (http://fseg.gre.ac.uk/SMARTFIRE/), PHOENICS (http://www.cham.co.uk/), CFX (http://www.ansys.com/) and FLUENT (http://www.fluent.com/).

Fairweather and Woolley [2003] investigated predictions using the classical k-ε turbulence model and a more sophisticated Reynolds stress turbulence model. They found the predictions were better when using the Reynolds stress turbulence model. This was also the conclusion of the CFD model development in the NATURALHY project (Section 2.5.4). DNS (direct numerical simulation) is the most intensive approach resolving all the flow without a turbulence model.
The most computationally expensive method is DNS (direct numeric simulation) where the fluid flow equations are solved directly. Therefore models are used to simplify the solution of the fundamental equations. Two advanced solutions techniques used for the fluid flow are the RANS or FANS (Reynolds averaged Navier-Stokes or Favre averaged Navier-Stokes) approaches [Liu and Wen, 2002]. However, these approaches require much computing power [Liu and Wen, 2002] hindering their wide application. A promising technique for use in modelling fires in CFD codes is the Large Eddy Scale (LES) model, it is computationally less expensive than DNS, but still capable of tackling the scale-dependent dynamic behaviour [Wen et al., 2007]. In LES models, flow features which are larger than the grid size are solved explicitly, otherwise the flow structures are modelled using sub grid scale (SGS) models [Xu et al., 2005].

Similar techniques applicable to combustion modelling in explosions are also used in fire modelling. The mixture fraction approach is frequently used to avoid needing to solve the conservation equation for each species [Brannan, 2000]. Another frequently used concept in turbulent non-premixed flame modelling is the laminar flamelet concept where an ensemble of instantaneous laminar flamelets represent the turbulent flame in which the properties are a function of the mixture fraction [Brannan, 2000]. A link between turbulence and the chemistry has to be made in the model. A PDF (probability density function) is often used for this purpose [Cleaver et al., 2003]. The laminar flamelet equations can be solved in advanced, by using a chemical kinetic scheme, to reduce computational time resulting in flamelet ‘libraries’ [Cleaver et al., 2003]. Advanced computation can also be done for assumed shapes of PDF functions.

For a sonic jet release, under-expanded supersonic jets are formed immediately after the orifice [Brannan, 2000]. Hereafter the flow rapidly accelerates and expands to atmospheric pressure through a single shock or through a series of expansion shocks. The computational grid would need to be sufficiently refined over the large length scale (compared to the exit diameter) involved which would be computationally expensive. To avoid this,
the concept of an effective source diameter has been developed [Brannan, 2000].

To obtain incident radiation predictions the CFD code needs a radiation transfer model. Some examples of radiation transfer models for use in CFD are listed in Section 8.5.1. However, defining the flame surface for use in radiative transfer models in a CFD model is not straightforward [Ledin, 2010], and different codes may use different methods. Similar to explosion modelling, there can be problems resolving the flame properly and adaptive gridding, for example based on the gradient of temperature or intermediate species, can be used to improve the resolution [Ledin, 2010]. Cleaver et al. [2001] using the discrete transfer method, evaluates the temperature and participating species concentration in the finite-volume cells that the ray traverses when travelling from a receiver to the fire.

8.7 **Assessment of Fire Predictions by Comparison with Experimental Data**

When comparing predictions of incident radiation with experimental data, two factors must be considered. Firstly, the variability of the measured values from large scale experiments, often as a result of variability in the atmospheric conditions and secondly the degree of accuracy realistically expected of predictions from models.

The variability of the measured incident radiation values during in experiments has been reported by Selby and Burgan [1998] and Lowesmith [2008 Apr, 2008 Aug] to be within ± 5%.

Selby and Burgan [1998] present predictions for incident radiation and flame geometry (length) for unconfined jet fire predictions and compare them against experimental data. The models chosen were a mix of phenomenological and CFD type models. Selby and Burgan report that some predictions of the incident radiation were outside a factor of two whilst the
majority were within a factor of two. Similarly for the flame length, the majority of predictions were within the factor of two band whilst there were some predictions over a factor of two.

Cowley and Jonhnson [1992] present comparisons of predictions for the flame length and the incident radiation levels for a selection of models against experimental data. For sonic natural gas release the flame length was overpredicted by up to 2.7 times but generally within a factor of 2 and never underpredicted. The incident radiation predictions ranged from a minimum factor 0.7 to a maximum factor of 1.9. The presentation also shows that near field and far field predictions have similar performance for the studied models.

For fires following release from a high pressure ruptured pipeline Cleaver et al. [2001] achieved incident radiation predictions within 30%. Caulfield et al. [1993b] report that 72% of the incident radiation predictions were within 1/3 of the measured values and Cook et al. [1987] report that approximately 80% of predictions lie within 30% of the experimental value.

As there appears to be no clear consensus, some judgement is required. Based on the above, predictions within +20% would be very acceptable. Within +40% they might be tolerable. Hence, these criteria are applied to the predictions presented in Chapters 9 and 10.

8.8 **Conclusions**

Engineering models for predicting the incident radiation from fires resulting from the release of high pressure gas have been developed for natural gas and validated against large scale experimental data.

The focus of this study is engineering models (empirical and phenomenological) which are used for routine hazard assessment within the oil and gas industry.
In Chapters 9 and 10 the fire models have been chosen to represent a variety of modelling approaches, that is both empirical and phenomenological. Both the point source and solid surface radiation approaches are used.
9 Predicting Large Scale Jet Fires

9.1 Introduction

In this chapter the size and incident thermal radiation characteristics of a jet fire, resulting from a release of natural gas and hydrogen mixtures from a hole in a high pressure pipe or vessel, is modelled and validated against the NATURALHY experimental programme. The approach taken is outlined first, and then predictions, using the experimental test conditions (Table 9-1), are presented and compared with the experimental data.

9.2 Experiments

A series of large scale experiments were undertaken by Loughborough University at the Advantica Spadeadam test site in the north of England as part of the NATURALHY project [Lowesmith, Apr, 2008].

Gas at an absolute pressure of 61bar was released horizontally through a small orifice. The release height was 3.25m above ground. A steel pipe target of diameter 0.9m is placed at the same height as the release. The distance between the pipe target and release point was varied depending on the mass flow rate. The pipe target had sensors attached to record the temperature of the steel and to measure the heat loads to the pipe from the fire although this aspect will not be modelled here. In the field there were radiometers orientated to point towards the centre of the pipe, which was also expected to be the location of the centre of the flame, to measure the incident radiation from the flame. Thermovision thermal imaging film and video film records were also made of the flame.
The releases were in a nominally easterly direction which was also nominally downwind. The prevailing weather conditions were also monitored including the wind speed and direction so that the actual wind angle relative to the release direction could be determined.

Figure 9-1 shows a typical schematic of the experimental arrangement used although the distances to the radiometers from the flame and the separation of the release point from the pipe target varied between tests. The labelled points with prefix ‘R’ are the locations of the radiometers.

![Figure 9-1: Schematic of horizontal jet fire experiment arrangement with target in view](image)

[Lowesmith, Apr, 2008]
Six tests in total were undertaken in this series of experiments, the fuel compositions used were natural gas for tests 1 to 3, and a 75% natural gas/25% hydrogen mixture for tests 4 to 6. The natural gas contained, by volume, 93% methane and 4.9% ethane and 1.7% nitrogen. The orifice hole was varied from 20mm, 35mm and 50mm to increase the mass flow rate, but the release gauge pressure was nominally 60 bar for all the tests.

Table 9-1 lists the test conditions and the observed visual flame length determined from the video footage.

<table>
<thead>
<tr>
<th>Test</th>
<th>Fuel NG:H₂ (by vol.)</th>
<th>Exit Diameter (mm)</th>
<th>Measured Mass Flow Rate (kg/s)</th>
<th>Measured Flame Length (m)</th>
<th>Wind Speed at release height (m/s)</th>
<th>Wind angle, relative to release axis (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>01</td>
<td>100:0</td>
<td>20</td>
<td>2.9</td>
<td>19.8</td>
<td>5.0 ±0.9</td>
<td>1° to S (+11°)</td>
</tr>
<tr>
<td>02</td>
<td>100:0</td>
<td>35</td>
<td>9.6</td>
<td>37.8</td>
<td>5.1 ±0.7</td>
<td>27° to S (+5°)</td>
</tr>
<tr>
<td>03</td>
<td>100:0</td>
<td>50</td>
<td>19.5</td>
<td>49.9</td>
<td>3.4 ±0.7</td>
<td>3° to N (+13°)</td>
</tr>
<tr>
<td>04</td>
<td>75:25</td>
<td>20</td>
<td>2.7</td>
<td>17.6</td>
<td>1.4 ±0.7</td>
<td>7° to N (+10°)</td>
</tr>
<tr>
<td>05</td>
<td>75:25</td>
<td>35</td>
<td>7.2</td>
<td>30.7</td>
<td>1.4 ±0.2</td>
<td>14° to S (+6°)</td>
</tr>
<tr>
<td>06</td>
<td>75:25</td>
<td>50</td>
<td>16.9</td>
<td>45.2</td>
<td>1.6 ±0.3</td>
<td>3° to N (+8°)</td>
</tr>
</tbody>
</table>

Table 9-1: Jet fire experimental conditions and visible flame length [Lowesmith, Apr, 2008]

Figure 9-2 shows a photograph of a jet fire in progress. The release point is on the far left of the picture and the gas expansion and lift-off region can be seen prior to the start of the flame. As can be seen, the tail of the flame bends upwards on the right hand side of the picture as the buoyancy of the flame becomes more dominant.
9.3 Modelling Methodology

In this section the methodology used in the modelling work is discussed.

Three models were used in this work:

1. the flame length correlation from Lowesmith et al. [2007] and the (single and multi) point source model;
2. the flame dimension model and thermal radiation model from Johnson et al. [1994];
3. the model JBurn from GL Industrial Services.

Computer codes of the models (1) and (2) were created by the author whereas a computer code for (3) was provided by GL and then modified by the author.

9.3.1 Multi Point Source Model

9.3.1.1 Description of the Flame and Radiative Characteristics

For this model, the flame is considered as a line rather than a solid body. The length is calculated using the correlation from Lowesmith et al. [2007],
\[ L = 2.8893Q^{0.3728} \]  \hspace{1cm} (9-1)

where \( Q \) is the power of the flame in MW. This length is used to place point sources along in the following radiation model.

To predict the radiation at locations in space the multi point source (MPS) is used. In this type of model radiation is assumed to be emitted from a number of point source(s) that lie evenly spaced along the length of the flame and emit in all directions. An example diagram is shown in Figure 9-3. A special case of the multi point source model is when the number of sources is just one in which case the model is the single point source (SPS) model.

![Diagram of the multi-point source model](image)

\( Q_r \) (W), the input power of the flame which can be calculated by the product of, \( \dot{m} \), the mass flow rate (kg/s) and, \( H \), the net calorific value (J/kg). The fraction of heat radiated, \( F \), accounts for how much radiation is radiated, as an average, from the whole flame.
The incident radiation, \( q \) (W), received at a point in space from one point source can be calculated as,

\[
q = \frac{\tau FQ}{4\pi S^2}
\]  

(9-3)

where \( S \) is the absolute distance from the point source to the point target and \( \tau \) is the atmospheric transmissivity along that path.

For multiple point sources along the flame’s trajectory, each point radiates a proportion of the total emitted power of the flame, and each contributes to the incident radiation on the target. The approach is to arrange the points on the flame into \( n \) points each radiating \( 1/n \)th of the total emissive power, \( Q_r \). Thus the radiation leaving a point source, \( Q_i \), are equally weighted,

\[
Q_i = \frac{1}{n} FQ
\]  

(9-4)

Note that realistically the points may not lay on a straight line, but on a curved line, though in many models the trajectory of the flame is something that is often neglected. Other methods include weighting each point so that some point sources contribute more to the incident radiation than others. For example, the point sources could be weighted by the variation along the flame of flame temperature raised to the fourth power (eg. GL model JBurn, see Section 9.3.3). In general the strength of a point source with some weight \( w_i \) is then,

\[
Q_i = w_i FQ
\]  

(9-5)

where \( \sum w_i = 1 \).

In general the multi point source model can be expressed as,

\[
q = \sum_{i=0}^{n} \frac{\tau_i Q_i}{4\pi S_i^2}
\]  

(9-6)

where the subscript \( i \) refers to a variable that depends on the distance between the target and \( i \)th point source on the flame.
The multiple point source approach is much preferred over using a single source as it behaves better in the near field giving more realistic answers but in the far field the single point source model performs well enough [Cowley and Johnson, 1992].

Figure 9-4 shows how the calculated fraction of heat, $F$, (from experimental data [Lowesmith, Apr, 2008]) varies with how many points are used to represent the flame. For $n$ under 10 the fraction of heat radiated changes much more, whereas above $n=10$ the value of $F$ increases very slowly and after $n=100$ the changes are insignificant. The number of points was varied beyond 100 but the difference is negligible and there is no reason for the extra computation. Therefore, the number of point sources used in this work was chosen to be 100.
As can be seen from Figure 9-4 the fraction of heat radiated for the point source model can depend upon the number of sources taken. Hence, care has to be taken to make sure the number of points being used is similar to that used to derive $F$ from the data.

### 9.3.1.2 Fraction of heat radiated for methane/hydrogen mixtures

To use the multi-point source model the fraction of heat radiated must be known, which is usually derived from experimental data. Further, if data are available for pure fuels, an appropriate method for deriving the fraction of heat radiated for the mixture would be desirable, especially as there has been little work undertaken for flames involving mixtures of methane and hydrogen.
From the experimentally measured incident radiation at each radiometer location, the fraction of heat radiated can be calculated based on a 100-point source approach. The values of fraction of heat radiated were found to be as summarised in Table 9-2 for the 6 tests. The values of $F$ for natural gas compare favourably with the value of 0.13 recommended by Lowesmith 2007, bearing in mind the experimental scatter noted in the paper, with some data exhibiting fractions of heat radiated over 0.2 and noting that the values of $F$ given by Lowesmith et al. [2007] were calculated on a single point source basis. The average for the pure methane tests (1 to 3) is 0.165 and for the 75:25 tests (4 to 6) is 0.15. It is also apparent that the mixtures produced similar values to the natural gas.

<table>
<thead>
<tr>
<th>Test</th>
<th>$F$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.126799</td>
</tr>
<tr>
<td>2</td>
<td>0.173615</td>
</tr>
<tr>
<td>3</td>
<td>0.189985</td>
</tr>
<tr>
<td>4</td>
<td>0.124376</td>
</tr>
<tr>
<td>5</td>
<td>0.167499</td>
</tr>
<tr>
<td>6</td>
<td>0.185016</td>
</tr>
</tbody>
</table>

Table 9-2: Calculated value of $F$ from experimental data (based on 100 point sources)

There is also limited data available for hydrogen flames and the available information is very small scale compared to the kind of fires of interest. For example, work on hydrogen flames and their radiation characteristics include work by:

- Choudhuri and Gollahalli [2000]
  Laminar flame experiments with exit Reynolds number varied between 150 to 3000
  Value of $F=0.038$
- Schefter et al [2006]
  Turbulent flame experiments with mass release rates of 0.021 g/s to
23.17 g/s.
Value of $F$ start from 0.04, increasing with flame residence time

- Mogi and Horiguchi [2008]
  Turbulent flame Experiments with mass release rates of 1 g/s to 100 g/s.
  Value of $F$ is 0.03 or 0.08
  (There is a dependency on the fraction of heat radiated value on whether the adiabatic flame temperature or measured flame temperature is used to calculate the value from experimental incident thermal radiation measurements.)

A value of $F$ for hydrogen of 0.15 was suggested by GL. This assertion is supported by recent confidential information made available to Loughborough University which suggests that the fraction of heat radiated from large scale hydrogen jet fires may be similar to large scale natural gas jet fires.

Having established values for the pure fuels, some kind of mixing formula is needed to derive fractions of heat radiated for mixtures. Possible options include formulae based on volume fraction, mass fraction or power fraction.

Figure 9-5 shows the three options for deriving the fraction of heat radiated for a mixture of natural gas and hydrogen based on a linear relationship with volume fraction, mass fraction and power fraction. For this figure, the fraction of heat radiated for hydrogen of 0.04 was taken based on small scale data [Choudhuri and Gollahalli, 2000] and 0.14 for methane from [Choudhuri and Gollahalli, 2003]. Also shown on the figure is some literature data for mixtures, also at small scale, from the same references. The 2000 data set was for a limited range of hydrogen addition and for a laminar co-flowing flame, while the 2003 data set was for a turbulent jet flame and also for a limited range.
Figure 9-5: The fraction of heat radiated value for methane addition to hydrogen

From Figure 9-5 it would be reasonable to conclude that the fraction of heat radiated for a mixture should be based on the volume fraction. However, this may not apply to the large scale situation.

Figure 9-6 shows a similar plot, assuming 0.165 for natural gas (average value derived from tests 1 to 3) and 0.15 for hydrogen. The values of $F$ derived from the experimental tests of NATURALHY, as summarised in Table 9-3, are also shown. It can be seen that, in the limit of the small difference between the value of $F$ for pure natural gas and pure hydrogen, that any of the three methods of mixing $F$ may be candidates.
Therefore, for the purposes of the 100-point source model adopted here, a fraction of heat radiated for pure hydrogen of 0.15 was used and a value for natural gas as derived from the tests 1 to 3. For mixtures, the value of $F$ will be derived based on the mass fraction approach, to provide conservative values, as follows,

$$F_{\text{mix}} = (1 - x_{H_2})F_{CH_4} + x_{H_2}F_{H_2}$$  \hspace{1cm} (9-7)

where $x$ is the mass fraction of hydrogen. All the point sources (100) are equally weighted and so have the same fraction of heat radiated.

9.3.1.3 **Computer Implementation of the Model and Application to the NATURALHY Jet Fires**

The model was implemented in a computer program and the flame length, used to determine where to place the point sources, determined via the correlation from Lowesmith et al. [2007] (Equation (9-1)). The mass flow rate which was calculated using the standard equation for choked flow through an orifice with the coefficient of discharge set at 0.9. The computational solution was performed in 3 dimensional space so the real target sensor locations...
were used. The flames were horizontal so for all point sources the height component was constant and set at the release height (3.25 m). Similarly the distance perpendicular from the release axis coordinate was set as 0 for all the point sources as the model does not predict the flame trajectory. The origin was set as the source of the release.

The power of the release was calculated using the net calorific value (also called the heat of combustion), which is the amount of heat released by combustion. This was calculated from the difference of the sums of the heat of formation for, the products, and that of the reactants. The heats of formation for the interested components come from the NASA database (see APPENDIX C). For pure natural gas the net calorific value calculated is approximated by pure methane and is taken as 50.03 MJ/kg. For 75% natural gas and 25% hydrogen the calorific value calculated is slightly larger at 52.84 MJ/kg.

The model then predicted the flame length and the incident radiation at each radiometer location. The results were analysed in spreadsheet software.

9.3.2 Johnson et al. [1994]

The model presented by Johnson et al. [1994] is the basis of the model that can be found in the Shell Global Solution risk assessment package FRED\(^7\). However, to investigate the applicability of this model to natural gas/hydrogen fires it was necessary to be able to apply modify the model and its inputs. Hence, the author produced a version of the model based on the equations published in literature in Johnson et al. [1994] with supporting information from, Chamberlain [1987] and Becker and Liang [1978].

This model builds on the work by Beck and Liang [1978], in which vertical flames in still air were studied. Indeed it uses the correlation results as a starting point. Chamberlain states that the flame length depends on a number

---

\(^7\) This software has been discontinued
of variables. The rate of air entrainment determines the rate at which the 
concentration of gas reaches the lower flammable limit at the tip of the flame. 
The entrainment rate depends on the momentum flux ratio (between the wind 
and the jet), Reynolds number, Richardson number (ratio of buoyancy to the 
input momentum flux) and effective source diameter.

9.3.2.1  Flame Geometry

Johnson et al. [1994]

This model predicts the dimensions of an ideal representation of sonic and 
subsonic jet fires. In this model the flame is represented as the frustum of a 
cone, and equations are presented to determine the dimensions and 
orientation of the frustum. The model includes the effects of wind and different 
release angles on the resulting flame size and location in space. The model 
geometry is shown in Figure 9-7.

![Figure 9-7: Diagram of flame shape and dimensions [Chamberlain, 1987]](image)

The following dimensions are predicted:
visible flame length \((L_b)\),
and width of tip \((W_2)\).

- lift of height \((b)\),
- width of base \((W_1)\),
- angle between the frustum axis and the release axis in the \(x-y\) plane \((\alpha)\)
  (flame tilt),
- angle between the frustum axis and the release axis in the \(x-z\) plane
  (flame twist).

(The order in which these values are calculated are as they are presented above, as some use previous results to complete).

The expanded jet momentum flux, \(G\), is given by

\[
G = \frac{\pi \rho_j u_j^2 d_j^2}{4} \tag{9-8}
\]

where \(\rho_j\) is the expanded jet density \((\text{kg/m}^3)\), \(u_j\) is the expanded jet velocity \((\text{m/s})\) and \(d_j\) is the expanded jet diameter \((\text{m})\). The Richardson number, \(\xi\), which characterises the balance between the initial jet momentum flux and buoyancy, is defined as,

\[
\xi(L) = \left[\frac{\pi \rho_{av} g}{4G}\right]^{1/3} L \tag{9-9}
\]

where \(g\) is the acceleration due to gravity \((\text{m/s})\) and \(L\) is a representative length scale of the flame \((\text{m})\). This length scale is the flame length for a vertical flame in still air, \(L_{b0}\). \(L_{b0}\) is given by the solution of the equation,

\[
\varphi = 0.2 + 0.02\xi(L_{b0}) \tag{9-10}
\]

where,

\[
\varphi = \frac{2.85D_s}{L_{b0} w} \tag{9-11}
\]

and \(w\) is the mass fraction of fuel in a stoichiometric mixture of air and \(D_s\) is an effective source diameter (see Eq. (9-29)).

The balance between the wind momentum flux and the initial jet momentum flux in the \(x\) and \(z\) directions is expressed by,
\[ \Omega_x = \left[ \frac{\pi \rho_{\text{air}}}{4G} \right]^{1/2} L_{b0} u_{\text{air}} \]  
\[ \Omega_z = \left[ \frac{\pi \rho_{\text{air}}}{4G} \right]^{1/2} L_{b0} w_{\text{air}} \]  
(9-12)

where \( u_{\text{air}} \) and \( w_{\text{air}} \) are the wind velocity components in the x and z direction respectively.

To calculate, \( X \) (in Figure 9-7), the following equation is used,

\[ \frac{X}{L_{b0}} = f(\xi)(1 + r(\xi)\Omega_x) \]  
(9-13)

where

\[ f(\xi) = 0.55 + (1 - 0.55)e^{-0.168\xi} \quad \xi \leq 5.11 \]  
(9-14)

\[ f(\xi) = 0.55 + (1 - 0.55)e^{-0.168\xi - 0.3(\xi - 5.11)^2} \quad \xi > 5.11 \]

and

\[ r(\xi) = 0.0 \quad \xi \leq 3.3 \]  
(9-15)

\[ r(\xi) = 0.082\left(1 - e^{-0.5(\xi - 3.3)}\right) \quad \xi > 3.3 \]

To calculate, \( Y \) (in Figure 9-7), the following equation is used,

\[ \frac{Y}{L_{b0}} = h(\xi)(1 + c(\xi)\Omega_x) \]  
(9-16)

where

\[ h(\xi) = \frac{1}{\left(1 + \frac{1}{\xi}\right)^{8.78}} \]  
(9-17)

and

\[ c(\xi) = 0.02\xi \]  
(9-18)

The flame length, \( L_b \), can be calculated by,

\[ L_b = \sqrt{X^2 + Y^2} \]  
(9-19)

The flame tip width, \( W_2 \), is calculated as follows,
The lift-off length, \( b \), is calculated as,

\[
b = 0.141 (G \rho_{\text{air}})^{1/2}
\]  \hspace{1cm} (9-21)

The flame base width, \( W_{1} \), is calculated as follows,

\[
\frac{W_{1}}{b} = -0.18 + 0.081 \xi
\]  \hspace{1cm} (9-22)

The flame is the angle the frustum axis makes with the horizontal plane for the horizontal releases in this study, \( \alpha \), is calculated as follows,

\[
tan(\alpha) = \frac{Z}{(X - b)} = 0.178 \Omega_{z}
\]  \hspace{1cm} (9-23)

### 9.3.2.2 Gas Jet Properties

The expanded jet gas velocity is given by,

\[
u_{j} = M_{j} \sqrt{\frac{\gamma_{g} R_{c} T_{j}}{W_{gk}}}  \hspace{1cm} (9-24)
\]

where \( R_{c} \) is the gas constant, \( \gamma_{g} \) is the ratio of specific heats in the expanded jet, \( W_{gk} \) is the molecular weight of gas (kg/mol) \( M_{j} \) is the jet Mach number and \( T_{j} \) is the expanded jet temperature. All pressures and temperatures are in SI units.

For choked flow,

\[
M_{j} = \left( \frac{\gamma_{g} + 1}{\gamma_{g} - 1} \right)^{1/2} \left( 1 - \frac{P_{c}}{P_{0}} \right)^{(\gamma_{g} - 1)/\gamma_{g}} - 2
\]  \hspace{1cm} (9-25)

where \( P_{0} \) it the atmospheric pressure. The static pressure, \( P_{c} \), at the hole exit plane is given by,
\[ P_c = 3.6713 \frac{\dot{m}}{d_0^2} \sqrt{\frac{T_c}{\gamma g W_{gk}}} \]  
(9-26)

where \( d_0 \) is the diameter of the release orifice and \( \dot{m} \) is the mass flow rate (kg/s). The expanded jet gas temperature, \( T_j \), is given by,

\[ T_j = \frac{2T_s}{2 + (\gamma g - 1)M_j^2} \]  
(9-27)

The static temperature, \( T_c \), at the hole exit plane is given as,

\[ T_c = \frac{2T_s}{1 + \gamma g} \]  
(9-28)

and \( T_s \) is the stagnation temperature.

The effective source diameter \( D_s \) is the throat diameter of an imagined nozzle from which air of density \( \rho_{air} \) issues at mass flow rate \( \dot{m} \) and uniform velocity \( u_s \). For choked flow,

\[ D_s = d_j \left( \frac{\rho_j}{\rho_{air}} \right)^{1/2} \]  
(9-29)

where \( \rho_j = \rho_{g0} \frac{273}{T_j} \), \( d_j = \left( \frac{4\dot{m}}{\pi u_j \rho_j} \right)^{1/2} \), and the subscript \( j \) represent the property in the expanded jet and the superscript \( 0 \) represent the property at standard conditions.

### 9.3.2.3 Radiative Characteristics

For this model, the flame has defined surface (a truncated cone) and hence incident radiation is calculated based on an approach using the surface emissive power and the view factor between the flame surface and the receiver (see Section 8.5.2. The radiation model is given by [Johnson et al., 1994]

\[ I = \pi (V_{side} E_{side} + V_{end} E_{end}) \]  
(9-30)

where \( V \) is the view factor and \( E \) is the surface emissive power, the subscript \( side \) represents that value contribution from just the side of the flame and the subscript \( end \) represents that value contribution from just the end of the flame.
The model assumes a uniform surface emission power, SEP (kW/m²), \( E_\infty \), given by the following expression

\[
E_\infty = \frac{F_q Q}{A}
\]  

(9-31)

where \( F_q \) is the fraction of heat factor for a flame which emits black body radiation and is given, for natural gas, as a function of jet velocity, \( u_j \), [Johnson et al., 1994],

\[
F_q = 0.21e^{-0.00323u_j} + 0.14
\]  

(9-32)

\( A \) is the surface area (including ends) and can be calculated, from the predicted flame dimensions, as,

\[
A = \pi \left( \frac{W_1^2}{4} + \frac{W_2^2}{2} \right) + \frac{\pi}{2} \left( W_1 + W_2 \right) \sqrt{R_L^2 + \left( \frac{W_1 - W_2}{2} \right)^2}
\]  

(9-33)

Johnson et al. [1994] introduced a method that takes into account the effect the varying pathlengths through the flame by assigning different values of SEP for the ends and sides of the flame geometry,

\[
E = \frac{1}{1 - e^{-kL}} E_\infty
\]  

(9-34)

where \( k \) is the grey gas absorption coefficient (m⁻¹) and \( L \) is a length scale (m) representing the emitting pathlength. \( k \) was found to be best fitted by 0.4. \( L \) is set as \( W_2 \) for calculations of the SEP for the sides of the flames and \( R_L \) for the ends of the flame.

The view factor between a flame of surface area \( A_2 \) and an infinitesimal target is defined as [Hankinson, 1985],

\[
V = \int_{\theta_1}^{\theta_2} \cos \theta_1 \cos \theta_2 dA_2
\]  

(9-35)

To calculate the view factor the geometry of the flame and receiving surface needs to be specified.

For anything but simple geometric shapes the integral cannot be expressed analytically and should be solved numerically [Hankinson, 1985]. Briefly, in
this method the flame surface is subdivided into triangles, and then the view factor between a triangle and a target can be expressed as,

\[
V_{12} = \frac{\cos \theta_1 \cos \theta_2 A_2}{\pi r^2}
\]  

(9-36)

where subscript 2 represents the triangle on the flame and 1 the target point.

The analysis is done using vector methodology. Thus \( \cos \theta_1 \) is the angle that the triangle normal makes with the vector from the centre of the triangle to the target, and \( \cos \theta_2 \) is the angle that the target normal makes with the vector from the target to the centre of the triangle element on the flame surface. Note that there is an angle of orientation of the target at which maximum incident radiation is received. This will be when the target normal is pointing along the direction vector to the triangle element. Then the view factor between the flame and the target is the vector sum of all \( V_{12} \) for those triangular elements on the flame surface that can be “seen” from the location and orientation of the target, and that can “see” the location of the target from their position and orientation,

\[
V = \sum_{\cos \theta_1 \geq 0, \cos \theta_2 \geq 0} V_{12}
\]  

(9-37)

First points on the surface of a vertical frustum and end circles were calculated and then the centres of the triangles formed by these points calculated. All the points were then transformed by rotation matrices. The normals to the triangles centres were also calculated. Finally the view factor for each target was calculated using the vector analysis method of Hankinson [1985] as described above. This was checked visually in 3 dimensions by plotting the triangular elements and the vector normals.

**9.3.2.4 Computer Implementation of the Model and Application to the NATURALHY Jet Fires**

A range of input parameters were needed for this model, the source fuel, the mass flow rate, the wind speed, and the locations and orientations of targets. All of these parameters were taken from the experimental conditions apart from the mass flow rate which was calculated using the standard equation for
choked flow through an orifice with the coefficient of discharge set at 0.9. The equations were incorporated into a computer program. This allowed changes to be made so a range of fuel compositions could be modelled. The fraction of heat radiated was calculated using Equation (9-32). This equation predicts that the fraction of heat radiated decreases with increasing jet velocity which will increase with increasing hydrogen addition.

The results were analysed in spreadsheet software. Predictions included the flame geometry and location in space and the incident radiation at selected locations. A three dimensional coordinate system was used.

9.3.3 GL Model JBurn [2006]

GL Industrial Services kindly donated the source code for this model [JBurn, 2006]. It is an extension of the model found in Cleaver and Edward [1990] where they developed an integral type model for gas dispersion for a turbulent jet in a cross flow.

9.3.3.1 Flame Geometry

It starts with the conservation of horizontal and vertical momentum taking into account a crosswind (parallel to ground) and density difference between the jet and the surrounding air. Further conservation equations for energy and species are also presented. In these equations the “bulk” mean values of jet properties such as specific heat capacity and density are used. The profiles of variables across the jet can be found by using an assumed cosine profile for velocity, concentration and temperature. The entrainment rate is the sum of different entrainment mechanism terms; the relative flow between the jet and cross flow and atmospheric turbulence.

This model predicts the trajectory of the jet, that is, the centre line of the jet (where fuel concentration is a maximum). It then predicts the temperature, the velocity and concentration profiles across the jet at intervals along the trajectory.
The flame length is set to be twice the distance to the maximum temperature.

9.3.3.2 Radiative Characteristics

The radiation model is of the multiple point source type; the number of points is determined by how many steps were used in stepping along the trajectory and is calculated automatically within the model. The radiation leaving the $i$'th point are weighted by the flame temperature, $T$, at that point to the fourth power over the sum of the temperature to the fourth power along the trajectory,

$$\frac{T_i^4}{\sum T_i^4}$$

Thus those parts of the flame where the temperature is higher radiate a greater amount of heat.

The fraction of heat for natural gas was calculated as,

$$F = 0.3213 - 0.4179x10^{-3}u_s$$

(9-39)

where $u_s$ is the speed of sound in the gas at atmospheric conditions [Cowley and Johnson, 1992, p125]. For hydrogen the value of $F$ is fixed, in the software, as 0.15. The model was modified to allow the fraction of heat radiated for natural gas/hydrogen mixtures to be calculated based on a mass fraction basis.

9.3.3.3 Application to the NATURALHY tests

A range of input parameters were needed for this model, the fuel composition, the mass flow rate, the exit and ambient temperature, the wind speed at a specified height, and the locations and orientation of targets. The parameters were taken from the experimental test conditions apart from the mass flow rate which was calculated using the standard equation for choked orifice flow with the coefficient of discharge set at 0.9. The results were imported and analysed in spreadsheet software.
9.4 **Results – Comparison of predictions with experimental data**

During the experiments, radiometers were positioned in 3 areas around the flame, crosswind to the north, crosswind to the south and downwind around the tail of the flame (see Figure 9-1). When comparing the data with predictions it is important to consider these groups separately as the effects of the wind on the flame may result in the measured values being higher than predicted on one side crosswind and lower on the other side.

In this section, predictions of the flame length and incident thermal radiation are compared against experimental observations using each of the 3 modelling approaches described above in Section 9.3.

### 9.4.1 Multi Point Source Model

The mass flow rate was calculated from the standard orifice flow equation for choked flow.

#### 9.4.1.1 Flame geometry

Table 9-3 lists the predicted flame length (from Lowesmith et al. [2007]) and the visible experimental value. It also lists the predicted flame power.

<table>
<thead>
<tr>
<th>Test</th>
<th>Predicted Mass Flow Rate (kg/s)</th>
<th>Predicted Flame Power (MW)</th>
<th>Flame Length (m) Predicted</th>
<th>Flame Length (m) Experiment</th>
<th>Factor*</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.01</td>
<td>150.7</td>
<td>18.7</td>
<td>19.8</td>
<td>0.94</td>
</tr>
<tr>
<td>2</td>
<td>9.61</td>
<td>480.5</td>
<td>28.9</td>
<td>37.8</td>
<td>0.77</td>
</tr>
<tr>
<td>3</td>
<td>18.85</td>
<td>943.0</td>
<td>37.1</td>
<td>49.9</td>
<td>0.74</td>
</tr>
<tr>
<td>4</td>
<td>2.75</td>
<td>145.1</td>
<td>18.5</td>
<td>17.6</td>
<td>1.05</td>
</tr>
<tr>
<td>5</td>
<td>8.55</td>
<td>451.0</td>
<td>28.2</td>
<td>30.7</td>
<td>0.92</td>
</tr>
<tr>
<td>6</td>
<td>17.08</td>
<td>902.2</td>
<td>36.5</td>
<td>45.2</td>
<td>0.80</td>
</tr>
</tbody>
</table>

*Factor is predicted divided by measured length

*Table 9-3: Experimentally observed [Lowesmith, Apr, 2008] and predicted flame length*
Figure 9-8 compares the flame length, derived from the experiments and the predictions, the y=x line is also drawn. Also shown are lines representing ±20% (factor 0.8-1.2) and ±40% (factor 0.6-1.4). In general, the predictions are within ±20% although tend to under-predict the length for the larger release tests. This may be due to the fact that during these experiments, the releases were horizontal in a downwind direction, which will tend to produce a longer flame length than other orientations relative to the wind. The correlation was derived from a large body of data from tests where the releases were both vertical and horizontal. It was derived from many different hydrocarbon fuel jet fires (some having heavier molecular weights than natural gas) and the correlation is a best fit through all the observed flame lengths which exhibited a range of flame lengths for the same flame power.

It can also be seen that the correlation correctly predicts that the addition of hydrogen results in a reduced flame length, due to the lower power of the flame. (Although the calorific value of the mixture is higher than for natural gas, the mass outflow is lower and overall the power is lower).
9.4.1.2 **Incident Radiation**

The model does not account for the effect of the wind on the location of the flame, so it is assumed to be coincident with the release direction. For most of the experiments, the wind direction was close to the release direction, except for Test 2, where the wind direction was 27 degrees to the south and Test 5, where the wind direction was 14 degrees to the south from the release direction. The location of the flame was not determined experimentally (only length) so in what follows, both the measured and predicted flame lengths are shown along the release axis on a plan view of the test arrangement which also includes the location of the radiometers.

Incident radiation was predicted for each radiometer location and compared with the measured values, with the crosswind south (S), crosswind north (N), and downwind locations identified separately.

Hence for each test, two figures are presented ((a) and (b)), the first (a) showing the predicted and measured flame length and radiometer locations and the second (b) comparing the predicted and measured incident radiation levels. Also shown on the second figure (b) are the y=x line and lines representing ±20% (factor 0.8-1.2) and ±40% (factor 0.6-1.4). Figure 9-9 to Figure 9-14 present this information for tests 1 to 6 respectively.

For all the tests, the predicted incident radiation is mostly within ±20% of the measured values across the measurement positions. The exceptions arise as follows:

- There is a tendency to underpredict for radiometer locations 7 and 9, located downwind of the flame tip. This is probably due to the flame length being generally slightly underpredicted. As radiometers 7 and 9 are close to the flame tip they will be sensitive to any difference in the location of the flame tip.
• For Tests 2 and 5 (Figure 9-10 and Figure 9-13) where the wind was blowing significantly off the release axis (and to the south) there was a tendency to overpredict the radiation to the north (more than +20%).

Ideally, this model would have a way of accounting for the effect of the prevailing wind conditions on the flame geometry and this is likely to improve the predictions of incident radiation. The program is implemented in three dimensional space so it would be possible to include a correlation for the effect of the wind on the flame trajectory.
(a): Test 1 – Plan view of radiometers (stars) and flame geometry (line)

(b): Test 1 - Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-9: Predictions using multi point source model for Test 1
(a) Test 2 – Plan view of radiometers (stars) and flame (line)

(b): Test 2 - Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]
Figure 9-10: Predictions using multi point source model for Test 2
(a) Test 3 - Plan view of radiometers (stars) and flame (line)

(b): Test 3 - Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-11: Predictions using multi point source model for Test 3
(a) Test 4 - Plan view of radiometers (stars) and flame (line)

(b): Test 4 - Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-12: Predictions using multi point source model for Test 4
(a) Test 5 – Plan view of radiometers (stars) and flame (line)

(b) Test 5 - Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-13: Predictions using multi point source model for Test 5
(a) Test 6 – Plan view of radiometers (stars) and flame (line)

(b) Test 6 - Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-14: Predictions using multi point source model for Test 6
9.4.2 Johnson et al. [1994]

The model was run for conditions representing tests 1-6. The flame geometry and incident radiation are compared to experimental values below.

9.4.2.1 Flame Geometry

Table 9-4 and Figure 9-15 show a comparison of the flame length predicted by this model to the observed visible lengths. As can be seen, the predictions of flame length are generally within ±20%.

This model predicts the flame geometry as a truncated cone, located in space, based on the release momentum, wind conditions and buoyancy. Overlays of the predicted flame geometry on photographs of the experiments are presented in Appendix B.1, from which it can be seen that the model tends to predict the flame locations as higher than the photographic evidence, especially for the natural gas/hydrogen mixture tests (Tests 4 to 6).

<table>
<thead>
<tr>
<th>Test</th>
<th>Predicted Flame Length (m)</th>
<th>Experimental Estimated Flame Length (m)</th>
<th>Factor*</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>21.2</td>
<td>19.8</td>
<td>1.07</td>
</tr>
<tr>
<td>2</td>
<td>35.6</td>
<td>37.8</td>
<td>0.94</td>
</tr>
<tr>
<td>3</td>
<td>47.2</td>
<td>49.9</td>
<td>0.95</td>
</tr>
<tr>
<td>4</td>
<td>21.6</td>
<td>17.6</td>
<td>1.23</td>
</tr>
<tr>
<td>5</td>
<td>35.4</td>
<td>30.7</td>
<td>1.15</td>
</tr>
<tr>
<td>6</td>
<td>48.0</td>
<td>45.2</td>
<td>1.06</td>
</tr>
</tbody>
</table>

* Factor is predicted divided by measured length.

Table 9-4: Experimental observed [Lowesmith, Apr, 2008] and predicted flame lengths
9.4.2.2 Incident Radiation

For this model, the fraction of heat radiated was calculated for each test using Equation (9-32) and then SEP values calculated using (9-31) and (9-34). For the six tests, the SEP values were calculated and can be found in Table 9-5.

<table>
<thead>
<tr>
<th>Test</th>
<th>$F_{\infty}$</th>
<th>Predicted SEP from side of flame (kW/m²)</th>
<th>Predicted SEP from end of flame (kW/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.191</td>
<td>199.2</td>
<td>304.4</td>
</tr>
<tr>
<td>2</td>
<td>0.191</td>
<td>252.3</td>
<td>286.9</td>
</tr>
<tr>
<td>3</td>
<td>0.192</td>
<td>271.8</td>
<td>284.2</td>
</tr>
<tr>
<td>4</td>
<td>0.182</td>
<td>163.5</td>
<td>226.3</td>
</tr>
<tr>
<td>5</td>
<td>0.183</td>
<td>204.8</td>
<td>225.0</td>
</tr>
<tr>
<td>6</td>
<td>0.183</td>
<td>220.5</td>
<td>227.5</td>
</tr>
</tbody>
</table>

Table 9-5: Surface Emissive Power (SEP) values
As can be seen lower SEP values are predicted for the natural gas/hydrogen mixture. For each test, two figures are presented, the first (a) showing the predicted flame geometry and radiometer locations and the second (b) comparing the predicted and measured incident radiation levels. Also shown on the second figure are y=x line and lines representing ±20% (factor 0.8 – 1.2) and ±40% (factor 0.6 – 1.4). Figure 9-16 to Figure 9-21 present this information for tests 1 to 6 respectively.

As can be seen from Figure 9-16 to Figure 9-21 the incident radiation is underpredicted by more than 20% and sometimes underpredicted by more than 40%. Possible factors which may contribute to this underprediction of radiation are:

- As noted above, the flame location in space is predicted to be higher than observed during the experiments. This will cause the distance from the flame to the radiometer locations to increase and hence results in lower incident radiation levels.
- The correlation for the fraction of heat radiated, $F_\infty$ (Equation (9-32)), was derived for natural gas and may not be applicable to natural gas/hydrogen mixtures. The higher velocity of the mixture results in a lower value of $F_\infty$ being derived for these cases, and hence lower incident radiation levels will result.
(a) Test 1 – Plan view of radiometers (stars) and flame geometry (line)

(b) Test 1 - Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-16: Prediction using the Johnson et al. [1994] model for Test 1
(a) Test 2 – Plan view of radiometers (stars) and flame geometry (line)

(b) Test 2 - Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-17: Prediction using the Johnson et al. [1994] model for Test 2
(a) Test 3 – Plan view of radiometers (stars) and flame geometry (line)

(b) Test 3 – Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-18: Prediction using the Johnson et al. [1994] model for Test 3
(a) Test 4 – Plan view of radiometers (stars) and flame geometry (line)

(b) Test 4 – Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-19: Prediction using the Johnson et al. [1994] model for Test 4
(a) Test 5 – Plan view of radiometers (stars) and flame geometry (line)

(b) Test 5 – Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-20: Prediction using the Johnson et al. [1994] model for Test 5
(a) Test 6 – Plan view of radiometers (stars) and flame geometry (line)

(b) Test 6 – Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-21: Prediction using the Johnson et al. [1994] model for Test 6
9.4.3 GL JBurn [2006]

The model was run for conditions representing tests 1-6. The flame geometry (a curved line) and incident radiation are compared to experimental values. Additional results can be provided by this model including the flame radius, flame temperature, and the fuel concentration profile along the flame trajectory; these can be found in Appendix B.2.

9.4.3.1 Flame Geometry

Figure 9-22 displays a comparison of the flame length as predicted by the model and the experimental data together with lines showing $\pm 20\%$ and $\pm 40\%$ variation. The flame length is taken to be twice the distance to the maximum flame temperature. It is unknown whether this is meant to be for visible flame length or chemical flame length. On this basis, the model overpredicts the flame length by more than 20\% although generally within $\pm 40\%$. However, also shown on the figure (with the ‘mod.’ suffix) is a flame length based on 1.7 times the distance to the maximum flame temperature which correlates better with the experimental data, generally within $\pm 20\%$. The model predicts the observed trend that adding 25\% hydrogen to natural gas shortens the flame (apart from the small tests where the model predicts a slight increase of the flame length). However, the predicted reduction in flame length due to the addition of hydrogen is much less than observed.
### Table 9-6: Experimental observed [Lowesmith, Apr, 2008] and predicted flame lengths

<table>
<thead>
<tr>
<th>Test</th>
<th>Predicted Flame Length (m)</th>
<th>Modified Predicted Flame Length (m)</th>
<th>Experimental Estimated Flame Length (m)</th>
<th>Factor* (modified flame length)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>27.4</td>
<td>23.3</td>
<td>19.8</td>
<td>1.18</td>
</tr>
<tr>
<td>2</td>
<td>46.9</td>
<td>39.9</td>
<td>37.8</td>
<td>1.05</td>
</tr>
<tr>
<td>3</td>
<td>64.0</td>
<td>54.4</td>
<td>49.9</td>
<td>1.09</td>
</tr>
<tr>
<td>4</td>
<td>28.2</td>
<td>23.8</td>
<td>17.6</td>
<td>1.35</td>
</tr>
<tr>
<td>5</td>
<td>46.2</td>
<td>39.3</td>
<td>30.7</td>
<td>1.28</td>
</tr>
<tr>
<td>6</td>
<td>62.5</td>
<td>53.1</td>
<td>45.2</td>
<td>1.18</td>
</tr>
</tbody>
</table>

* Factor is predicted divided by observed length

9.4.3.2 **Incident Radiation**

The calculated fraction of heat radiated used in the incident radiation predictions are listed in Table 9-7. These were derived using Equation (9-39)
for tests 1 to 3, a value of 0.15 was taken for hydrogen and calculating $F$ for mixtures was done on a mass fraction basis. The value of $F$ for the mixed gas tests 4 to 6 are higher because the value of $F$ for hydrogen is actually slightly larger than what is predicted for natural gas using Equation (9-39).

<table>
<thead>
<tr>
<th>Test</th>
<th>$F$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.145</td>
</tr>
<tr>
<td>2</td>
<td>0.147</td>
</tr>
<tr>
<td>3</td>
<td>0.147</td>
</tr>
<tr>
<td>4</td>
<td>0.148</td>
</tr>
<tr>
<td>5</td>
<td>0.149</td>
</tr>
<tr>
<td>6</td>
<td>0.149</td>
</tr>
</tbody>
</table>

Table 9-7: Calculated value of $F$ used in JBURN

For each test, two figures are presented, the first (a) showing the predicted flame trajectory and radiometer locations and the second (b) comparing the predicted and measured incident radiation levels. Also shown on the second figure are the $y=x$ line and lines representing $\pm 20\%$ (factor 0.8-1.2) and $\pm 40\%$ (factor 0.6-1.4). Figure 9-23 to Figure 9-28 present this information for tests 1 to 6 respectively.

As can be seen from Figure 9-23 to Figure 9-28 there is a tendency to significantly overpredict incident radiation (up to 40\% lower) for the lowest release rate (Tests 1 and 4 on Figure 9-23 and Figure 9-26) and significantly underpredict (by up to 40\% for the highest release rates (Tests 3 and 6 on Figure 9-25 and Figure 9-28). In Tests 3 and 6, it is the locations downwind that are the most underpredicted. This is probably due to predictions of flame trajectory (see Appendix B.2) where it can be seen that the flame tip is predicted to be about 70m above ground level for Tests 3 and 6 compared to the observed height of approximately 22m. This means that at the downwind locations, the model predicts the distance between the radiometer and the flame to be much larger than in reality and this perhaps explains why the incident radiation is underpredicted.
Chapter 9

(a) Test 1 – Plan view of radiometers (stars) and flame trajectory (line)

(b) Test 1 – Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-23: Prediction using the JBurn model for Test 1
(a) Test 2 – Plan view of radiometers (stars) and flame trajectory (line)

(b) Test 2 – Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-24: Prediction using the JBurn model for Test 2
(a) Test 3 – Plan view of radiometers (stars) and flame trajectory (line)

(b) Test 3 – Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-25: Prediction using the JBurn model for Test 3
(a) Test 4 – Plan view of radiometers (stars) and flame trajectory (line)

(b) Test 4 – Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-26: Prediction using the JBurn model for Test 4
(a) Test 5 Plan view of radiometers (stars) and flame trajectory (line)

(b) Test 5 – Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-27: Prediction using the JBurn model for Test 5
(a) Test 6 – Plan view of radiometers (stars) and flame trajectory (line)

(b) Test 6 – Comparison of maximum incident radiation from predictions and experimental data [Lowesmith, Apr, 2008]

Figure 9-28: Prediction using the JBurn model for Test 6
9.5 **Discussion and Conclusions**

Three models have been applied to predict the flame geometry and incident radiation field for conditions representing the experiments tests and the predictions compared with experimental data. All these models (with the exception of JBurn) are empirically based. Flame geometry is determined as simple length, a truncated cone or a curvilinear trajectory by the three models considered respectively. Only in JBurn is the flame geometry determined phenomenologically. Incident radiation is based on a multi point source approach or by using a solid flame geometry, view factor and surface emissive power.

The relative performance of the predictive methods compared to the experimental data is discussed below.

### 9.5.1 Flame Geometry

For the experimental test conditions studied, the flame geometry predictions for the three approaches can be summarised as:

- Flame correlation from Lowesmith [2007]: Slightly underpredicted but within 25%.
- Johnson et al. [1994]: Length predicted within +20% but location of flame in space higher than observed.
- JBurn [2006]: length overpredicted by 20-40% and flame tip higher than observed.

However, the experimental test conditions were limited to 25% (by volume) hydrogen addition to natural gas. The question arises of how flame length would vary as hydrogen addition increases for the above methods.

Work has been carried out with hydrogen diffusion flames for example work by Choudhuri and Gollahalli [2000, 2003], Mogi and Horiguchio [2008] and Schefer et al. [2006]. The authors Choudhuri and Collahalli and Schefer et al. use the same correlation form, from Delichatsios [1993], but determine
different constants giving a non dimensional flame length 1.4 times higher than the correlation given by Delichatsios [1993]. Choudhuri and Gollahalli [2003] report that adding hydrogen increases the combustion performance via faster burning, as expected. This reduces the time, and distance, it takes for combustion which shortens the length of the flame. Further, the luminosity of hydrogen blended flames reduces, which reduces the measurement of the visible flame length. The authors Cozzi and Coghe [2005] report the same, but also present evidence for longer fuel jet penetration in blended fuels.

Table 9-8 details the predicted flame lengths for the above three models for compositions ranging from 100% natural gas to 100% hydrogen. These are also plotted in Figure 9-29. The source mass flow was calculated using the pressure behind the orifice in the experiments and the atmospheric conditions were taken from test 4, 5, and 6.

As can be seen from Figure 9-29 the flame length predicted by the correlation from Lowesmith et al. [2008] suggests that the flame length decreases up to 75% hydrogen addition before rising slightly for the 100% hydrogen case, reflecting the variation in power (also shown on the figure). However, the variation across the fuel range is not large.

However, the flame length predicted by the model from Johnson et al. [1994] increases consistently with hydrogen addition, resulting in a significantly increased flame length for 100% hydrogen. This is markedly different from the prediction from the Lowesmith et al. correlation.

The GL model JBurn behaves in an unusual fashion in that the flame length predicted decreases with the exception of the smaller release where the flame length increases to 50% hydrogen addition before decreasing thereafter. Once again, quite different to other approaches.
Overall, it is clear that further research is needed (ideally with large scale experiments) to resolve the behaviour of these flames as different trends with hydrogen addition are currently predicted by these 3 models.
Figure 9-29: Predicted flame length from 0 to 100% hydrogen addition to methane, (a) 20mm release, (b) 35mm release, (c) 50mm release
### 9.5.2 Incident radiation

For the experimental test conditions studied, the incident radiation predictions for the 3 modelling approaches can be summarised as follows:

- **Multi point source with length by Lowesmith et al. [2007]:** Predicted mostly within ±20% of measured values except where the wind direction significantly affects the flame location and for positions downstream of the flame.

- **Johnson et al. [1994] model:** Underpredicted by more than 20% and sometimes over 40% underpredicted. Possibly due to the flame location being incorrect, and an inappropriate correlation for hydrogen containing fuels when determining the SEP.

- **JBurn model [2006]:** Overpredicts by up to 40% for the lowest studied release rates but underpredicts by a similar amount for the highest release rates. The latter is probably due to incorrect prediction of the flame trajectory.

On this basis, it would appear the first method provides the better predictions. However, this is probably to be expected since the fractions of heat radiated used are based on values determined from large scale experiments. This is also the case for JBurn which used a fixed value of $F$ for 100% hydrogen. For the Johnson et al. [1994] model the value of $F$ (used to determine the SEP) was calculated based on the jet velocity and whilst this correlation may have been validated for natural gas it may be inappropriate for hydrogen. As the hydrogen content increase, this will result in lower SEPs being determined.

Overall it can be concluded that further research is required to develop these models with large scale experimental data at higher hydrogen concentration levels being essential to provide validation.
10 Predicting Fires Following High Pressure Gas Pipeline Ruptures

10.1 Introduction

In this chapter the size and incident radiation characteristics of fires resulting from failed pipelines is predicted and validated against the NATURALHY experiments. The experiments are first introduced before the modelling approach taken is outlined. Then predictions are compared with the experimental data.

10.2 Experiments

Two experiments were undertaken within the NATURALHY project [Lowesmith, Aug, 2008] to study full scale pipeline fires following underground high pressure pipeline ruptures. This scenario represents the result of a failing high pressure gas transmission pipeline.

The pipeline had a diameter of 150mm and was pressurised to a gauge pressure of 70 bar. The pipe was failed catastrophically by removing a 1.67m section using shaped high explosive charges, allowing gas to discharge from both ends of the severed pipe. The section of the pipe that was failed was situated in a pre-fabricated steel crater of a shape similar to that observed after actual underground pipeline ruptures. Figure 10-1 shows a schematic of the experimental set up. The points with the label with a prefix ‘R’ are the locations of the radiometers and the points with the prefix ‘T’ are the locations
of pressure transducers. There were incendiary devices to make sure the gas was ignited.

Incident thermal radiation was measured using 15 radiometers, the overpressure was measured using 6 pressure transducers, and video footage of the experiment was captured.

Two tests were carried out, one with a natural gas/hydrogen mixture with 22.5%v/v hydrogen addition and one with natural gas. Table 10-1 lists the test conditions.
<table>
<thead>
<tr>
<th>Condition</th>
<th>Test 1</th>
<th>Test 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel</td>
<td>77.5:22.5 (NG:H₂)</td>
<td>NG</td>
</tr>
<tr>
<td>Initial Pressure (barg)</td>
<td>71.4</td>
<td>70.5</td>
</tr>
<tr>
<td>Atmospheric Pressure (mbar)</td>
<td>997</td>
<td>1023</td>
</tr>
<tr>
<td>Relative Humidity (%)</td>
<td>88</td>
<td>88</td>
</tr>
<tr>
<td>Ambient Temperature (°C)</td>
<td>3.4</td>
<td>3.5</td>
</tr>
<tr>
<td>Wind Direction</td>
<td>318 ±7</td>
<td>246 ±16</td>
</tr>
<tr>
<td>Wind Speed @2.9m (m/s)</td>
<td>1.4 +0.3</td>
<td>4.8 +0.3</td>
</tr>
<tr>
<td>Wind Speed @4.7m (m/s)</td>
<td>1.2 +0.4</td>
<td>5.1 +0.4</td>
</tr>
<tr>
<td>Wind Speed @8.4m (m/s)</td>
<td>2.0 +0.3</td>
<td>5.6 +0.3</td>
</tr>
<tr>
<td>Wind Speed @10.9m (m/s)</td>
<td>2.1 +0.3</td>
<td>5.7 +0.3</td>
</tr>
</tbody>
</table>

Table 10-1: Pipeline fire test conditions [Lowesmith, Aug, 2008]

Figure 10-2 shows a photograph of a pipeline fire in progress in the early stages where there is a fireball. After the fireball burns out, a steadily declining fire is formed which reduces in size as the pipeline depressurises. Figure 10-3 shows the pipeline after the tests, showing how the failed pipeline section ‘folded’ out leaving gas to escape from both severed ends at the full diameter of the pipeline.
Figure 10-2: Photograph of a pipeline fire experiment in progress [Lowesmith, Aug, 2008]

Figure 10-3: Photograph of the pipeline after the test [Lowesmith, Aug, 2008]
10.3 Modelling Methodology

Due to time constraints and the success of the flame length correlation of Lowesmith et al [2007], see Section 9.3.1, only this flame length model was used along with the multi point source model (MPS) for predicting the pipeline fires.

The flame correlation of Lowesmith et al [2007] (Equation (9-1)) is a function of the flame power in MW. The flame power is calculated as the product of the mass flow rate (kg/s) and the heat of combustion or calorific value of the fuel (J/kg). The current model implementation does include the affect of wind so flame tilt is not predicted. The fire is modelled as a vertical flame. Unlike the constant source mass flow rate found in a jet fire scenario, the gas pressure at the release point decreases in a ruptured pipeline which reduces the mass flow rate from the severed ends until the gas pressure reaches atmospheric pressure. This is a transient problem and needs to be treated as such. Therefore, at selected times it is possible to calculate the flame length using the mass flow rate at that time, either from experimental data or predictions from an outflow model. If it is assumed that the instantaneous flame length corresponds to the instantaneous outflow then, using the multi point source (MPS) (see Section 9.3.1.1) model, it should be possible to calculate the incident thermal radiation. However, the validity of this approached must be demonstrated by comparing predictions with the large scale data. Note in particular that this approach is not expected to replicate the early stages of the event when the fireball occurs since during this stage, the assumption that the flame length corresponds to the instantaneous outflow will be invalid.

Figure 10-4 shows how the models are link together in progression.

---

Figure 10-4: Link between models
To implement this, the Lowesmith et al [2007] (Equation (9-1)) flame length correlation was applied many times at specified times using the measured mass flow rate. The predicted flame length was then input into the MPS model, at every time step, which then calculated n points on the flame between the release source (a point on the ground) and the predicted flame length. The incident thermal radiation is then calculated at this time step. Essentially this method is calling models that are used for steady state calculation, but using a time dependent mass flow rate, creating a series of 'virtual' steady state problems.

The predictions of outflow from a ruptured pipeline as it depressurises is a complex problem and outside the scope of this work. Hence, in order to demonstrate the validity of the model for flame length and incident radiation, experimental data on the mass outflow was used.

The heat of combustion (calorific value) is calculated by the difference of the sum of heat of formation of the products and the sum of heat of formation of the reactants [Kuo, 2005]. The heat of formation is taken from an electronic file provided by the new format of the database from Bonnie McBride of NASA Glenn Research Centre. The calculated calorific values for the studied fuel composition are listed in Table 10-2.

<table>
<thead>
<tr>
<th>Test</th>
<th>Fuel</th>
<th>Calculated Calorific Value (MJ/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>01</td>
<td>77.5% natural gas :</td>
<td>50.03</td>
</tr>
<tr>
<td></td>
<td>22.5% hydrogen</td>
<td></td>
</tr>
<tr>
<td>02</td>
<td>natural gas</td>
<td>52.84</td>
</tr>
</tbody>
</table>

Table 10-2: Fuel properties

10.4 Results – Comparison of Predictions with Experimental Data

The model was used to calculate the flame length and the incident radiation at the radiometer locations as used in the experiments (Figure 10-1).
10.4.1 Flame Geometry

The flame length of the experiments was determined by analysis of the video footage and infra-red thermal imaging of the experiments.

Figure 10-5 shows the flame length with time for test 1, using 77.5% natural gas 22.5% hydrogen (mixed gas), from the experimental observations, derived from the 2 video cameras and the thermal imaging camera, and the predictions from the flame length model. Overall the agreement is very good with the exception of the initial stage immediately after the rupture, where the fireball is formed (as expected). During this initial stage, the validity of the assumption that the instantaneous outflow corresponds to the instantaneous flame length breaks down. However, as can be seen, after this stage, the flame length can be calculated from the instantaneous outflow using the flame length correlation.

![Pipeline Test 1: Flame Length with Time](image)

**Figure 10-5: Test 1 –Predicted and observed [Lowesmith, Aug, 2008] flame length with time**
Figure 10-6 shows the flame length with time for test 2, using natural gas, from the experimental observations, derived from the 2 video cameras and the thermal imaging camera, and the predictions from the model. Once again the predictions are in good agreement after the initial stage. There is a greater degree of experimental scatter for this test due to the higher wind speed which prevailed.

![Pipeline Test 2: Flame Length with Time](image)

**Figure 10-6: Test 2 – Predicted and observed [Lowesmith, Aug, 2008] flame length with time**

The flame width was also calculated from experimental film footage using the same techniques as used to derive the flame length. It was found that the maximum flame width can be calculated by taking 0.45 of the flame length.

Figure 10-7 shows the maximum flame width for test 1 for experimental derivations and predictions. The simple correlation for flame width gives a good prediction apart from the initial stages where the fire ball exists.
Figure 10-7: Test 1 – Predicted and observed [Lowesmith, Aug, 2008] flame width with time

Figure 10-8 shows the maximum flame width for test 2 for experimental derivations and predictions. Again the correlation provides a good prediction giving the right trend, apart from the initial stages.

Figure 10-8: Test 2 – Predicted and observed [Lowesmith, Aug, 2008] flame width with time
The calculation of flame width, along with the flame length, would allow a 3 dimensional volume to be constructed (such as a cone or cylinder) to represent an idealisation of the flame shape to be used in modelling. This could then be used in a solid geometry approach to modelling the incident radiation. However, the approach adopted here is to use only the flame length and a multi point source model of the incident radiation.

10.4.2 Fraction of Heat Radiated

The value of the fraction of heat radiated was calculated from experimental data with time. For reduction of data processing and display, the incident radiation and mass flow rate was averaged over successive 10 second periods. The predicted flame length was used. The number of point sources for the MPS model, \( n \), was chosen to be 100.

Figure 10-9 is for test 1, where the gas was a mixture of natural gas and hydrogen. The figure also shows the value of \( F \) if a single point source approach was taken. As can be seen, the difference in the fraction of heat radiated between a single point source and 100 point sources is minimal for this test. This is because the radiometer locations are far away (the closest radiometer is 40 m away from crater). The fraction of heat radiated steadily increased with time as the flame became shorter. The fraction of heat radiated has a minimum value at approximately 0.25 and slowly rises to 0.43, before spiking at 0.57 after 170 s. The reasons for the apparent increase in F with time are not known. The average fraction of heat radiated, averaging up to 170 s was 0.31.
Figure 10-9: Test 1 – Fraction of heat calculated values

Figure 10-10 is for test 2, where the gas was pure natural gas. The difference of the fraction of heat radiated between $n=1$ and $n=100$ is again seen to be small. The fraction of heat radiated does not follow the same trend as for test 1, with no apparent trend with time. The fraction of heat radiated has a minimum value at approximately 0.25 and rises to a maximum 0.35. The average fraction of heat radiated, averaging up to 180 s, was 0.30. Hence, the average fraction of heat value is very similar to that calculated for the mixed gas test.
10.4.3 Predicting Incident Radiation (Test 1)

The incident radiation predicted by the MPS model is now compared against the experiment data for test 1, a mixture of 77.55% natural gas and 22.25% hydrogen. First, the incident radiation predicted with time at three selected locations (crosswind) are presented, and then all the incident radiation predictions are presented at time intervals of 20 s up to 120 s. The number of point sources was taken to be 100. The fraction of heat radiated is taken to be a constant equal to 0.31. Due to the light wind speeds prevailing, the flame experienced negligible tilt. As the flame model does not include the effects of the wind on the flame these are the ideal conditions to compare the model against.

10.4.3.1 Incident radiation at specific locations

Figure 10-11 to Figure 10-13 shows the incident radiation at radiometer 11 (40m to the south of the crater) radiometer 13 (76m to the south) and radiometer 14 (144m to the south). The results are in good agreement except for the fireball stage. In the very first stage where the fireball occurs it is seen
that the incident radiation rises to a maximum and the sharply declines and while the model does not predict the peak at the correct time, the maximum value of the incident radiation predicted is similar to that measured. After the fireball phase the predictions agree well with the observe values, especially as time progresses.

Figure 10-11: Test 1 – Comparison of incident radiation prediction and experimental data [Lowesmith, Aug, 2008] at R11, 40m to the south
Comparison of Incident Radiation at R13, 76m to South

![Graph showing comparison of incident radiation prediction and experimental data at R13, 76m to the south.](image)

Figure 10-12: Test 1 Comparison of incident radiation prediction and experimental data [Lowesmith, Aug, 2008] at R13, 76m to the south

Comparison of Incident Radiation at R14, 144m to South

![Graph showing comparison of incident radiation prediction and experimental data at R14, 144m to the south.](image)

Figure 10-13: Test 1 – Comparison of incident radiation prediction and experimental data [Lowesmith, Aug, 2008] at R14, 144m to the south
10.4.3.2 Incident radiation at all locations at 20s intervals

Figure 10-14 to Figure 10-19 show the incident radiation at all targets away from the failure point, in West, East, South, South east, and North-east lines, at different time intervals, 20, 40, 80, 100 and 120 seconds after the rupture respectively. It is important to distinguish the direction as the distance from the flame to the radiometers will change as the position of the flame varies due to the wind. To this end the radiometer locations are grouped into the categories: west (W), east (E), south east (SE), south (S) and north east (NE).

Initially the predictions tend to overpredict by up to 40% but after about 60 s the prediction tend to be within ±20% of the measured values.

---

**Pipeline Test 1: Incident Radiation at t~20s**

![Graph showing measured vs predicted radiation at different locations](image)

*Figure 10-14: Test 1 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations, 20s after rupture*
Figure 10-15: Test 1 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations, 40s after rupture

Figure 10-16: Test 1 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations, 60s after rupture
Figure 10-17: Test 1 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations, 80s after rupture

Figure 10-18: Test 1 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations, 100s after rupture
10.4.4 Predicting Incident Radiation (Test 2)

The incident radiation predicted by the MPS model is now compared against the experiment data for test 2, pure natural gas. First, the incident radiation predicted with time at three selected locations (crosswind) are presented, and then all the incident radiation predictions are presented at time intervals of 20 s up to 120 s. The number of point sources was taken to be 100. The fraction of heat radiated is taken to be a constant equal to 0.3. The wind in this test was much stronger than in test 1 and it can be seen in the tilt of the flame in Figure 10-20.
10.4.4.1 *Incident radiation at specific locations*

Figure 10-21 to Figure 10-23 show the incident radiation predictions with time for radiometer locations 11, 13 and 14. They are all located south of the release positions at distances 40m 76m and 144m away from the release position respectively. The predictions seen in the figures are in general agreement with the experimental observations, after the fireball state, and the level of agreement increases as time progresses.
Comparison of Incident Radiation at R11, 40m to South

Figure 10-21: Test 2 – Comparison of incident radiation predictions and experimental data [Lowesmith, Aug, 2008] at R13, 76m to the south

Comparison of Incident Radiation at R13, 76m to South

Figure 10-22: Test 2 – Comparison of incident radiation predictions and experimental data [Lowesmith, Aug, 2008] at R13, 76m to the south
10.4.4.2 Incident radiation at all locations at 20s intervals

Figure 10-24 to Figure 10-29 show the incident radiation at all targets away from the crater, in West, East, South, South east, and north east lines, at different time intervals, 20, 40, 80, 100 and 120 seconds after the rupture respectively. It is important to distinguish the direction as the distance from the flame to the radiometers will change as the position of the flame varies due to the wind. To this end the radiometer locations are grouped into the categories: west (W), east (E), south east (SE), south (S) and north-east (NE).

As can be seen from these figures (compared to Figure 10-14 to Figure 10-19 for Test 1) there is a greater degree of scatter. This is primarily due to the increased wind speed during the test which caused the flame to tilt to the east. Consequently there is a tendency to overpredict radiation levels to the west and underpredict radiation levels to the east. The level of agreement between predictions and the data to the south (crosswind) improves with time from initially more than 40% overprediction at 20 s (Figure 10-24) to extremely good agreement at 120 s (Figure 10-29). The level of agreement is also
generally better for radiometers in the far field where the flame tilt is less important.

Figure 10-24: Test 2 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations at 20s.

Figure 10-25: Test 2 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations at 40s.
Figure 10-26: Test 2 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations at 60s

Figure 10-27: Test 2 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations at 80s
Figure 10-28: Test 2 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations at 100s

Figure 10-29: Test 2 – Incident radiation predictions compared against experiments data [Lowesmith, Aug, 2008] at all locations at 120s
10.5 **Conclusions**

In this chapter the MPS model has been extended, implemented and validated against large scale pipeline fire experiments. The flame length, flame width and thermal radiation have been shown to have reasonable agreement with observations (after the initial fireball phase) and the fraction of heat radiated has been calculated for pipeline fires involving natural gas or natural gas/hydrogen mixtures containing up to 22.5% hydrogen.

The major limitations of this model are:

- The inability to predict the initial fireball stage
- The need to input the mass flow rate with time from data or obtain prediction from other models.
- The lack of flame tilt due to the wind
- The lack of data for other hydrogen concentration levels in order to determine fractions of heat radiated.

In future work, the easiest to rectify in the above list would be to include the affect of wind on the flame tilt as several correlations for the effect of a crosswind on a flame are available [Cowley et al., 1992].

Nevertheless, this model of pipeline fires has been subsequently incorporated within a risk assessment methodology (called LURAP) developed within the NATURALHY project and shown to be able to predict individual and societal risk for pipelines successfully.
References to electronically available articles are provided with their DOI reference (document object identifier), please visit http://www.doi.org/ and enter the DOI reference to find the corresponding article online.

• Delichatsios, M.A., 1993, “Transition from momentum to buoyancy-controlled turbulent jet diffusion flames and flame height relationships”,

- JBurn, 2006, GL JBurn source code, private communication with A. Halford, GL.
In this chapter the main conclusions are summarised for the work presented in this thesis. Also, summarised are suggestions on possible future research topics or suggested extensions to further improve the models.

This work was part of the NATURALHY project safety work package aimed at assessing the effect on safety of adding hydrogen to the natural gas infrastructure. The objective of the thesis was to look at some available engineering models used for hazard analysis for natural gas and assess if they could be modified and applied to natural gas and hydrogen mixtures.

12.1 Predicting Explosion Hazards involving Natural gas/Hydrogen Mixtures

- The different properties of mixtures of natural gas and hydrogen were considered which identified the need to determine the burning velocity and Markstein number, in order to be able to develop and apply explosion models. Starting with some available experimental data obtained at an elevated temperature, a methodology was applied to temperature correct the laminar burning velocity to a standard temperature. Polynomial functions of the laminar burning velocity as a function of equivalence ratio were derived for several natural gas and hydrogen compositions.
- It has been shown that for confined vented explosions, the Shell explosion model SCOPE was capable of predicting the maximum internal
overpressure by using new laminar burning velocity data and Markstein numbers.

- For VCEs in compact regions of congestion two engineering models were assessed. The Shell CAM2 model was used unmodified but using new laminar burning velocity data and expansion ratios, whereas, the author developed a second model (CCEM) which was based on a previous model from GL. To allow for the effect of hydrogen addition to natural gas, the flame speed correlation within the CCEM model was generalised in terms of the laminar burning velocity, thereby enabling the model to be used for any fuel and equivalence ratio. Both models predicted the overpressure satisfactorily, for fuels containing up to 50% hydrogen, which is the range of most interest to the Naturalhy project. At 100% hydrogen, a detonation was observed during an experiment involving a compact congested region. Predicting a detonation event is outside the expectations for engineering models, nevertheless, both models predicted very high overpressures.

- For VCEs in a long congested region, an existing model provided by GL was used (HAREM). The flame speed model was then modified to allow for different fuels, stoichiometry, an initially moving flame with incoming speed and turbulence entering the congested region, and sensitivity to flame stretch through the Markstein number was incorporated. The model assumed that a limiting stable speed would be reached whereas experimental data showed that this was not always the case. For tests where a limiting speed was reached, the revised model performed well and generally provided satisfactory predictions of the flame speed and the overpressure. This indicates that the modifications made, satisfactorily accounted for the different fuels and initial flame parameters.

However, the revised model was still unable to address situations where an accelerating flame occurred, due to the assumed flame speed profile. Furthermore, in these situations the model underpredicted the final flame speed and maximum overpressure. However, the model did manage to predict flame speed about halfway along the congestion showing that some aspect of the flame acceleration was being represented. The
conditions where continued flame acceleration occurred were for fuels involving more than 40% hydrogen or high speed, highly turbulent flames for fuels with more than 20% hydrogen in the natural gas. The level of congestion was also found to be important in generating flame acceleration. This suggests that there is a feedback mechanism for the more reactive fuels, whereby the turbulence generated produces continued flame acceleration. This is an area suggested for further study, perhaps using CFD predictions which could be used to assess the turbulence levels downstream of obstacles and the response of the burning velocity of different mixtures of natural gas and hydrogen to this turbulence.

- Overall, in most cases, it has been shown that engineering models originally developed for natural gas explosions can be modified and applied to predict the hazard presented by explosions involving natural gas/hydrogen mixtures. Up to about 30% hydrogen addition to natural gas, no significant increase in overpressure is predicted, but for 40% or more hydrogen, there is, potentially, a large increase in explosion overpressure and an increased risk of transition to detonation in situations where a long path length through congestion is possible or high turbulence is generated.

### 12.1.1 Recommendations for future work on explosion models

- Determination of expressions for Markstein numbers and laminar burning velocities for the full range of natural gas/hydrogen mixtures.
- Develop a criteria which would identify when a continually accelerating flame might be generated, taking account of the hydrogen content in the fuel and the level of turbulence generated by the confinement and congestion.
12.2  Predicting Fire Hazards for Natural Gas/Hydrogen Mixtures

- For high pressure jet fires, 3 different approaches were used to predict the flame length (2 empirical and 1 phenomenological). Compared with experimental observations the predictions were all satisfactory for natural gas and approximately 25% hydrogen addition to natural gas. However, for mixtures that contain higher amounts of hydrogen, the correlations exhibited markedly different behaviour, so, without further experimental evidence, it is not possible to determine the effect of increased hydrogen addition on flame length.

- It has been demonstrated that a simple correlation for the flame length based on the power of the release can predict the flame length of a jet fire and also the flame length of a pipeline rupture with time (after the initial fireball phase), for natural gas and natural gas/hydrogen mixtures with approximately 25% hydrogen addition.

- A solid geometry model, using a truncated cone, was found to predict the flame tip to be higher above ground than observed (especially with some hydrogen addition), suggesting that buoyancy effects in the model are overstated.

- It has been shown that a multi-point source approach can successfully predict the incident radiation from jet fires and also from pipeline fires provided that suitable fractions of heat radiated can be obtained, which relies upon experimental data.

- There are some known limitations of the pipeline fire model in this work, in particular, no account is made for the initial fireball stage following the rupture and the transient mass outflow has not been modelled. Furthermore, to extend the model to other levels of hydrogen addition, values of the fraction of heat radiated will need to be obtained from large scale experiments.
12.2.1 Recommendations for future work on fire models

- It is recommended that a suitable correlation for flame tilt due to the wind is incorporated into the fire models which do not already account for the effect of the wind.

- Comprehensive large scale data is needed on the radiative characteristics of fires involving the full range of mixtures of natural gas and hydrogen.

- The Johnson et al. model of jet fires requires modifications in order to improve the prediction of the flame location in space. This will also improve the incident radiation predictions.

- To obtain a fully predictive model for pipeline fires, a pipeline mass outflow model will need to be obtained/developed which can account for the highly transient outflow following a pipeline rupture.
## A.1 Burning Velocity Data

The following table lists the power law equations derived for both the GRI and Konnov mechanisms.

<table>
<thead>
<tr>
<th>ER</th>
<th>% H₂</th>
<th>GRI Equation</th>
<th>Konnov Equation</th>
<th>GRI R²</th>
<th>Konnov R²</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.6</td>
<td>0</td>
<td>11.597(T/T₀)^2.1671</td>
<td>8.9159(T/T₀)^2.3254</td>
<td>0.9986</td>
<td>0.9998</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>12.554(T/T₀)^2.156</td>
<td>9.7638(T/T₀)^2.2987</td>
<td>0.9986</td>
<td>0.9999</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>13.691(T/T₀)^2.1247</td>
<td>10.655(T/T₀)^2.4421</td>
<td>0.9982</td>
<td>10.655</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>15.045(T/T₀)^2.1189</td>
<td>12.031(T/T₀)^2.4723</td>
<td>0.998</td>
<td>12.031</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>16.82(T/T₀)^2.1043</td>
<td>13.958(T/T₀)^2.4421</td>
<td>0.9979</td>
<td>13.958</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>18.767(T/T₀)^2.2962</td>
<td>16.333(T/T₀)^2.5559</td>
<td>0.9998</td>
<td>16.333</td>
</tr>
<tr>
<td>0.7</td>
<td>0</td>
<td>19.824(T/T₀)^1.8944</td>
<td>15.602(T/T₀)^2.0072</td>
<td>0.9987</td>
<td>15.602</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>21.246(T/T₀)^1.9086</td>
<td>16.757(T/T₀)^2.1155</td>
<td>0.9983</td>
<td>16.757</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>23.099(T/T₀)^1.894</td>
<td>18.338(T/T₀)^2.1155</td>
<td>0.9991</td>
<td>18.338</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>25.352(T/T₀)^1.844</td>
<td>20.519(T/T₀)^2.1155</td>
<td>0.9982</td>
<td>20.519</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>28.144(T/T₀)^1.849</td>
<td>23.198(T/T₀)^2.1923</td>
<td>0.9976</td>
<td>23.198</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>31.419(T/T₀)^1.8029</td>
<td>26.96(T/T₀)^2.2596</td>
<td>1</td>
<td>26.96</td>
</tr>
<tr>
<td>0.8</td>
<td>0</td>
<td>28.012(T/T₀)^1.7509</td>
<td>22.414(T/T₀)^1.829</td>
<td>0.9987</td>
<td>22.414</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>30.253(T/T₀)^1.7511</td>
<td>24.066(T/T₀)^1.9546</td>
<td>0.9989</td>
<td>24.066</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>32.519(T/T₀)^1.7515</td>
<td>26.28(T/T₀)^1.9367</td>
<td>0.9992</td>
<td>26.28</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>35.617(T/T₀)^1.729</td>
<td>28.969(T/T₀)^1.9947</td>
<td>0.9993</td>
<td>28.969</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>39.714(T/T₀)^1.6885</td>
<td>32.622(T/T₀)^2.0249</td>
<td>0.9994</td>
<td>32.622</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>44.394(T/T₀)^1.8297</td>
<td>37.622(T/T₀)^2.0922</td>
<td>1</td>
<td>37.622</td>
</tr>
<tr>
<td>0.9</td>
<td>0</td>
<td>34.951(T/T₀)^1.6522</td>
<td>28.394(T/T₀)^1.7719</td>
<td>0.9989</td>
<td>28.394</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>37.479(T/T₀)^1.658</td>
<td>30.593(T/T₀)^1.7992</td>
<td>0.9987</td>
<td>30.593</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>40.622(T/T₀)^1.6413</td>
<td>33.103(T/T₀)^1.8572</td>
<td>0.9992</td>
<td>33.103</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>44.483(T/T₀)^1.6338</td>
<td>36.459(T/T₀)^1.8953</td>
<td>0.9996</td>
<td>36.459</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>49.734(T/T₀)^1.5813</td>
<td>40.896(T/T₀)^1.942</td>
<td>0.9994</td>
<td>40.896</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>55.625(T/T₀)^1.717</td>
<td>47.165(T/T₀)^1.9907</td>
<td>1</td>
<td>47.165</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>39.192(T/T₀)^1.5907</td>
<td>32.97(T/T₀)^1.6465</td>
<td>0.9988</td>
<td>32.97</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>42.012(T/T₀)^1.5907</td>
<td>35.947(T/T₀)^1.5462</td>
<td>0.9985</td>
<td>35.947</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>45.79(T/T₀)^1.5832</td>
<td>39.223(T/T₀)^1.5557</td>
<td>0.9988</td>
<td>39.223</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>50.282(T/T₀)^1.5637</td>
<td>43.463(T/T₀)^1.5435</td>
<td>0.999</td>
<td>43.463</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>56.157(T/T₀)^1.5416</td>
<td>48.67(T/T₀)^1.6191</td>
<td>1</td>
<td>48.67</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>63.434(T/T₀)^1.6485</td>
<td>56.526(T/T₀)^1.6269</td>
<td>1</td>
<td>56.526</td>
</tr>
<tr>
<td>1.1</td>
<td>0</td>
<td>39.433(T/T₀)^1.5803</td>
<td>34.252(T/T₀)^1.6205</td>
<td>0.9999</td>
<td>34.252</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>42.311(T/T₀)^1.5724</td>
<td>37.198(T/T₀)^1.5561</td>
<td>0.9992</td>
<td>37.198</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>46.188(T/T₀)^1.5741</td>
<td>40.99(T/T₀)^1.5325</td>
<td>0.9999</td>
<td>40.99</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>51.25(T/T₀)^1.5639</td>
<td>45.827(T/T₀)^1.521</td>
<td>0.9999</td>
<td>45.827</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>57.77(T/T₀)^1.5422</td>
<td>52.204(T/T₀)^1.5099</td>
<td>1</td>
<td>52.204</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>66.066(T/T₀)^1.625</td>
<td>60.694(T/T₀)^1.5713</td>
<td>1</td>
<td>60.694</td>
</tr>
</tbody>
</table>
The following series of graphs displays the detailed modelling laminar burning velocity predictions for 0-50% hydrogen addition against the temperature increase from the standard temperature we set at 298K. The left hand column contains results derived from the GRI mechanism modelling and the right hand side for Konnov.
Laminar Burning Velocity for E.R. of 0.8

(GRI)

Laminar Burning Velocity for E.R. of 0.8

(Konnov)

Laminar Burning Velocity for E.R. of 0.9

(GRI)

Laminar Burning Velocity for E.R. of 0.9

(Konnov)
Laminar Burning Velocity for E.R. of 1.0

(GRI)

Temperature Increase from T0 (T/298K)

Ul [cm/s]

Laminar Burning Velocity for E.R. of 1.1

(Konnov)

Temperature Increase from T0 (T/298K)

Ul [cm/s]
Laminar Burning Velocity for E.R. of 1.4

(GRI)

Laminar Burning Velocity for E.R. of 1.5

(GRI)

Laminar Burning Velocity for E.R. of 1.4

(Konnov)

Laminar Burning Velocity for E.R. of 1.5

(Konnov)
APPENDIX B  Fires

B.1  *Extended Jet Fire Predictions* - *Johnson et al. 94*

B.1.1  Test 1
Appendix B

B.1.2 Test 2

B.1.3 Test 3
B.1.4 Test 4
B.1.5 Test 5

B.1.6 Test 6
B.2  **Extended Jet Fire Predictions - GL JBurn**

Graphs of the flame profile, temperature, gas jet velocity, concentrations and radius along the jet as predicted by the model are presented here.

B.2.1  **Test 1**

The following graph shows the flame trajectory in the x-z plane (vertical) and x-y plane (plan view) as you move along the x axis away from the release. The ‘wings’ along the centre line represent the radius of the flame along the x axis. Note that the way this is plotted is that the radius is shown in the vertical axis and not perpendicular to the flame trajectory due to limitations in the graphing software. This will become more pronounced as the flame trajectory becomes steeper. The triangles represent the targets in the x-u plane (plan view), the negative y co-ordinates represent the south crosswind direction, and positive y co-ordinates the north crosswind direction.
The following two graphs are for the temperature along the centre line, and the volume concentration of fuel.

The following two graphs are for the jet velocity, and the radius along the trajectory.
### B.2.2 Test 2

#### Test 1: Jet Velocity

![Graph of Test 1: Jet Velocity](image)

#### Test 1: Radius

![Graph of Test 1: Radius](image)

#### Test 2: Flame Profile

![Graph of Test 2: Flame Profile](image)
B.2.3 Test 3

Test 3: Flame Profile

Test 3: Temperature

Test 3: Volume Concentration
B.2.4 Test 4
Appendix B

Test 4: Temperature

Test 4: Volume Concentration

Test 4: Jet Velocity

Test 4: Radius
B.2.5 Test 5

Test 5: Flame Profile

Test 5: Temperature

Test 5: Volume Concentration
B.2.6 Test 6
C.1  **Equation of State**

The state of gas was calculated using the standard perfect gas equation of state,

$$PV = nRT$$

Density is calculated as follows,

$$\rho = \frac{m}{V} = \frac{nM_v}{\frac{nRT}{P}} = \frac{M_vP}{RT}$$

In the program the default state was, in SI units, 101325 Pa and 298K.

C.2  **Thermodynamic**

Thermodynamic data was calculated using electronic sources. The latest database was produced by NASA, 1996

[http://www.grc.nasa.gov/WWW/CEAWeb/RP-1311P2.htm, 17/09/08] which are based on polynomial fits of up to nine coefficient constants for a database of species. This shall be referred to as NASA-9. The format of the file and database was obtained from


There are three correlations provided by the NASA, for the non-dimensional specific heat capacity at constant pressure, the enthalpy and the entropy. In the file there is a set of coefficients for every specie, and sometimes multiples sets for different temperature ranges. Also included in the files is the heat of
formation values, which has been used to calculate the heat of combustion and the adiabatic combustion temperature.

C.3  Transport

Transport coefficients for viscosity (momentum transfer/diffusion), thermal conductivity (energy transport) and mass transport for pure species were calculated from equations found in Bird et al. [2002] and Kee et al. [2003]. Further, rules for determining the properties for mixtures are also found in the references. Extra information was needed for these calculations; this was obtained from the open source project http://sourceforge.net/projects/cantera as an electronic text file.

The following equations are for low densities, and are not meant to determine the properties for polar or elongated molecules. They are derived from kinetic theory, however it is possible to fit the coefficient by a log-log polynomial of the coefficient against temperature (viscosity and thermal conductivity independent of pressure).

C.3.1  Viscosity

The formula derived from fundamental theory for viscosity (see Bird et al. [2002], pp26 for full details) is written as,

$$
\mu = \frac{5}{16} \frac{\sqrt{\pi m K T}}{\pi \sigma^2 \Omega_{\mu}}
$$

where $m$ is the atomic weight [kg], $K$ is the Boltzmann constant, $T$ is the temperature [°K], $\sigma$ is a characteristic diameter of the molecule (also called the collision diameter) [m] and $\Omega_{\mu}$ is called the collision integral (for viscosity) and is a slowly varying function of the reduced temperature $K T/\varepsilon$. A correlation is available for this on page 866.

For mixtures of $N$ components, the following relation can be used giving satisfactory results,
\[ \mu_{\text{mix}} = \sum_{a}^{N} \sum_{b}^{N} x_a \mu_a x_b \phi_{ab} \]

where

\[ \phi_{ab} = \frac{I}{\sqrt{8}} \left( I + \frac{M_a}{M_b} \right)^{-1/2} \left( I + \left( \frac{\mu_a}{\mu_b} \right)^{1/2} \left( \frac{M_b}{M_a} \right)^{1/4} \right)^2 \]

where \( x \) is the mole fraction of that component, and \( M \) is the molecular weight.

### C.3.2 Thermal Conductivity

The formula for thermal conductivity (Bird et al. [2002], pp275) in monatomic gases is,

\[ k = \frac{25 \sqrt{\pi n k T}}{32 \pi \sigma^2 \Omega_k} \hat{C}_v \]

where \( \hat{C}_v \) is the molar specific heat capacity at constant volume, the rest are the same as for viscosity, see previous heading. For polyatomic gases the following formula should be used,

\[ k = \left( \hat{C}_p + \frac{5 R}{4 M} \right) \mu \]

where \( \mu \) is the viscosity.

For mixtures of \( N \) components, the following relation can be used giving satisfactory results,

\[ k_{\text{mix}} = \sum_{a}^{N} \sum_{b}^{N} x_a k_a x_b \phi_{ab} \]

where the variable are the same as for viscosity. The standard deviation is about 4%. Furthermore, an extension to this theory is shown in Kee et al, 2003, pp516, which was used in the coding, the above is shown for its functional dependence and simplicity.

### C.3.3 Mass Diffusion

For binary diffusion the expression from Warnatz et al. [2001], p57 is used,
\[ D_{12} = \frac{3}{8} \frac{\sqrt{\pi KT} 2m_{12}}{\pi \sigma_{12}^2 \Omega_{1,1}^T T_{12}} \frac{1}{\varrho} \]

where \( m_{12} \) is the reduced mass, \( m_{12} = \frac{m_1 m_2}{m_1 + m_2} \), \( T^*_{12} \) is the reduced temperature, \( KT/\varepsilon_{12} \), where \( \varepsilon_{12} = \sqrt{\varepsilon_1 \varepsilon_2} \).

For mixtures, the empirical relation can be used,

\[ D^M_j = \frac{1 - w_j}{\sum_{j=1}^{M} x_j D_j} \]

where \( w \) is the mass fraction, and \( x \) the mole fraction.