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INVESTIGATION OF THE EFFECTS OF PREHEATING ON THE CHARACTERISTICS OF MICRO COMBUSTION

by

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Abstract

The requirement for efficient power sources for portable electronics and miniature mechanical devices, such as laptops, micro robots or micro aerial vehicles, has led to research on ultra micro gas turbine (UMGT). The ultra micro gas turbine is one of the most promising power sources for small scale applications due to its higher power and energy densities compared to currently used batteries.

In order to realise UMGT as a viable power source, its individual components have to be developed, since downscaling introduces new problems for each component. Since the micro combustor is one of the key components of UMGT, it is an obvious area for investigation and improvement. Until now, it has been very difficult for micro combustors to achieve wide flame stability, high combustion efficiency and clean combustion with low pressure loss, due to the associated downscaling problems, such as high heat loss ratio and small residence time.

In order to overcome the issues associated with smaller residence time, preheating the reactants was investigated in the present study, both experimentally and numerically. Two different domains were used in the two different methods.

The effects of preheating the reactants on the flame stability and combustion characteristics were investigated experimentally on a 46 mm inner diameter quartz-walled flat flame combustor. The preheating was provided with external heaters. The flame shape and behaviour were observed with different air mass flow rates and equivalence ratios. The experimental results showed that preheating widened the flame stability limit. From the experimental results a new correlation was developed between mass flow rate, reactant temperature, air to fuel ratio and the diameter of the micro combustor. With this correlation, it is possible to determine the minimum combustor diameter required for stable flat flame combustion. Also, in order to have a stable flat flame at higher mass flow rates, the correlation enables the calculation of the required reactants temperature, and is a major contribution to the design of micro combustors. Furthermore, it was found that with the flat flame combustor, very clean, that is, almost complete combustion was achieved with both natural gas and methane as fuels. In addition, different flame holder materials were investigated for their pressure loss characteristics and usability for UMGT applications.

On the other hand, the effects of preheating on the flame stability and species concentrations were investigated numerically within a 2 mm diameter micro combustor tube, over two-dimensions. The simulations were performed with both adiabatic walls and non-adiabatic walls. At high incoming flow velocities, preheating was shown to widen the flame
stability limit. On the other hand, there is no advantage in preheating for low incoming flow velocities or low mass flow rates. A comparison of employing different skeletal and detailed reaction mechanisms was made. Furthermore, in the non-adiabatic case the effect of heat loss through the outer wall via convection and radiation were investigated with different heat transfer coefficients.

In conclusion, preheating widens the flame stability limit and provides flame sustainability even at very small scales. The information generated in this research will help the development of UMGT as a viable alternative to conventional power sources at small scale.
Dedicated to my love, Altan
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# Table of Contents

Abstract ....................................................................................................................................... i  
Acknowledgements .................................................................................................................... v  
Table of Contents ..................................................................................................................... vii  
List of Figures ........................................................................................................................... xi  
List of Tables ............................................................................................................................ xix  
Nomenclature ............................................................................................................................ xxi  
1 INTRODUCTION ............................................................................................................. 1  

1.1 Downscaling problems of combustors ........................................................................ 3  

1.1.1 Smaller residence time ........................................................................................... 3  

1.1.2 Increasing heat loss ............................................................................................... 4  

1.2 Application of UMGТ ............................................................................................... 5  

1.3 Objectives .................................................................................................................. 7  

1.4 Thesis Outline ............................................................................................................ 9  

2 LITERATURE REVIEW ................................................................................................ 11  

2.1 Literature review on ultra micro gas turbine ............................................................ 11  

2.2 Literature review on micro combustors ...................................................................... 15  

2.3 Literature review on flat flames ................................................................................ 24  

2.3.1 Flame holder materials and geometry ................................................................ 26  

2.3.2 Burning velocity.................................................................................................... 28  

2.3.3 Flame temperature ............................................................................................... 31  

2.3.4 The effect of flame holder on flame temperature ................................................ 32  

2.3.5 Flame location and stand-off distance .................................................................. 33  

2.3.6 Flame instabilities ............................................................................................... 35  

2.3.7 Emissions ............................................................................................................ 37  

2.4 The effect of the reactants temperature on burning velocity .................................... 39  

2.5 Premixed laminar flame ............................................................................................ 40  

2.6 Summary .................................................................................................................... 42  

3 EXPERIMENTAL APPARATUS AND METHODOLOGY ........................................ 43  

3.1 Flat flame combustor ................................................................................................. 43  

3.2 Flame holders ............................................................................................................. 44  

3.3 Mixing chamber ........................................................................................................ 45  

3.4 Fuels .......................................................................................................................... 47
<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.4.1</td>
<td>Natural gas</td>
<td>48</td>
</tr>
<tr>
<td>3.4.2</td>
<td>Methane</td>
<td>48</td>
</tr>
<tr>
<td>3.5</td>
<td>Mass flow controllers</td>
<td>49</td>
</tr>
<tr>
<td>3.6</td>
<td>Flame stability limit</td>
<td>50</td>
</tr>
<tr>
<td>3.7</td>
<td>Flame visualization</td>
<td>51</td>
</tr>
<tr>
<td>3.8</td>
<td>Pressure measurements</td>
<td>51</td>
</tr>
<tr>
<td>3.9</td>
<td>Emission measurements and combustion efficiency</td>
<td>53</td>
</tr>
<tr>
<td>3.9.1</td>
<td>Exhaust gas analyzers</td>
<td>53</td>
</tr>
<tr>
<td>3.10</td>
<td>Temperature measurements</td>
<td>55</td>
</tr>
<tr>
<td>3.11</td>
<td>Summary</td>
<td>58</td>
</tr>
<tr>
<td>4</td>
<td>EXPERIMENTAL RESULTS AND DISCUSSION</td>
<td>59</td>
</tr>
<tr>
<td>4.1</td>
<td>Pressure loss through flame holders</td>
<td>59</td>
</tr>
<tr>
<td>4.2</td>
<td>Operating conditions for different flame holders without heating</td>
<td>62</td>
</tr>
<tr>
<td>4.3</td>
<td>The usability of different plates as flame holders for flat flame combustion</td>
<td>64</td>
</tr>
<tr>
<td>4.4</td>
<td>The effects of preheating the reactants on the flame stability limit</td>
<td>67</td>
</tr>
<tr>
<td>4.5</td>
<td>The effects of preheating the reactants on the flat flame stabilization</td>
<td>68</td>
</tr>
<tr>
<td>4.6</td>
<td>The flame behaviour with changing air to fuel ratio</td>
<td>71</td>
</tr>
<tr>
<td>4.7</td>
<td>The relationship between burning velocity and the incoming flow velocity</td>
<td>76</td>
</tr>
<tr>
<td>4.8</td>
<td>The proposed correlation for flat flame burners</td>
<td>80</td>
</tr>
<tr>
<td>4.9</td>
<td>Exhaust emissions</td>
<td>84</td>
</tr>
<tr>
<td>4.9.1</td>
<td>CO\textsubscript{2}, O\textsubscript{2} and CO emissions</td>
<td>84</td>
</tr>
<tr>
<td>4.9.2</td>
<td>NO\textsubscript{x} emission</td>
<td>88</td>
</tr>
<tr>
<td>4.9.3</td>
<td>Unburned hydrocarbon emissions</td>
<td>92</td>
</tr>
<tr>
<td>4.10</td>
<td>Equivalence ratio calculation from exhaust gas constituents</td>
<td>93</td>
</tr>
<tr>
<td>4.11</td>
<td>Combustion efficiency</td>
<td>96</td>
</tr>
<tr>
<td>4.12</td>
<td>Flame temperature</td>
<td>98</td>
</tr>
<tr>
<td>4.13</td>
<td>Summary</td>
<td>99</td>
</tr>
<tr>
<td>5</td>
<td>NUMERICAL STUDY</td>
<td>101</td>
</tr>
<tr>
<td>5.1</td>
<td>Introduction and literature review on numerical micro combustion research</td>
<td>101</td>
</tr>
<tr>
<td>5.2</td>
<td>Numerical model</td>
<td>103</td>
</tr>
<tr>
<td>6</td>
<td>NUMERICAL RESULTS AND DISCUSSION: ADIABATIC CASE</td>
<td>106</td>
</tr>
<tr>
<td>6.1</td>
<td>Boundary conditions</td>
<td>106</td>
</tr>
<tr>
<td>6.2</td>
<td>Validation of the model</td>
<td>107</td>
</tr>
</tbody>
</table>
6.3 Comparison of chemical reaction mechanisms ....................................................... 109
6.4 Effect of initial temperature and incoming flow velocity ....................................... 113
   6.4.1 Effect of initial reactant temperature ............................................................... 113
   6.4.2 Effect of increasing incoming flow velocity .................................................... 114
   6.4.3 Effect of equivalence ratio ............................................................................... 117
6.5 Summary ................................................................................................................. 118
7 NUMERICAL RESULTS AND DISCUSSION: NON-ADIABATIC CASE .............. 119
   7.1 Boundary conditions ............................................................................................... 119
   7.2 Comparison of chemical reaction mechanisms ....................................................... 119
   7.3 Comparison between adiabatic and non-adiabatic wall conditions .................. 122
   7.4 Effect of initial temperature and incoming flow velocity ....................................... 124
      7.4.1 Effect of initial reactant temperature ............................................................... 124
      7.4.2 Effect of increasing incoming flow velocity .................................................... 126
   7.5 Effect of equivalence ratio ...................................................................................... 127
   7.6 Effect of heat loss .................................................................................................... 128
      7.6.1 Heat loss via convection only .......................................................................... 128
      7.6.2 Effect of heat transfer coefficient with and without radiation ......................... 131
   7.7 The effect of preheating at the same mass flow rate ............................................... 133
   7.8 Summary ................................................................................................................. 135
8 CONCLUSIONS AND SUGGESTIONS FOR FUTURE STUDIES ........................... 137
Appendices ............................................................................................................................. 142
   A1 Estimation of molar mass and LHV of natural gas ...................................................... 142
   A2 Sierra Smart Trak mass flow controller working principle .......................................... 144
   A3 K-Factor calculation using Sierra Smart-Trak 2 Series with other gases .................. 145
   A4 Micro Motion mass flow meter working principle ...................................................... 148
   A5 Uncertainty calculation of the K type thermocouples ............................................... 149
      A5.1 K type reactants thermocouple .............................................................................. 149
      A5.2 0.25 mm diameter K type thermocouple ............................................................... 149
      A5.3 0.5 mm diameter K type thermocouple ................................................................. 150
   A6 Thermocouple radiation correction .............................................................................. 151
   A7 SK16 reaction mechanism ........................................................................................ 152
   A8 SK17 reaction mechanism ........................................................................................ 154
   A9 GRI 3.0 reaction mechanism ...................................................................................... 156
References
List of Figures

Figure 1-1 Comparison of specific energies [3]........................................................................................................2
Figure 1-2 Specific energy and applications [7]........................................................................................................6
Figure 2-1 a) Schematic of the baseline design of the MIT’s ultra micro gas turbine engine b) cross-section of half of the axisymmetric 6-wafer static structure [5, 31] .................................................................11
Figure 2-2 a) Schematic layout of Tohoku University’s UMGT b) compressor and turbine [32] ..........................12
Figure 2-3 Schematic layout of Palm-type UMGT (left) [8], turbine rotor of finger-top UMGT (right) [7] ..........................................................................................................................................................13
Figure 2-4 Schematic layout of Belgian PowerMEMS [11] ......................................................................................13
Figure 2-5 ONERA’s UMGT designs a) single stage UMGT [34] b) Cocoon architecture [14] .....................14
Figure 2-6 Schematic and a photo of the UMGT prototype at the University of Roma [37] .........................14
Figure 2-7 Schematic of catalytic combustors a) three-wafer combustor, b) six-wafer combustor [38] .......16
Figure 2-8 Schematic design of seven-wafer micro combustor [40] .................................................................17
Figure 2-9 a) Canister type micro combustor, b) Doughnut type micro combustor [41] .................................17
Figure 2-10 Schematic of flat flame micro combustor for a) H₂ b) Methane [25] .............................................18
Figure 2-11 Schematic design of prototype annular micro combustor for the palm-top UMGT [8] .........18
Figure 2-12 Schematic and a photo of prototyped propane-air flat flame micro combustor [43] .............18
Figure 2-13 Schematic of engineering model of propane-fuelled flat flame micro combustor [44] .......19
Figure 2-14 Schematic of micro combustors of Marbach et al. [26, 27] .........................................................20
Figure 2-15 a) Cross section view of prototyped HEX-Combustor, b) Prototyped HEX-Combustor [46]..........................21
Figure 2-16 Swiss roll combustors [49] ..............................................................................................................22
Figure 2-17 Combustion chamber layout of Belgian PowerMEMS [11] .........................................................22
Figure 2-18 ONERA’s first micro combustor and its position in the pressurised vessel [13] ...................23
Figure 2-19 Combustion chamber and spiral heat exchanger of the University of Roma Sapienza [57] ..........................................................................................................................................................23
Figure 2-20 Flat flame burners .........................................................................................................................25
Figure 2-21 a) Schematic of Powling’s flat flame burner, photographs of b) rich ether/air flame [70], and c) methyl nitrite [69] obtained with the burner ............................................................................................................26
Figure 2-22 Effect of equivalence ratio on the laminar burning velocity of methane–air mixtures, P=1 bar, T=288.15–298.15 K [80] .................................................................................................................................................. 29

Figure 2-23 Flame location vs inlet velocity [89] ......................................................................................... 33

Figure 2-24 The dependence of flame temperature on burning velocity (left) (Ø is the fuel-air equivalence ratio, ψ is the molar nitrogen to oxygen ratio of the reactants) and the dependence of stand-off distance on flame temperature (right) (solid curves are the theoretical results) [66] ............. 34

Figure 2-25 Computed and measured flame stand-off distance as functions of the mass flow rate (left)
Computed and measured flame temperature as functions of the mass flow rate (right)[65] ............... 35

Figure 2-26 Concentration and temperature profiles of a one-dimensional, premixed, adiabatic flame[106] ............................................................................................................................................. 41

Figure 2-27 Flame front of a conical flame .................................................................................................. 41

Figure 3-1 Drawing and photo of the test rig .......................................................................................... 43

Figure 3-2: Photo of flame holders ........................................................................................................... 44

Figure 3-3: Mixing chamber improvements a)foams, b)stainless steel wool, c) glass beads, d)extended air inlets ............................................................................................................................................... 46

Figure 3-4 Different coloured flames due to improper mixing ............................................................... 46

Figure 3-5 Mixing chamber improvements-2 .......................................................................................... 47

Figure 3-6 Extended mixing chambers, 60 mm (left), 120 mm (right) ................................................. 47

Figure 3-7 Micro Motion mass flow meter calibration set-up .............................................................. 50

Figure 3-8 Calibration of Micro Motion mass flow meter with water .................................................... 50

Figure 3-9 Observing flat flame with the help of a black cylinder ......................................................... 51

Figure 3-10 a) Sintered stainless steel flame holder b) View of quartz tube combustor ....................... 52

Figure 3-11 Pressure transducers, Betz micromanometer and a U-tube manometer ............................ 52

Figure 3-12 a) Emission probe 60 mm far from the flame holder surface, b) flame at low equivalence ratio, c) flame at high equivalence ratio, d) deposits from the melting of the emission probe affecting the flame .......................................................................................................................... 54

Figure 3-13 a) Extended exhaust chimney, b) Signal oven, c) Gas analyzers rack .............................. 55

Figure 3-14 a) Schematic of Medtherm fine wire thermocouple b) Tip detail (G. Luft from Medtherm Corporation, email to author, January 27, 2012) .......................................................... 56

Figure 3-15 a) Thermocouple with the cone shaped holder, b) thermocouple very close to the flame 57

Figure 3-16 a) Thermocouple with robust holder, b) vertical traverse, c) water cooling for fine wire thermocouples ........................................................................................................................................... 57
Figure 3-17 A photo of ISOTECH Jupiter 650B dry block high temperature calibrator
Figure 4-1 Pressure loss vs incoming velocity with different flame holders
Figure 4-2 Percentage of pressure loss vs incoming velocity with different flame holders
Figure 4-3 Operating conditions for different flame holders showing the region in which flat flame combustion occurred
Figure 4-4 Blue flat flame combustion on the surface of FA060 alumina ceramic flame holder: air mass flow rate of 0.38 g/s, equivalence ratio of 0.75, a) before crack and b) after crack
Figure 4-5 Flat flame combustion on the surface of perforated plate flame holder: air mass flow rate of 0.22 g/s, equivalence ratio of 0.66
Figure 4-6 Flat flame combustion on the surface of a) SS filter flame holder, b) R100 flame holder and c) R200 flame holder at an air mass flow rate of 0.22 g/s and Ø=0.66
Figure 4-7 Flame stability limit of natural gas-air mixture for reactants at room temperature and 600 K
Figure 4-8 Flame photos at an air mass flow rate of 0.38 g/s and an equivalence ratio of 0.57 when the reactants are at a) room temperature and b) 600 K
Figure 4-9 Flame photos at an air mass flow rate of 0.38 g/s and an equivalence ratio of 0.62 when the reactants are at a) room temperature, b) 343 K, and c) 600 K
Figure 4-10 Flame photos at an air mass flow rate of 0.38 g/s and an equivalence ratio of 0.68 when the reactants are at a) room temperature, b) 360 K, and c) 600 K
Figure 4-11 Flame photos at an air mass flow rate of 0.76 g/s and an equivalence ratio of 0.64 when the reactants are at a) room temperature, b) 600 K
Figure 4-12 Flame photos at an air mass flow rate of 0.38 g/s and equivalence ratios of a) 0.51 and b) 0.54
Figure 4-13 Flame photos at an air mass flow rate of 0.38 g/s and equivalence ratios of a) 0.75 and b) 0.82
Figure 4-14 Flame photos at an air mass flow rate of 0.38 g/s and equivalence ratios of a) 0.88 side view, b) 0.88 closer view from top, c) 0.95 side view, and d) 0.95 closer view from top
Figure 4-15 Flame photos from the side view, at an air mass flow rate of 0.38 g/s and equivalence ratios of a) 1.00, b) 1.02, c) 1.06, d) 1.08, e) 1.14, f) 1.20
Figure 4-16 Flame photos at an air mass flow rate of 0.38 g/s and equivalence ratios of a) 1.32 side view, b) 1.32 closer view from top
Figure 4-17 Flame photos at an air mass flow rate of 0.31 g/s and equivalence ratios of 1.30
Figure 4-18 At an Ø=0.68, air mass flow rates with increasing reactants temperature, when d=46 mm and uₐ=5SL
Figure 4-19 CO₂, O₂ and CO emissions of natural gas at an air mass flow rate of 0.38 g/s with varying equivalence ratios.................................................................................................................................. 85

Figure 4-20 Comparison of CO₂, O₂ and CO emissions of natural gas at air mass flow rates of 0.31 g/s and 0.38 g/s with varying equivalence ratios .................................................................................................................................. 86

Figure 4-21 CO₂, O₂ and CO emissions of methane at an air mass flow rate of 0.38 g/s with varying equivalence ratio .................................................................................................................................. 87

Figure 4-22 Comparison of CO₂, O₂ and CO emissions of methane and natural gas at an air mass flow rate 0.38 g/s with varying equivalence ratios .................................................................................................................................. 87

Figure 4-23 Effect of equivalence ratio on NOₓ emissions of natural gas at an air mass flow rate of 0.38 g/s ........................................................................................................................................ 88

Figure 4-24 Effect of mass flow rate on NOₓ emissions at stoichiometric natural gas-air flame ........ 89

Figure 4-25 Reactants temperature at stoichiometric natural gas-air flame with increasing air mass flow rate ........................................................................................................................................ 90

Figure 4-26 NOₓ emissions of natural gas-air flame at an equivalence ratio of 0.68 with increasing air mass flow rate ........................................................................................................................................ 90

Figure 4-27 Effect of equivalence ratio on NOₓ emissions of methane at air mass flow rate of 0.38 g/s ........................................................................................................................................ 91

Figure 4-28 Comparison of NOₓ emission of methane and natural gas at an air mass flow rate of 0.38 g/s with varying equivalence ratios ........................................................................................................................................ 92

Figure 4-29 Unburned hydrocarbon (UHC) emissions of methane at an air mass flow rate of 0.38 g/s ........................................................................................................................................ 92

Figure 4-30 Equivalence ratio from the exhaust gas emissions versus set fuel flow rate .............. 95

Figure 4-31 Comparison of equivalence ratios calculated from exhaust gas constituents and mass flow meter readings ........................................................................................................................................ 95

Figure 4-32 Combustion efficiency of natural gas-air flames at an air mass flow rate of 0.38 g/s ....... 97

Figure 4-33 Combustion efficiency of methane-air flames at an air mass flow rate of 0.38 g/s ........ 98

Figure 4-34 Flame temperature at an air mass flow rate of 0.38 g/s and an equivalence ratio of 0.68 99

Figure 5-1 Schematic diagram of the micro combustor tube .......................................................... 103

Figure 6-1 Schematic diagram of the micro combustor tube .......................................................... 106

Figure 6-2 Temperature profile for stoichiometric methane-air flame. Experimental data extracted from Bechtel et al. [143] ........................................................................................................................................ 108

Figure 6-3 Temperature and major species profiles for stoichiometric methane-air flame. Ò=1.0, uₐ=0.3 m/s, Tₑ=300 K Experimental data extracted from Bechtel et al. [144] ........................................................................................................................................ 108
Figure 6-4 Temperature, velocity and CH$_4$ mass fraction contours for methane-air flame at atmospheric pressure. $\varnothing$=1.0, $u_{in}$=0.3 m/s, $T_r$=300 K. These figures are not to scale. (d=2 mm, L=12 mm).................................................................................................................110

Figure 6-5 CO$_2$, CO and H$_2$O mass fraction contours for methane-air flame at atmospheric pressure, $\varnothing$=1.0, $u_{in}$=0.3 m/s, $T_r$=300 K (d=2 mm, L=12 mm).........................................................................................................................110

Figure 6-6 Comparison of predicted centreline temperature, velocity and major species concentration profiles for methane-air flame, $\varnothing$=1.0, $u_{in}$=0.3 m/s, $T_r$=300 K.................................................................................................................111

Figure 6-7 Temperature, velocity and CH$_4$ mass fraction contours of methane-air flame at an incoming velocity of 0.3 m/s and equivalence ratio of 0.9 with increasing initial temperature (d=2 mm, L=12 mm) .................................................................................................................................111

Figure 6-8 CO$_2$, CO and H$_2$O mass fraction contours of methane-air flame at an incoming velocity of 0.3 m/s and equivalence ratio of 0.9 with increasing initial temperature (d=2 mm, L=12 mm).................................................................................................................................114

Figure 6-9 Temperature, velocity and CH$_4$ mass fraction contours of methane-air flame at an incoming velocity of 1 m/s and equivalence ratio of 0.9 with increasing initial temperature (d=2 mm, L=12 mm) .................................................................................................................................114

Figure 6-10 CO$_2$, CO and H$_2$O mass fraction contours of methane-air flame at an incoming velocity of 1 m/s and equivalence ratio of 0.9 with increasing initial temperature (d=2 mm, L=12 mm).................................................................................................................................115

Figure 6-11 Comparison of the effect of incoming flow velocity on flame temperature (left) and CH$_4$ and O$_2$ mole fraction profiles (right) at an initial temperature of 500 K and an equivalence ratio of 0.9 .................................................................................................................................................117

Figure 6-12 Temperature, velocity and CH$_4$ mass fraction contours of methane-air flame at an incoming velocity of 0.3 m/s and an initial temperature of 300 K with increasing equivalence ratio (d=2 mm, L=12 mm) .................................................................................................................................................118

Figure 6-13 CO$_2$, CO and H$_2$O mass fraction contours of methane-air flame at an incoming velocity of 0.3 m/s and an initial temperature of 300 K with increasing equivalence ratio (d=2 mm, L=12 mm).................................................................................................................................................118

Figure 7-1 Schematic diagram of the micro combustor tube.................................................................................................................................................119

Figure 7-2 Temperature, velocity and CH$_4$ mass fraction contours for methane-air flame at atmospheric pressure at an incoming velocity of 1 m/s, an equivalence ratio of 0.9 and an initial reactant temperature of 800 K (d=2 mm, L=12 mm) .................................................................................................................................................121

Figure 7-3 CO$_2$, CO and H$_2$O mass fraction contours for methane-air flame at atmospheric pressure at an incoming velocity of 1 m/s, an equivalence ratio of 0.9 and an initial reactant temperature of 800 K (d=2 mm, L=12 mm) .................................................................................................................................................121

Figure 7-4 Centreline flame temperature and CH$_4$ concentration profiles an incoming velocity of 1 m/s, an equivalence ratio of 0.9 and an initial reactant temperature of 800 K.................................................................................................................................................121

Figure 7-5 Temperature, velocity and CH$_4$ mass fraction contours of methane-air flame at an incoming velocity of 1 m/s and equivalence ratio of 0.9 with adiabatic and non-adiabatic wall (d=2 mm, L=12 mm) .................................................................................................................................................122
Figure 7-6 CO\textsubscript{2}, CO and H\textsubscript{2}O mass fraction contours of methane-air flame at an incoming velocity of 1 m/s and equivalence ratio of 0.9 with adiabatic and non-adiabatic wall ........................................ 122

Figure 7-7 Comparison of predicted centreline temperature, velocity and species concentration profiles with an adiabatic wall and non-adiabatic wall at an initial temperature of 800 K, an incoming flow velocity of 1 m/s, and an equivalence ratio of 0.9 ................................................................. 123

Figure 7-8 Temperature, velocity and CH\textsubscript{4} mass fraction contours of methane-air flame at an incoming velocity of 0.3 m/s and equivalence ratio of 0.9 with increasing initial temperature (d=2 mm, L=12 mm) .................................................................................................................. 125

Figure 7-9 CO\textsubscript{2}, CO and H\textsubscript{2}O mass fraction contours of methane-air flame at an incoming velocity of 0.3 m/s and equivalence ratio of 0.9 with increasing initial temperature (d=2 mm, L=12 mm)........ 125

Figure 7-10 Temperature, velocity and CH\textsubscript{4} mass fraction contours of methane-air flame at an incoming velocity of 1 m/s and equivalence ratio of 0.9 at initial temperatures of 700 K and 800 K (d=2 mm, L=12 mm) ........................................................................................................ 127

Figure 7-11 CO\textsubscript{2}, CO and H\textsubscript{2}O mass fraction contours of methane-air flame at an incoming velocity of 1 m/s and equivalence ratio of 0.9 at initial temperatures of 700 K and 800 K (d=2 mm, L=12 mm) ........................................................................................................................................ 127

Figure 7-12 Temperature, velocity and CH\textsubscript{4} mass fraction contours of methane-air flame at an incoming velocity of 0.3 m/s and an initial temperatures of 800 K with changing equivalence ratio (d=2 mm, L=12 mm) ................................................................................................................................. 128

Figure 7-13 Temperature, velocity and CH\textsubscript{4} mass fraction contours of methane-air flame: incoming velocity of 0.3 m/s, equivalence ratio of 0.9, initial temperature of 300 K, convective heat transfer coefficients of 5 W/m\textsuperscript{2}K and 10 W/m\textsuperscript{2}K (d=2 mm, L=12 mm) ................................................................................................. 129

Figure 7-14 CO\textsubscript{2}, CO and H\textsubscript{2}O mass fraction contours of methane-air flame: incoming velocity of 0.3 m/s, equivalence ratio of 0.9, initial temperature of 300 K, convective heat transfer coefficients of 5 W/m\textsuperscript{2}K and 10 W/m\textsuperscript{2}K (d=2 mm, L=12 mm) .................................................................................................................. 129

Figure 7-15 a) Temperature contours, b) Centerline outlet temperature profile with increasing number of iterations at an initial temperature of 300 K, an incoming velocity of 0.3 m/s and an equivalence ratio of 0.9, a convective heat transfer coefficient of 50 W/m\textsuperscript{2}K .................................................................................................................. 130

Figure 7-16 Temperature, velocity and CH\textsubscript{4} mass fraction contours of methane-air flame: incoming velocity of 0.3 m/s, equivalence ratio of 0.55, initial temperature of 800 K, convective heat transfer coefficients of 5 W/m\textsuperscript{2}K and 10 W/m\textsuperscript{2}K (d=2 mm, L=12 mm) .................................................................................................................. 131

Figure 7-17 CO\textsubscript{2}, CO and H\textsubscript{2}O mass fraction contours of methane-air flame: incoming velocity of 0.3 m/s, equivalence ratio of 0.55, initial temperature of 800 K, convective heat transfer coefficients of 5 W/m\textsuperscript{2}K and 10 W/m\textsuperscript{2}K (d=2 mm, L=12 mm) .................................................................................................................. 131

Figure 7-18 Temperature, velocity and CH\textsubscript{4} mass fraction contours of methane-air flame: incoming velocity of 0.3 m/s, equivalence ratio of 1.0, initial temperature of 800 K, convective heat transfer coefficients of 5 W/m\textsuperscript{2}K, 10 W/m\textsuperscript{2}K and 50 W/m\textsuperscript{2}K, emissivity of 0 and 0.2 ............................................. 132
Figure 7-19 CO₂, CO and H₂O mass fraction contours of methane-air flame: incoming velocity of 0.3 m/s, equivalence ratio of 1.0, initial temperature of 800 K, convective heat transfer coefficients of 5 W/m²K, 10 W/m²K and 50 W/m²K, emissivity of 0 and 0.2 (d=2 mm, L=12 mm) ........................................... 132

Figure 7-20 Temperature, velocity and CH₄ mass fraction contours of methane-air flame at a constant mass flow rate of 6.3742*10⁻⁷ kg/s and equivalence ratio of 0.9 at initial temperatures of 500 K and 800 K (d=2 mm, L=12 mm) ............................................................................................................ 134

Figure 7-21 CO₂, CO and H₂O mass fraction contours of methane-air flame at a constant mass flow rate of 6.3742*10⁻⁷ kg/s and equivalence ratio of 0.9 at initial temperatures of 500 K and 800 K (d=2 mm, L=12 mm) ............................................................................................................ 134

Figure A-1 a) Flow paths through Sierra Smart Trak 100 Series, b) Flow measuring principle [153] ....................................................................................................................................... 144

Figure A-2 Comparison of equivalence ratios calculated from mass flow meter and controller readings and exhaust emissions ......................................................................................................................... 147

Figure A-3 Heat balance of the thermocouple bead................................................................. 151
List of Tables

Table 1-1 Comparison of UMGT and LiSO₄ fuel cell [16] ................................................................. 2
Table 2-1 Comparison between conventional and micro combustors [30] .......................................... 15
Table 2-2 Experimental data and empirical expressions for the power exponent α for methane-air flames from [104] ......................................................................................................................... 40
Table 3-1 Specification of porous and sintered flame holders ................................................................ 45
Table 3-2 Molar gas composition of New Zealand natural gas in Auckland (July/2012) .................. 48
Table 3-3 Accuracy of the pressure transducers and Betz micromanometer ........................................ 52
Table 3-4 Specifications of the gas analyzers ..................................................................................... 53
Table 4-1 Burning velocity coefficients of methane-air [115] ............................................................. 77
Table 4-2 Comparison of burning velocities ..................................................................................... 80
Table 6-1 Comparison of reaction mechanisms of stoichiometric methane-air flame at atmospheric pressure ........................................................................................................................................ 112
Table A-1 Chemical compositions of natural gas with the corresponding mole and mass fractions and $Q_{LHV}$ of its constituents ........................................................................................................ 142
Table A-2 Correction factor for the molecular structure of the gas [154] ........................................... 146
Nomenclature

A  Surface area (m²)
Aₖ  Pre-exponential factor of reaction rate
B  Stoichiometric fuel/air ratio
C  Form drag coefficient
Cₚ  Specific heat at constant pressure (kJ/kg-K)
d  Diameter (m)
Dₐₜ  Damköhler number
E  Output voltage
Eₐ  Activation energy
Eₖ  Activation energy for the i-th reaction
h  Convective heat transfer coefficient (W/m²K)
H  Heat
K  K-factor or permeability
kᵢ  Reaction mechanism rate coefficients
L  Length (m)
M  Mass (kg)
M  Molar mass (kg/kmol)
ṁ  Mass flow rate (kg/sec)
mᵢ  Mass fraction
N  Correction factor
n  Number of moles
P  Pressure (Pa)
ΔP  Pressure drop
Q  Volumetric flow rate (m³/s)
Qᵢ  Lower heating value
Δq  Enthalpy loss
Q  Heat loss
R  Gas constant (kJ/kg-K)
Rᵤ  Universal gas constant
Rᵢ  Specific gas constants of each i-th species
Sᴸ  Laminar burning velocity (m/s)
Sᵣᴸ,₀  Reference or adiabatic laminar burning velocity (m/s)
Sᵣᴸ,₀  Burning velocity coefficients
Sᵣᴸ,₁  Burning velocity coefficients
Sᵣᴸ,₂  Burning velocity coefficients
Sᵣᴸ,₃  Burning velocity coefficients
Sᵣᴸ,₄  Burning velocity coefficients
T  Temperature (K)
Tₐ  Ambient temperature (K)
Tᵣₜ  Adiabatic flame temperature (K)
Tᵣᵇ  Non-adiabatic flame temperature (K)
\( T_0 \) Reference temperature (K)
\( T_w \) Wall temperature (K)
\( \Delta T \) Temperature difference
\( U \) Uncertainty
\( u \) Velocity (m/s)
\( V \) Volume (m\(^3\))
\( \bar{x} \) Wet mole fraction
\( \bar{x}^* \) Dry mole fraction
\( y \) Molar fraction
\( \alpha \) Cone angle or power exponent
\( \beta_k \) Temperature exponent of the \( i \)th reaction
\( \rho \) Density (kg/m\(^3\))
\( \varepsilon \) Effective emissivity
\( \lambda \) Thermal conductivity (W/mK)
\( \tau_{res} \) Residence time
\( \tau_{rec} \) Chemical reaction time
\( \mu \) Viscosity
\( \varnothing \) Equivalence ratio
\( \sigma \) Stefan Boltzmann constant
\( \eta_{comb} \) Combustor efficiency

**Subscripts**

a air or ambient
ad adiabatic
b non-adiabatic or burned
conv convection
exp expanded
f fuel
hys hysteresis
in incoming flow or thermocouple inhomogeneity
L laminar
mix mixture
rad radiation
res residual
surf surface
surr surroundings
T total
u unburned
w wall
0 unburned or reference
### Acronyms

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>UMG</td>
<td>Ultra Micro Gas Turbine</td>
</tr>
<tr>
<td>MIT</td>
<td>Massachusetts Institute of Technology</td>
</tr>
<tr>
<td>MEMS</td>
<td>Micro-Electro-Mechanical Systems</td>
</tr>
<tr>
<td>MAV</td>
<td>Micro Aerial Vehicle</td>
</tr>
<tr>
<td>UAV</td>
<td>Unmanned Air Vehicle</td>
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<tr>
<td>TPV</td>
<td>Thermo Photovoltaic</td>
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<tr>
<td>DARPA</td>
<td>Defence Advanced Research Projects Agency</td>
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<td>IHI</td>
<td>Ishikawajima-Harima Heavy Industries</td>
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<td>TMU</td>
<td>Tokyo Metropolitan University</td>
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<tr>
<td>HEX</td>
<td>Heat Exchanger</td>
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<tr>
<td>NG</td>
<td>Natural gas</td>
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<tr>
<td>NDIR</td>
<td>Non-dispersive Infra-red</td>
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<tr>
<td>UHC</td>
<td>Unburned hydrocarbon</td>
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<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
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<tr>
<td>CEA2</td>
<td>NASA-Glenn Chemical Equilibrium with Applications Program</td>
</tr>
<tr>
<td>SK16</td>
<td>Methane-air skeletal reaction mechanism of Correa, consisting of 16 species and 41 reactions</td>
</tr>
<tr>
<td>SK17</td>
<td>Methane-air skeletal reaction mechanism of Lu et al., consisting of 17 species and 73 reactions</td>
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<tr>
<td>LFE</td>
<td>Laminar flow element</td>
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<tr>
<td>RTD</td>
<td>Resistance temperature detector</td>
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<td>TC</td>
<td>Thermocouple</td>
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**Chapter 4- Experimental Results and Discussion**


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- in cases where the PhD candidate was the lead author of the work that the candidate wrote the text.

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**Chapter 4- Experimental Results and Discussion**

**Clean Flat Flame Combustor for Ultra Micro Gas Turbine, in Proceedings of the 19th Australasian Fluid Mechanics Conference, RMIT University, Melbourne, Australia, 8-11 December 2014.**

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1 INTRODUCTION

Energy and pollution are two important and vital problems of the 21st century. As technological improvements are made, our lives become more comfortable but at the same time our dependency on energy sources increases day by day. This is especially on fossil fuels, since the majority of our current energy needs are met from fossil fuels. If the consumption of fossil fuels continues at the same rate as it is today, the available resources which were formed over billions of years will run out in less than a century. At the same time, more clean energy resources are required because pollution from fossil fuels has become one of the most serious issues facing planet earth and its inhabitants. In addition to exhaust gas emissions from aircraft, cars etc., methane emission is also one of the biggest problems facing agricultural countries such as New Zealand. Therefore, it is necessary to look for new, efficient, and clean energy resources for sustainable life for both our generation and generations to come.

As pointed out by Dunn-Rankin et al. [1] “While the technology to create personal autonomy for communications, information processing and mobility has accelerated, similar breakthroughs for the systems powering these devices have not yet occurred”. Since energy requirements increase in parallel with technological developments, especially in micro devices such as micro robots and computers, more powerful and compact power sources are therefore required. Ultra micro gas turbine (UMGT) is a promising candidate to meet this requirement with its higher power density and higher energy density compared to currently used batteries, which are the primary power supply for portable devices [2, 3]. Batteries currently in use are not compact and constitute most of the volume and weight of devices in which they are utilised. In addition to this, they also need long recharging times.

The concept of UMGT was first developed by Epstein at the Massachusetts Institute of Technology’s (MIT) Gas turbine Laboratory using Micro-Electro-Mechanical Systems (MEMS) technology around 1995 [4]. Gas turbine technology has been used in power plants to generate electricity and as a propulsion system for aircraft. Basically, the gas turbine consists of a turbomachinery part, compressor and turbine, a combustor and a heat exchanger. In the last two decades smaller size gas turbines, known as micro gas turbines with 1-100 kW capacity, have become popular for power generation for single home use or for factories. With MIT’s research using MEMS technology, the UMGT concept was introduced. The objective of MIT’s UMGT project was to micro fabricate a gas turbine engine with an integral electric generator on a silicon chip with a power output of 10-50 W. The overall size of MIT’s UMGT
was about 2.1 cm x 2.1 cm x 0.38 cm and it was manufactured by fusion bonding six silicon wafers [5, 6]. This was followed by other UMGT research projects conducted around the world like the University of Tokyo’s ‘palm top’ and ‘finger top’ UMGT projects [7, 8], Belgian PowerMEMS project [9-11] and ONERA’s DecaWATT project [12-14].

Although the efficiency of UMGT is projected to be around 10%, which is much lower than that of the gas turbine (~40%) [15], the UMGT is still superior to the most advanced batteries with respect to power density and specific energy. The comparison of the specific energy of batteries and UMGT with 10% efficiency is shown in Figure 1-1.

![Specific energy comparison](image)

**Figure 1-1 Comparison of specific energies [3]**

Furthermore, UMGT is also superior compared to the fuel cell. The energy density of the fuel cell is not sufficient for many of its intended applications. However, UMGT generates one to two orders higher energy densities for the same volumes or weights than those of fuel cell systems [16]. A comparison of the specific energies and energy densities of UMGT and the LiSO₄ fuel cell are listed in Table 1-1.

**Table 1-1 Comparison of UMGT and LiSO₄ fuel cell [16]**

<table>
<thead>
<tr>
<th></th>
<th>UMGT</th>
<th>LiSO₄</th>
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<tbody>
<tr>
<td>Power (W)</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>Energy (Whr)</td>
<td>175</td>
<td>175</td>
</tr>
<tr>
<td>Engine weight (g)</td>
<td>50</td>
<td>1100</td>
</tr>
<tr>
<td>Engine volume (cc)</td>
<td>50</td>
<td>880</td>
</tr>
<tr>
<td>Specific energy (Whr/kg)</td>
<td>3500</td>
<td>175</td>
</tr>
<tr>
<td>Energy density (Whr/cc)</td>
<td>3</td>
<td>0.2</td>
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The UMGT has twenty times the specific energy and fifteen times the energy density of those of LiSO$_4$ fuel cell. Specific energy is defined as energy per unit mass, while energy density is defined as energy per unit volume.

More efficient and clean energy resources may be achieved by utilising methane as a fuel for UMGT, thereby generating power for portable electronic and mechanical devices, in addition to propulsion systems for micro aerial vehicles (MAV). This may also help to reduce the methane emissions from animal farming in agricultural countries such as New Zealand.

In order to realize UMGT as a viable power source it is necessary to develop three micro scale technologies since downscaling introduces new challenges for each of these components. These are rotating machinery, combustor technology and high temperature material fabrication technology. Since the micro combustor is one of the key components of both UMGT and other combustion based power generators such as micro thermo photovoltaic (TPV) system, it has to be developed in order to realize the miniaturization of these systems and thus their utilisation as viable power sources. It is not easy to achieve stable, high combustion efficiency, wide flame stability with less pollutants in small scale combustors because downsizing reveals many problems that do not occur on conventional combustors. In the next sections the downscaling problems of micro combustors are specified.

1.1 Downscaling problems of combustors

Downscaling the combustor introduces new problems which do not occur in typical gas turbine combustors. Yuasa et al. [17] specified the fundamental downscaling problems of micro combustors as smaller residence time for mixing and combustion, high heat loss, and high pressure loss. It can be said that the two most important downscaling problems of combustors are smaller residence time and high heat loss. These in turn result in flame quenching, incomplete combustion and increased pollutant emissions [6, 12, 17, 18].

1.1.1 Smaller residence time

Damköhler number ($Da_h$) is the ratio of the residence time to the characteristic chemical reaction time [19].

$$Da_h = \frac{\tau_{res}}{\tau_{rec}} \quad (1-1)$$
For complete combustion to occur $D_{a_h}$ has to be greater than unity. To have a $D_{a_h}$ greater than 1, it is necessary to increase the residence time or decrease the chemical reaction time.

Residence time can be defined as the volume of the combustor divided by the volumetric flow rate,

$$
\tau_{res} = \frac{Volume}{Volumetric\ flow\ rate} = \frac{VP}{mRT}
$$

(1-2)

where $V$ is volume, $P$ is pressure, $m$ is mass flow rate, $T$ is temperature and $R$ is the gas constant.

When the size of the combustor decreases, the residence time gets smaller. Smaller residence time may lead to incomplete combustion, low combustion efficiency and high pollutant emissions. To increase the residence time, it is necessary to either increase the volume or pressure or decrease the mass flow rate. But to have a high power density, it is necessary to have a high mass flow rate and a small volume. Also, with a small size compressor it is not possible to get a higher compression ratio. Therefore, it is not possible to increase the residence time. In that case, to ensure complete combustion the chemical reaction time has to be reduced.

Chemical reaction time can be defined by an Arrhenius type expression [19]:

$$
\tau_{rec} \approx \frac{[fuel]}{A[O_2]^b e^{-\frac{E_a}{RT_h}}}
$$

(1-3)

where $E_a$ is the activation energy while $A$, $a$, and $b$ are empirically determined constants.

Since chemical reaction time is a function of both the fuel properties and the mixture temperature and pressure, it can be increased through increasing the reactants temperature. Fernandez-Pello [2] emphasized the importance of having small chemical reaction time to assure completion of the combustion process within micro combustors. He also clarified that small chemical reaction times can be achieved by reducing the heat losses in the combustion chamber, preventing radial depletion at the wall, increasing the reactants temperature, using stoichiometric mixtures and utilizing highly energetic fuels.

1.1.2 Increasing heat loss

The second important challenge of downsizing the combustor is higher heat loss. As the size of the combustor decreases, the surface-to-volume ratio increases. Heat loss is
proportional to the surface area while heat release is proportional to the volume. As the surface-to-volume ratio increases, the ratio of heat loss to the heat release also increases. Therefore, the micro combustor performance decreases by lowering overall efficiency and narrowing the flammability limits.

Higher heat loss rate also causes increasing quenching distance. Quenching distance is a distance between plates or a tube diameter through which a flame will not propagate. If the heat loss is too high, this will consequently decrease the temperature of the reaction zone, and therefore the reaction will slow down. When the reaction slows down, the heat release rate is lowered, the temperature drops below the ignition temperature, and the flame will be quenched.

Before outlining the objectives of this research, the probable applications of UMGT will be introduced.

1.2 Application of UMGT

UMGT has two potential applications. The first one is as a power source for portable electronic and miniature mechanical devices while the second one is as a propulsion system for micro aerial vehicles (MAV) or unmanned air vehicles (UAV), commonly known as drones. Portable power generation is also divided into two main categories; military and civil applications.

According to Defence Advanced Research Projects Agency (DARPA), there are three separate regimes of UMGT for future army applications [3]. These are 20 W average with a 50 W peak, 100 W average with a 200 W peak and 1 to 5 kW high power draw applications. The 20 W regime includes power sources for computers, radios, sensors and displays. Whereas, the 100 W regime would allow applications such as a laser target designator and microclimate cooling (ventilation for soldiers wearing protective clothing) and a portable recharger for rechargeable batteries. The high power regime, the 1 to 5 kW regime includes power-intensive capabilities such as exoskeletons which are robotic human performance augmentation systems which artificially reduce the load felt by the soldier.

Power generation for civil applications may be divided into two regimes, 10 to 100 W and 0.1 to 10 kW regimes. The first regime includes mass market electronics such as cordless drills, recharging units for a cell phone battery or sheep shears. The second regime covers the applications for domestic appliances, golf cart, rolling armchair, garden tools, milking machines and sailboat engines, to name a few.
The examples of the possible applications of UMGT and the specific power and specific energy of these applications are presented in Figure 1-2.

![Diagram showing specific energy and applications](image)

**Figure 1-2 Specific energy and applications [7]**

For aerial vehicle propulsion, UMGT is one of the most promising propulsion systems. The propulsion of micro aerial vehicles and distributed propulsion, where several small engines are used to propel either a large unmanned vehicle or a small manned aircraft, may be two possible applications of UMGT in vehicle propulsion. Military applications may include reconnaissance and surveillance, sensing of nuclear, biological and chemical contaminants, and urban war fighting. Civil applications such as counter drug support, assistance in finding survivors after disasters like earthquakes, and in the domain of security tasks, are also potential applications. In late 2013, Amazon started testing drones for package delivery and also Zoookal, an Australian textbook rental company, announced that they would start using drones to make deliveries from 2015, if approved by Australia's Civil Aviation Safety Authority [20]. Other civil purposes of using UAV includes conservation, biosecurity, mineral exploration, fisheries management and traffic monitoring. Examples of using UAV in conservation include skimming over Indonesia's jungle canopy to photograph orangutans, protecting rhinos in Nepal and studying invasive aquatic plants in Florida [21]. In New Zealand also, using UAV’s in farming, for livestock counting and tracking, and for vegetation growth tracking is becoming common practice [22]. For New Zealand, earth science, coastal patrol and land management may be classified as possible UAV missions since using UAV instead of manned aircraft is both cheaper and safer. These missions include coastal ocean observations, vegetation structure, coastal patrol and forest fire damage assessment. However currently, similar to the other portable devices, UAV’s are powered by batteries and therefore require long recharging.
times and are heavy in weight. On the other hand, with an UMGT, a UAV would be able to fly longer and more efficiently than is currently possible with batteries.

In 2010 Jaguar also introduced its new hybrid car, C-X75 that uses twin 70 kW micro gas turbines running on a choice of natural gas, liquefied petroleum gas, diesel or biofuels, mixed with air [23]. The micro gas turbines can power the electric motors directly or can be used to recharge the battery. This example shows probable applications of micro gas turbine as an electric power generator, or charger, for electric cars. This may be possible by using clusters of UMGTs.

1.3 Objectives

The motivation for this study is to develop a micro combustor using methane or natural gas as a fuel, with high combustion efficiency and wide flame stability, that burns cleanly and can be utilised in UMGT applications as well as other small power generators such as thermo photovoltaic power generators. As Fernandez-Pello [2] stated, preheating the reactants may reduce the chemical reaction time to less than the residence time, thus achieving complete combustion in a small scale. Although in the literature, it has been shown that preheating the reactants increases the burning velocity, at micro scale it has not been shown how preheating affects flame stability or combustion characteristics. Therefore, the main objective of this study is to investigate the effects of preheating on the flame stability and combustion characteristics at small scale both experimentally and numerically.

The main objective of the experimental research is to investigate the fundamentals of flat flame combustion at small scale. The specific objectives of the experimental research are to investigate the effect of preheating on the flame stability within a 46 mm diameter flat flame combustor and lastly exhaust emissions. Although, flat flame burning method has been used for a long time for flame investigations, the behaviour of the flame over a wide range of equivalence ratio on the surface of uncooled flat flame burners has not been reported. Therefore, one of the specific objectives of this study is to observe the flame behaviour and location over a wide range of stoichiometry and varying mass flow rates on the surface of uncooled flat flame burners.

Although the flat flame burner method was first developed and applied to UMGT by Yuasa [24, 25], and also applied by Marbach and Agrawal [26, 27] there is a lack of data showing the effect of using different flame holders and their ability to provide flat flame
combustion with minimum pressure loss. Therefore, another objective of this study is to investigate the effect of using flame holders of different material and geometric parameters for flat flame combustion, in addition to measuring pressure losses through them. Other objectives of the experimental work are to show the relationship between the incoming flow velocities and burning velocities for obtaining flat flame combustion and to obtain a correlation between mass flow rate, reactant temperature, air to fuel ratio and diameter of the micro combustor. A final objective of the experimental work, is to calculate the equivalence ratios and combustion efficiencies from the exhaust emissions.

The main objective of the numerical research is to investigate two-dimensional modelling of laminar premixed methane-air flame within a 2 mm diameter micro combustor. Similar to the experimental work, the main focus of the numerical work is also to investigate the effect of preheating the reactants on the combustion stability and characteristics. The specific objectives are to obtain flame temperature, velocity and major species at varying initial temperatures and incoming flow velocities, as well as air to fuel ratios at both adiabatic and non-adiabatic cases. Other objectives include comparing the flame location, shape and thickness, as well as different reaction mechanisms, with the available experimental data. Finally, the last objective of the numerical work is to investigate and analyse the effects of convective heat transfer coefficients and heat loss, with and without radiation, on the flame stability and combustion characteristics.

For the experimental investigation, a flat flame burning method was chosen because it provides clean and stable flames whose location is known. Knowledge of the flame location helps the design of the engine. Furthermore, in the literature, very few studies applied flat flame burning method at small scale, and there are many issues which have not yet been elucidated, such as the effect of preheating, or utilizing different flame holders. On the other hand, for numerical investigation, a 2 mm diameter combustor tube was chosen because this is smaller than the quenching distance for stoichiometric methane-air flame, at atmospheric pressure and room temperature [28]. The numerical study helps to understand the effect of preheating on the flame stability and combustion characteristics at a very small scale, which the experimental investigations are not able to replicate. Furthermore, in the adiabatic case this model simulates a single tube of a micro combustor which consists of a bundle of micro tubes, similar to the Meker burner [29]. However, in the numerical work combustion occurs inside the tubes instead of on top of them, as in the Meker burner.
This study will lead to a better understanding of the effects of preheating on the flame stability and combustion characteristics at small scale in order to develop a methane fuelled micro combustor with high combustion efficiency, wide flame stability and clean emissions, which is required for the realization of UMGT as a viable power source.

1.4 Thesis Outline

This thesis consists of eight chapters. Chapter 1 introduces the concept of UMGT and its downscaling problems. This chapter also outlines the requirements for developing micro combustors for UMGT applications as well as the downscaling problems of micro combustors. Lastly, the objectives of this study are presented.

Chapter 2 presents a comprehensive literature review on UMGT and micro combustor research around the world. While introducing these studies, the gaps in the literature will be emphasized. Furthermore, a literature review on flat flame studies and the different topics which were investigated, is detailed.

Chapter 3 describes the experimental methodology and set-up. The equipment used in the experiment, their working principles and specifications as well as calibration methods are given. In addition, modifications to the test rig are explained.

Chapter 4 presents the experimental results and discussion. The experimental results include the pressure loss measurements through the flame holders, the effects of preheating the reactants on the flame stability and flat flame stabilization, the usage of different flame holder materials and geometric parameters for flat flame combustion. In addition to the flame behaviour with varying mass flow rates and equivalence ratios, exhaust emissions, combustion efficiencies and flame temperatures are also presented. Finally, a correlation for flat flame burning method is proposed and introduced.

Chapter 5 presents the background of the two-dimensional numerical micro combustion research around the world. The two-dimensional computational model for the present numerical research is described.

Chapters 6 and 7 present the simulation results both for adiabatic and non-adiabatic cases, respectively. In the adiabatic case, the simulation results include a validation of the numerical model, a comparison of the employment of different skeletal and detailed reaction mechanisms on the prediction of flame temperature, species concentrations and flame
thickness. In both adiabatic and non-adiabatic cases, the effects of preheating the reactants, incoming flow velocity, and equivalence ratio, on the flame stability and combustion characteristics are presented. Furthermore, in the non-adiabatic case, the effects of heat loss via convection and radiation and convective heat transfer coefficients on the flame stability are detailed.

Finally, the conclusions derived from this work and suggestions for future work are presented in Chapter 8.
2 LITERATURE REVIEW

In this chapter, the research on ultra micro gas turbine around the world is introduced. Then, the background of the micro combustor research, conducted by these UMGT research groups is presented. While introducing each micro combustor design, the shortcomings of the designs are outlined. Next, flat flame combustion is introduced and different research investigations on flat flames are detailed. The background of the two-dimensional numerical investigation of micro combustion around the world, which has emerged with the interest in UMGT and other combustion-based micro power generators, will be presented in Chapter 5. Finally, a brief description of premixed laminar flame is introduced.

2.1 Literature review on ultra micro gas turbine

The objective of the MIT’s UMGT project was to develop a micro gas turbine generator capable of producing 10-100 watts of electrical power while occupying less than 1 cm³ and consuming approximately 7 gr of jet fuel per hour [30].

The schematic of the baseline design of the MIT’s UMGT is shown in Figure 2-1a. As can be seen from this figure, air enters the engine axially through an inlet and makes a right angle turn into the compressor. Fuel is injected and mixes with air in the recirculation jacket, and then the premixture ignites and burns in the combustion chamber. Finally, the hot gases expand through the turbine. Although the individual components of the engine have been demonstrated independently, a complete device has not operated successfully.

![Figure 2-1 a) Schematic of the baseline design of the MIT’s ultra micro gas turbine engine b) cross-section of half of the axisymmetric 6-wafer static structure [5, 31]](image-url)
In Japan, at Tohoku University in collaboration Ishikawajima-Harima Heavy Industries (IHI), a micro scale gas turbine with a power output of 100 watts was developed in the year 2000. The UMGT developed at Tohoku University consisted of a centrifugal compressor and turbine, each of these were 10 mm in diameter, and hydrogen was chosen as the fuel. Following this study, in 2007 Tohoku University successfully built the World’s smallest UMGT in terms of the diameter of the impellers, fuelled with hydrogen [32]. The UMGT consisted of a compressor of 16 mm diameter, a turbine of 17.4 mm diameter, an annular combustor and a dummy electromagnetic generator. A schematic of the UMGT layout, and turbo machinery parts is shown in Figure 2-2.

In 2001, an international research project led by the University of Tokyo launched to develop palm-top and finger-top UMGT’s [7, 8]. The palm-top UMGT targeted a 2-3 kW power output while finger-top UMGT was expected to produce tens of watts power output. A schematic layout of the palm-top UMGT is shown in Figure 2-3. A compression ratio of 2.5 and turbine inlet temperature of 1223 K were chosen for both sized UMGTs. For palm-top UMGT a turbine rotor diameter of 40 mm was selected, while for finger-top UMGT a 8 mm rotor diameter was chosen. At the end of the project in 2003, all the components of the palm-top UMGT were prototyped and successfully operated with propane. A feasibility study, key components design and test were completed for the finger-top UMGT.

Figure 2-2 a) Schematic layout of Tohoku University’s UMGT b) compressor and turbine [32]
The Belgian PowerMems Project started to develop a micro gas turbine generator in the range of 1 kW using hydrogen as a fuel in 2003 with the collaboration of universities and research institutes [9-11, 33]. The micro turbine generator had a diameter of 95 mm and a length of 120 mm, and both the compressor and turbine impellers were 20 mm in diameter. In order to reduce the overall fuel consumption, the Belgian group inserted a recuperator in their design, however the development of a recuperator with high effectiveness and low pressure drop at small scale has been challenging.

In France, ONERA conducted a research program called DecaWatt which proposed a power output range between 50 to 100 Watts [12, 14, 34]. Two different designs were proposed by ONERA. A single stage micro turbine which is separated from the combustor chamber, as shown in Figure 2-5a and two stage micro turbine within a “Thermodynamical Cocoon”, as shown Figure 2-5b. The first design was prototyped and tested. It had a diameter of 22 mm and a height of 32 mm, and was based on the Brayton-Joule cycle. The purpose of the Cocoon type UMGТ is to limit the thermal fluxes, by keeping the hotter element, which is the combustor, at the core, while the compressors are at the periphery.
In Italy, at the University of Roma Sapienza UMGT based research launched in 2006 in order to develop a hybrid propulsion system for UAV [35, 36]. In the Italian UMGT, the axis of the turbo machinery part is parallel to the axis of the combustion chamber. The turbine used in the UMGT is a radial one and manufactured by Garret/Honeywell. The compressor is also a modified Barret GT14 radial compressor.

As it can be seen from the previous UMGT research, until now, only IHI claims to have successfully achieved a working palm sized micro gas turbine with a power output of 400 watts. For a smaller range of power output, there are still some challenges which are to be overcome. Even though IHI built the World’s smallest UMGT, a methane fuelled ultra micro gas turbine has yet to be manufactured. Therefore, this research is dedicated to the improvement of methane combustion at small scale in order to fulfil the requirements of micro combustion for UMGT applications.

At this stage, it would be beneficial to explain that micro gas turbines have been used in the hundred kilowatt range, while UMGT is defined for a power output range of a few watts to a few kilowatts. According to this power range description, in UMGT the size may change from micro to meso scale.
2.2 Literature review on micro combustors

In this section, UMGT based micro combustor research conducted around the world is presented. The functional requirements of a micro combustor do not change with downscaling and is similar to those of a conventional gas turbine combustor [38]. Some of these requirements are the efficient conversion of chemical energy to fluid thermal and kinetic energy with low pressure loss, wide flame stability limit and low pollutant emissions. However, to fulfill these requirements is not an easy task due to the downscaling problems which were explained in Chapter 1.

The introduction of UMGT at the Gas Turbine Laboratory of MIT, initiated the development of micro combustors. Thus, the first micro combustors were built and designed at MIT.

With downscaling, the design parameters of the micro combustor change substantially. Waitz et al. [30] listed a comparison between the design parameters of a conventional gas turbine combustor and those of MIT’s micro combustor, which is shown in Table 2-1.

<table>
<thead>
<tr>
<th>Design requirement</th>
<th>Conventional combustor</th>
<th>Micro combustor</th>
</tr>
</thead>
<tbody>
<tr>
<td>(sea level takeoff)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Length (m)</td>
<td>0.3</td>
<td>0.003</td>
</tr>
<tr>
<td>Volume (m$^3$)</td>
<td>$6 \times 10^{-2}$</td>
<td>$4 \times 10^{-8}$</td>
</tr>
<tr>
<td>Cross-sectional area (m$^2$)</td>
<td>0.2</td>
<td>4 $\times 10^{-5}$</td>
</tr>
<tr>
<td>Inlet total pressure (atm)</td>
<td>30</td>
<td>4.5</td>
</tr>
<tr>
<td>Inlet total temperature (K)</td>
<td>800</td>
<td>500</td>
</tr>
<tr>
<td>Mass flow (kg/s)</td>
<td>55</td>
<td>20 $\times 10^{-4}$</td>
</tr>
<tr>
<td>Average flow speed (m/s)</td>
<td>40-60</td>
<td>6</td>
</tr>
<tr>
<td>Residency time (ms)</td>
<td>5-8</td>
<td>0.5</td>
</tr>
<tr>
<td>Efficiency</td>
<td>&gt;99.5</td>
<td>&gt;99.5</td>
</tr>
<tr>
<td>Combustor pressure ratio</td>
<td>&gt;0.95</td>
<td>&gt;0.95</td>
</tr>
<tr>
<td>Exit temperature (K)</td>
<td>1800</td>
<td>1500</td>
</tr>
<tr>
<td>Allowable wall temperature (K)</td>
<td>1200</td>
<td>1600</td>
</tr>
<tr>
<td>Space heating rate (kW/m$^3$/atm)</td>
<td>3.8$\times 10^4$</td>
<td>3.3$\times 10^4$</td>
</tr>
</tbody>
</table>

At MIT, the first hydrogen micro combustion was performed in 0.13 cm$^3$ silicon carbide and stainless steel micro combustors over a range of equivalence ratios from 0.4 to 1.0 and mass flow rates between 0.045 g/s and 0.2 g/s [30]. Then, with silicon carbide two micro combustors were designed, one of those consists of three wafer [18], while, the other one consists of six wafer [5]. Experiments with the three-wafer combustor showed that although hydrogen combustion was possible in the device with combustor efficiencies in the range of
40%–60%, the hydrocarbon combustion could not be sustained due to the insufficient residence time. Both longer chemical reaction times and larger quenching distances of hydrocarbons prevent sustainable combustion. The quenching distance is approximately inversely proportional to pressure [39]. When the pressure increases, the quenching distance decreases. However, in UMGT, with the small size compressor, it is not possible to obtain a higher compression ratio, which in turn hinders a reduction in the quenching distance. Conversely, the quenching distance also decreases with increasing temperature. Therefore, preheating the reactants not only shortens the chemical reaction time, but also decreases the quenching distance, enabling combustion at small scales.

Introducing heterogeneous catalytic combustion into the same size combustor, combustion of both propane and ethylene was achieved, but efficiencies were still very poor and in the range of 40%–60% for both fuels [38]. Although the ability to sustain catalytic combustion at a lower lean flame stability limit than that of gas-phase combustion, catalytic combustion results in higher pressure loss and low exit temperatures. Furthermore, the combustion efficiencies for both hydrocarbon fuels were lower than that required for UMGT applications. Schematics of three-wafer and six-wafer catalytic combustors are presented in Figure 2-7.

![Schematic of catalytic combustors](image)

**Figure 2-7 Schematic of catalytic combustors a) three-wafer combustor, b) six-wafer combustor [38]**

Similar to the MIT’s UMGT, in Singapore Shan et al. [40] developed a seven wafer silicon carbide micro combustor for hydrogen, as shown in Figure 2-8. Shan et al. performed both numerical and experimental investigations of hydrogen-air combustion in the seven wafer micro combustor. Within the seven wafer micro combustor, it was possible to sustain hydrogen-air flame with a highest exit temperature of 1700 K [40].
In Japan, a group at Tohoku University, collaborating with IHI, developed canister type and doughnut type micro combustors for hydrogen-air, as shown in Figure 2-9 [41]. Both combustors showed self-sustainability of the flame over a wide range of equivalence ratios with a combustion efficiency very close to 100%. On the other hand, with natural gas the combustion efficiency was very poor and flame could not be sustained over a wide range of equivalence ratios.

Tokyo Metropolitan University (TMU) developed micro combustors [42] with the palm-top and finger-top UMGT projects. Yuasa introduced flat flame combustion at micro scale. For finger-top UMGT, a hydrogen flat flame micro combustor was developed and tested for measurements of combustion characteristics. A schematic of hydrogen flat flame micro combustor is shown in Figure 2-10. The hydrogen fuelled micro combustor had a total volume of 0.067 cm$^3$ and combustion efficiencies of more than 99.2% were achieved. A flat flame micro combustor with a diameter of 20 mm was manufactured for methane-air premixture. In this micro combustor, the effect of combustor height on the flame stability was investigated. An annular swirl type propane fuelled micro combustor was designed and tested for palm-top UMGT [8], as shown in Figure 2-11.
Flat flame micro combustor research at TMU has continued with the “Prototyped” and “Engineering” model propane flat flame micro combustors. The Prototyped propane flat flame micro combustor had a volume of 0.806 cm$^3$, could form a flat flame successfully, but high combustion efficiencies (around 99.4%) were only achieved between equivalence ratios of 0.5 and 0.7. When the equivalence ratio was increased above 0.7, the combustion efficiencies decreased dramatically. A schematic layout of the Prototyped propane-fuelled flat flame micro combustor and a typical flame appearance in it is shown in Figure 2-12.
In order to improve the combustion efficiency and flame stability of the prototyped propane fuelled flat flame micro combustor, an engineering model flat flame combustor was developed [44], as shown in Figure 2-13. In the engineering model, a recirculation channel and a flat plate were introduced. Through the recirculation channel, the reactants were heated from the burned gas before passing through the porous plate. The flat plate was inserted at the combustor exit, in order to create the stagnation flow field for a specific flat flame formation. Without the flat plate at the exit, the burned gas flow converged vertically in the exit tube like a converged nozzle flow, which resulted in decreasing the flame stability [45]. Introducing the flat plate provided the formation of flat flame combustion, but also increased the heat loss resulting in low combustor exit temperature and high CO emissions. Furthermore, the total pressure loss is about 5.5 % which is higher than the maximum allowable pressure loss ratio for micro combustors.

![Figure 2-13 Schematic of engineering model of propane-fuelled flat flame micro combustor [44]](image)

Flat flame combustion was also applied by Marbach et al. [26, 27]. The methane flat flame combustor of Marbach et al. is shown in Figure 2-14. The flame stabilized on the surface of silicon-carbide coated carbon foam, used as a porous inert media (PIM). Similar to the engineering model propane fuelled flat flame micro combustor of TMU, Marbach et al. used heat recirculation in an annulus around the combustor in order to preheat the reactants from the burned gas. Two similar configurations were tested by Marbach et al., one of them has porous inner media in both the combustor chamber and the preheating annulus, as shown in Figure 2-14b.
Both flat flame burning method and heat recirculation was also applied by Turkeli-Ramadan for methane-air within the triple tube HEX-Combustor [46, 47]. However, the HEX-Combustor design proposed the heat recirculation not only from the combustion products, but also the turbine exit gas which flows through the outer annulus. A schematic of triple tube HEX-Combustor is shown in Figure 2-15. Turkeli-Ramadan proposed the triple tube HEX-Combustor which possesses the characteristics of both preheating the reactants and reducing the heat loss in the combustion zone. This in turn shortens the chemical reaction time thus ensuring complete combustion within micro combustors [46-48]. The triple tube HEX-Combustor is a micro combustor with an integrated heat exchanger. The HEX-Combustor consists of a triple tube system; inner, middle, and outer tubes. Reactants enter and flow through the inner annulus. They then pass from the inner annulus to the inner tube passing through a flame holder. Flat flame combustion occurs on the downstream side of the flame holder and combustion products flow along the inner tube to the turbine in the opposite direction to the reactants. The turbine exit gas flows in the outer annulus in the same direction as the reactants. The HEX-Combustor enables the preheating of reactants from both the combustion products and turbine exit gas. Furthermore, the combustion zone is encapsulated and is not exposed to the cold surrounding air which aids in reducing the heat loss from the combustion zone.
The design of the HEX-Combustor was tested with a prototype which had an inner diameter of 14 mm and the gaps between the inner tube, middle tube and outer tube were 1.5 mm. An alumina ceramic porous plate was used as a flame holder. The experimental results of the prototype HEX-Combustor showed that in the triple tube system, using methane as a fuel, the flame stability limit was widened and high combustion efficiency was achieved by preheating the reactants from both the combustion products and turbine exit gases. However, these results introduced new questions, particularly concerning flat flame burners. First of all, in the prototype HEX-Combustor it was not possible to see either the flame shape or the exact location of the flame. Thus, a combustion chamber which allows observation of the flame should be considered. Secondly, since the main focus of the previous study was to investigate combustion the micro turbine was not a part of the test rig and the turbine exit gas was simulated by recirculating the combustion products through a circulation volume on the bottom side of the HEX-Combustor. Thus, the heating system of the reactants did not reflect the actual conditions and there was no control mechanism for the reactants temperature. Furthermore, although the flat flame burner method was first developed and applied to UMGT by Yuasa, and also applied by Marbach and Agrawal, as mentioned above, there is a lack of data showing the effect of using of different flame holders and their ability to provide flat flame combustion with minimum pressure loss. Finally, none of these studies investigated the effect of preheating on the flat flame stabilization as well as flame behaviour with varying equivalence ratios.

Swiss roll micro combustors also have a similar concept to the HEX-Combustor, which is to utilize the thermal energy in the combustion products to preheat the unburned premixture.
in order to extend the flame stability limit. Sitzki et al. developed the Swiss roll micro combustors [49]. Several studies have been performed on Swiss roll micro combustors [50-52]. However, the structure of the rolls increases the volume of the whole system and reduces the space heating in addition to providing a low exhaust gas temperature and high pressure loss; therefore this combustor is not suitable for UMGT applications. Because of that, the Swiss roll micro combustors were employed as heaters for thermoelectric power systems [49]. Swiss roll recuperators were also utilised in the micro turbine devices with power outputs in the range of 25-300 kW. A pressure drop of approximately 15% occurred across the recuperator [53, 54].

**Figure 2-16 Swiss roll combustors [49]**

Under the Belgian PowerMEMS project, the Royal Military School of Belgium (RMS) and the Aachen University of Applied Sciences in Germany worked together on hydrogen micro combustion. They developed micromix principles for diffusive hydrogen combustion [55, 56]. As shown in Figure 2-17 an annular combustor design was chosen.

**Figure 2-17 Combustion chamber layout of Belgian PowerMEMS [11]**

At ONERA, under the DecaWatt project, micro combustion research started with a cylindrical micro combustor with a diameter of 20 mm [13]. Hydrogen and propane were used as fuels. The combustion of hydrogen was tested at equivalence ratios of 0.3 to 0.7. The combustion efficiencies were found to vary from 0.46 to 0.92. The combustion tests were
performed in a pressurised vessel as shown in Figure 2-18. With propane, it was not possible to ignite propane-air mixture without hydrogen and also incomplete combustion was observed.

![Figure 2-18 ONERA’s first micro combustor and its position in the pressurised vessel [13]](image)

At the University of Roma, a combustion chamber with an integrated heat exchanger was developed. Similar to the HEX-Combustor, the reactants are heated from both the combustion products and the turbine exit gas. The heat exchanger spirals along the outer face of the combustion chamber, as shown in Figure 2-19 [57]. The combustion chamber is a cylindrical chamber with prewhirl and air is injected with an intense swirl motion [57, 58]. The overall length of the combustion chamber is 2.2 cm, the outer diameter is 4.2 cm, and the overall height is 13.0 cm. Although some combustion tests were performed, no combustion efficiency or flame stability data is given, therefore it is not possible to draw conclusions on this development.

![Figure 2-19 Combustion chamber and spiral heat exchanger of the University of Roma Sapienza [57]](image)

As can be seen from the previous micro combustion studies, most of the research groups have chosen hydrogen as a fuel because of its high heating value, high burning velocity and leaner flame stability. However, due to its storage problem hydrogen is not a good candidate as a fuel for UMGT applications [3]. Methane combustion at small scales, with high combustion efficiency and wide flame stability has not yet been achieved. Turkeli-Ramadan,
with HEX-Combustor design, did improve the flame stability by preheating the reactants with both the combustion products and turbine exit gas. However, it is not clear how preheating affects the flame characteristics and flat flame stabilization. Furthermore, Sakurai et al. [44] also developed the engineering model flat flame combustor, and without a flat plate at the combustor exit, it was shown that a converged flame was observed. In both the micro combustors of Marbach et al. [27] and Sakurai et al. [44], the combustor designs do not allow the visualization of the flame. They distinguished the flame as a flat flame but the shape of the flame was unclear. Therefore, in order to elucidate the issues mentioned above, a fundamental study on flat flame combustion in a combustor which enables the visualization of the flame is performed in the present study.

Furthermore, in the HEX-Combustor it was found that as the mass flow rate increased, the maximum flame temperature moved downstream, but it was not clear if the flame moved downstream in a flat shape or in a conical shape. Therefore, observation of the flame location and shape, with varying mass flow rate, is also required in the present study.

2.3 Literature review on flat flames

Flat flames are mostly used for calibration of techniques [59-62], burning velocity measurements [63], for detailed investigation of flame stabilization processes [64, 65] and flame structures [66]. In addition to this laboratory research based usage, flat flame burners exist in radiant furnaces for industrial and household applications.

Laser diagnostic techniques have been used to explore the temperature, species concentrations and flow fields. These techniques have become very popular because non-intrusive measurements are able to be obtained. These techniques are mostly calibrated by laminar flat flames in which temperature, concentration and flow patterns are stable.

Flat flame combustion has been used for a long time. Since they provide lean premixed laminar flame combustion, they are clean and stable. For calibration purposes, three major types are being used; these are Meker type, McKenna type and Hencken type, as shown in Figure 2-20. In laboratories, mostly McKenna type flat flame burners are chosen.

The special Meker type burner consists of a bundle of 100 tubes with inner diameters of 0.055 cm which forms the central part of the flame holder and an additional shielding is provided by an outer flame [29]. Another commercially available burner is the Hencken burner. This burner also consists of both central flow and co-flow which is used to prevent air
entrainment. Both flow regions are composed of a square, honeycomb structure which has a cross-section cell size of 0.8 mm. The flame holder is uncooled. This type is non-premixed burner in which the fuel and oxidizer are injected into alternating honeycomb channels. Although this type of burner provides the seeding of atom tracer species, it is not possible to form perfect flat flames.

Hartung et al. [60] developed a flat flame burner shown in Figure 2-20d. All parts are made from brass, except the cooling tube, which is made from copper. The thickness of the burner plate is 5 mm and consists of a brass disc with 2335 0.5 mm diameter holes. A single water cooling loop was used to remove the heat transferred to the burner. This burner allows for seeding of atomic tracer species for laser based thermometry techniques.

![Flat Flame Burners](image)

a) Meker burner [67]  
b) Hencken burner [68]  
c) McKenna burner [61]  
d) A flat flame burner developed for the calibration of laser thermometry techniques [60]

**Figure 2-20 Flat flame burners**
All of these burners form flat flames except the He ncken burner. But these burners do not offer a suitable configuration for micro combustion in UMG, since they all have complex configurations including co-flow and cooling systems. Conversely, a micro combustor requires a very compact design. The micro combustor should be both simple and efficient.

Flat flame burning method was developed by Powling [69, 70] in order to measure the burning velocity. His first flat flame burner is shown in Figure 2-21. With this burner, it was only possible to measure low burning velocities of 0.15 m/s or less.

![Figure 2-21 a) Schematic of Powling’s flat flame burner, photographs of b) rich ether/air flame [70], and c) methyl nitrite [69] obtained with the burner](image)

Following Powling, many studies were performed on flat flame burners. In flat flames, the flame front area as measured by shadow photography, Schlieren photography and the visible are all the same [39]. This is one of the reasons for using flat flames to understand combustion phenomena.

In the next section, a literature review on flat flames is presented. The literature review on flat flame is divided into subsections, where each subsection presents usage of flat flame in different areas. Therefore, the subsections are named according to these topics.

### 2.3.1 Flame holder materials and geometry

Porous plates, perforated plates, sintered plates and honeycomb are the main types of flame holder structures. Brass, stainless steel and ceramics are used as materials for flat flame holders. The flame can stabilize either within or on the downstream surface of the porous medium. The flame can propagate and stabilize within the porous medium when the size of the pores is relatively large, i.e, greater than the quenching distance. Downstream stabilization is
obtained when the size of the pores of the burner are much smaller than the quenching distance. On surface burners, combustion is more stable than the combustion within the porous medium because within the porous medium, the adiabatic burning velocity may increase by a factor of the order of 10 relative to the free burning velocity due to an increase of upstream energy transport [71, 72].

The flames on porous plates are very stable and the position of the flame can be fixed by the position of the porous plate, in addition, these flames can be made quite flat [73]. Since the pore size is in μm scale, porous plates are very suitable as a flame holder for providing flat flames. However, perforated plates are more suitable for the application of seeding particles for laser techniques. The size and the shape of the perforated plates are also important for designing flat flame burners since the thermal properties and the design of the perforated plate have considerable impact on the steady flame structure and the unsteady flame dynamics [74].

Altay et al. [74] and De Goey et al. [75] investigated numerically the effect of the perforated plate holes diameter on the flat flame burner.

De Goey et al. [75] found that the holes and flow obstacles at the outflow edge of the burner distort the flame shape, especially when both the dimensions of them and the burning velocities are large.

Snelleman and Smitt [76] introduced a flat plate with 0.9 mm diameter drilled holes with a distance between the holes of 0.7 mm for application of the sodium line reversal technique. Cone shaped flames stabilized above each hole due to the relatively large hole diameter and hole to hole distance [76].

Altay et al. [74] examined the impact of the operating conditions and the perforated plate design on the steady, lean premixed flame characteristics, by performing two-dimensional simulations of laminar flames using a reduced chemical kinetics mechanism for methane-air combustion, consisting of 20 species and 79 reactions. The results showed that the flame consumption speed, and the flame structure, depend significantly on the equivalence ratio, mean inlet velocity, the distance between the perforated-plate holes and the plate thermal conductivity. The calculation domain was very similar to that of de Goey et al. While de Goey et al. [75] investigated the flame properties at one equivalence ratio, Altay et al. [74] investigated those at varying equivalence ratios.
The conclusions of the study of Altay et al. can be explained as follows. The stand-off distance decreases with an increasing equivalence ratio, since the flame moves closer to the plate, causing its temperature to increase. As the mean inlet velocity increases, the flame stabilizes further downstream. The flame anchors at a finite distance away from the plate due to the flame-wall interactions. As the thermal conductivity of the plate increases, the flame stand-off distance also increases. It is important to note the dimensions of the computational domain which Altay investigated the flame structure on a perforated plate with a thickness of 1.32 cm and the hole diameter of 0.1 cm. The differences between the study of de Goey et al. and Altay et al. are in the incoming flow velocity, the thickness of the plates and the diameter of the holes. De Goey et al. simulated the flame structure with an incoming velocity of 0.35 m/s whereas Altay et al. performed computations with an incoming velocity of 1.3 m/s, which is much higher than the burning velocity. In both studies, the inlet temperature of the gas is uniform and equal to the environment temperature.

McIntosh and Clark [77] analytically investigated the effect of thermal conductivity of the flame holder on burner stabilized flames. They showed that the flame stand-off distance increases with increasing plate thermal conductivity. Similar results were obtained by Altay et al. [74]. McIntosh and Clarke also showed that the flame distance is zero for very low plate thermal conductivity whereas it becomes constant for very large plate thermal conductivity.

In these studies, the effects of preheating the reactants on the flame stability and combustion characteristics, as well as pressure loss through these burner surfaces were not investigated. When a porous plate is used as a flame holder, it is not known whether it behaves like a conical flame in each pore or a perfect flat flame. This phenomenon should also be investigated.

2.3.2 Burning velocity

Laminar burning velocity is one of the most important intrinsic properties of any combustible mixture and is dependent on mixture composition, temperature and pressure of the unburned mixture. The burning velocity is defined as the velocity at which unburned gases move through the combustion wave in the direction normal to the wave surface. It is highly useful for modelling turbulent burning velocity and for validation of theoretical chemical kinetics models.
Andrews and Bradley [78] and Rallis and Garforth [79] reviewed different experimental techniques for measurement of burning velocity of a methane-air mixture. Burning velocity can be measured by flat flame method, flame kernel method, soap bubble method, spherical constant volume vessel method, nozzle burner method and counter flow method.

There is neither consistency nor agreement on both the laminar burning velocities and the measurement technique, as can be understood from Figure 2-22, which was obtained by Dahoe and de Goey [80]. Dahoe and de Goey investigated and reviewed the studies on the laminar burning velocities for methane-air-mixture against varying equivalence ratios. They summarized their findings in Figure 2-22, from which we can conclude that the data shows wide scatter.

![Figure 2-22 Effect of equivalence ratio on the laminar burning velocity of methane–air mixtures, P=1 bar, T=288.15–298.15 K [80]](image)

Heat extraction and heat flux method will now be explained briefly since in these two methods flat flames were adopted. In the literature, there are many studies performed on the measurement of burning velocity of methane and other hydrocarbons against various equivalence ratios, since the burning velocity measurements are used to validate and optimize the chemical reaction mechanism. In flat flames, the heat loss from the flame to the burner provides the stabilization mechanism for these flames, thus these burners are not suitable to stabilize adiabatic flat flames [75]. However, flame stretch, flame curvature and heat losses are the main distortion mechanisms which affect the flame in these methods, the heat flux method being the exception. Heat flux method is a new method compared to others and it was introduced by de Goey and co-workers. The purpose of introducing the heat flux method was to stabilize adiabatic flat flames and measure the adiabatic burning velocity. De Goey and co-
workers proposed stabilized adiabatic stretchless flat flames with the heat flux method. In the heat flux method, the stabilization of the flame is obtained with a thin perforated plate burner. A heating jacket is used to heat the perforated plate and a cooling jacket is used to keep the premixture temperature uniform in the plenum chamber. The adiabatic burning velocity is obtained by the measurement of the temperature distribution of the burner plate with very small thermocouples located at different positions on the burner plate. With this system, the net heat loss is zero since the heat loss from flame front to the burner plate is compensated by the heat gain of the unburned premixture from the burner plate. Thus, the temperature of the burner plate becomes constant and the adiabatic burning velocity is obtained. Details of the heat flux method can be found in Bosschaart et al. [81] and de Goey et al. [64]. The burning velocity is obtained by interpolation of the measurement quantity which is different to the extrapolation of the data for zero heat loss method which was proposed by Botha and Spalding [82] with heat extraction from the flame on a cooled porous plate. Botha and Spalding determined the laminar burning velocity of combustible mixtures by linearly extrapolating experimental flame speeds with various heat loss rates to the state of zero heat loss.

The heat flux method is a promising method to measure adiabatic burning velocity. However, in small scale micro combustors it is not possible to have heating and cooling jackets since it makes the system both more complex and heavier.

In addition to the burning velocity measurements, there are some studies that focus on the response of burning velocity due to variations of the heat loss rate or hydrogen enrichment or nitrogen dilution. Spalding and Yumlu [83] investigated the response of the burning velocity to variations in the heat loss rate. Although the temperature decreases in the downstream of the flat flame due to radiative losses, the radiative losses have no significant influence on burning velocity according to numerical studies. Hermanns et al. [84] and Coppens et al. [85] both measured laminar burning velocity of methane-hydrogen-air mixtures with nitrogen dilution at atmospheric pressure with the heat flux method.

Dyakov et al. [86] used the heat flux burner with a heating jacket to keep the perforated plate flame holder at 353 K which is higher than the incoming premixture temperature of 298 K, and the temperature of the premixture is also kept constant by using a cooling jacket. The reason for applying the heating jacket temperature higher than the incoming premixture temperature is to increase the stability of the flame [87]. An experimental error analysis was performed by Dyakov et al. in addition to obtaining the adiabatic burning velocity of methane-
oxygen-nitrogen mixture with varying dilution ratio \((O_2/O_2+N_2)\). It was found that when the dilution ratio decreases, the adiabatic burning velocity decreases.

To what level can the mass flow rate be increased to obtain high power while keeping the incoming velocity lower than the burning velocity should also be determined in order to use flat flame burners as a component of micro combustors. In the HEX-Combustor, preheating the reactants results in increasing the mass flow rate significantly under which flat flames are formed in addition to widening of the flame stability limits [46]. In the present study therefore, a correlation between the temperature of the reactants and burning velocity and mass flow rate is obtained in order to elucidate the issues mentioned above.

2.3.3 Flame temperature

Bouma et al. [88] presented an analytical model in order to calculate the non-adiabatic flame and surface temperature based on the known behaviour of 1D flames on an externally cooled perfectly conducting burner.

An Arrhenius like equation between the non-adiabatic gas temperature and the burning velocity was obtained by Kaskan [73] for methane combustion, as shown in equation (2-1), which was used for the calculation of the non-adiabatic flame temperature.

\[
S_L = ke^{-E_a/2RT_b}
\]  

(2-1)

where \(T_b\) is the non-adiabatic flame temperature, \(S_L\) is the burning velocity, \(k\) is a constant, and \(E_a\) is the overall activation energy.

When the adiabatic flame temperature and the adiabatic burning velocity are known, Bouma et al. obtained the non-adiabatic flame temperature, as shown in equation (2-2) [88]:

\[
T_b = \left(\frac{1}{T_{ad}} - \frac{2R}{E_a} \ln \frac{S_L}{S_{L0}}\right)^{-1}
\]  

(2-2)

where \(T_{ad}\) is the adiabatic flame temperature and \(S_{L0}\) is the adiabatic burning velocity.

De Goey et al. [64] showed that this relation is also valid for other cooling-stabilized burners only if the reaction zone is not in contact with the heat absorbing material.

In ceramic foam burners the flame can only stabilize when the enthalpy loss of the flame is equal to the enthalpy loss of the burner due to radiation. Thus,
\[ \Delta q = \rho S_L c_p (T_{ad} - T_b) = \varepsilon \sigma \left( T_{surf}^4 - T_{surround}^4 \right) \]  

(2-3)

where \( \varepsilon \) is the effective emissivity of the surface, \( \sigma \) is the Stefan-Boltzmann constant, \( T_{surf} \) is the temperature of the ceramic foam at the outlet center and \( T_{surround} \) is the temperature of the surroundings which is assumed to be equal to the cold unburned gas temperature \( T_u \) for a burner.

The relation between the surface temperature and the burning velocity can be obtained as follows [88]:

\[ T_{surf}^4 = T_u^4 + \frac{\rho S_L c_p T_{ad}}{\varepsilon \sigma} \frac{2RT_{ad} \ln \left( \frac{S_L}{S_{L,0}} \right)}{2RT_{ad} \ln \left( \frac{S_L}{S_{L,0}} \right) - E_a} \]  

(2-4)

In this analytical model the surroundings, unburned mixture gas and ceramic temperatures are assumed to be equal. The enthalpy loss of the burner to the unburned mixture was not taken into account. A more accurate non-adiabatic flame temperature can be calculated by considering the heat loss from burner to the surroundings and the unburned mixture.

### 2.3.4 The effect of flame holder on flame temperature

There are two strategies to minimize the influence of flame holder on the flame temperature. The first one is to heat the flame holder above the temperature of the unburned mixture to appropriate temperature levels, thus the net heat losses from the flame to the burner are balanced. Thus a uniform radial temperature profile of the flame holder can be achieved. The second strategy is to reduce the heat loss from the flame to the flame holder by stabilizing detached flames at a distance far from the flame holder [59].

Detached flames can be obtained by controlling the incoming flow velocity. Gregor and Dreizler [59] were able to obtain detached flames at 1.5 to 2.5 mm from the flame holder by using 60 mm diameter sintered bronze flame holder with a thickness of 5.5 mm. The flame holder had a porosity of 32% with approximate pore size of 0.02 mm.

According to Gregor and Dreizler, to obtain detached flames requires spatially very homogeneous porous flame holders, suitable porosity and pore sizes in addition to precise control of the mass flows. The hot gas was measured 20 mm above the burner head by using Rayleigh thermometry. The thermokinetic state of the detached flames without any water cooling is very close to the freely propagating flames whose temperatures deviate from
adiabatic conditions only due to gas radiation [59]. Gregor and Dreizler minimized the effect of flame holder on the flame temperature using unique porosity, unique pore size and unique thickness but the effect of different porosity, pore size and thermal conductivity of the materials on the flame temperature have not been investigated.

2.3.5 Flame location and stand-off distance

The effect of inlet flow velocity on flame location was investigated by Norton and Vlachos [89] and Li et al [90] at small scale. Both studies stated that when the inlet velocity increases, the flame location shifts downstream and at very high flow velocities, blowout occurs. Similarly, when the inlet velocity decreases the flame location shifts downstream again. Further reduction in inlet velocity results in extinction due to the relative increase of heat loss to heat release rate. Flame location and flame stability limit plots are very similar in shape which is a U-shape as shown in Figure 2-23. The flame location versus inlet velocity plot was obtained with 2D elliptical model using a stoichiometric methane-air premixture at a reactants temperature of 300 K and atmospheric pressure [89].

![Figure 2-23 Flame location vs inlet velocity [89]](image)

Yuuki and Matsui [91] defined the stand-off distance as the distance between the burner surface and the point where the thermocouple shows the maximum temperature. The thermocouple was 0.1 mm in diameter and made of 10% Rh-Pt and the measurement of stand-off distance was done with the help of a reading microscope.

In the heat extraction method, Botha and Spalding [82] stated that if the burning velocity of the mixture exceeds the stream velocity, the flame travels upstream. Conversely, if
the stream velocity is greater than the burning velocity the flame travels downstream. The results were similar to studies obtained by both Norton and Vlachos [89] and Li et al [90].

The dependence of the burning velocity on the flame temperature on porous metal burners is given by

\[
\frac{S_L}{S_{L0}} = \exp \left[ -\frac{E_A}{2R} \left( \frac{1}{T_p} - \frac{1}{T_{ad}} \right) \right] \tag{2-5}
\]

Ferguson and Keck [66] using the above equation also developed a theoretical solution for a given stand-off distance of a laminar flame on a porous metal burner. They obtained two solutions for a given stand-off distance, one in the high speed flame region and the other one in the low speed flame region. The theoretical results were also compared with experimental results. The results of the dependence of flame temperature on burning velocity and the dependence of stand-off distance on flame temperature are shown in Figure 2-24.

![Figure 2-24 The dependence of flame temperature on burning velocity (left) (\(\Theta\) is the fuel-air equivalence ratio, \(\psi\) is the molar nitrogen to oxygen ratio of the reactants) and the dependence of stand-off distance on flame temperature (right) (solid curves are the theoretical results) [66]](image)

The physical reason behind two different solutions for a given stand-off distance can be explained by the fact that near adiabatic flame temperatures, stand-off distances will be large because in order to maintain a steady-state energy balance only a small amount of energy needs to be transferred to the burner. On the other hand, as the flame temperature decreases, the heat loss per unit mass increases, so the heat transfer to the burner increases thus the stand-off
distance must decrease. For very low temperatures, the energy generation decreases more rapidly than the heat loss per unit mass increases, therefore the heat transfer to the burner must decrease and the stand-off distance must increase.

In contrast to Ferguson and Keck’s dual response of flame speeds for a given flame stand-off distance, Eng et al. [65] demonstrated computationally and experimentally the uniqueness of the flame response when the flame burning rate is considered to be the independent variable. They also observed a wrinkled flame when the minimum stand-off distance was obtained and further increases in the mass flow rate caused the flame to be wrinkled. In addition to this, flame wrinkling was also observed for very small mass flow rates.

![Computed and measured flame stand-off distance as functions of the mass flow rate (left) Computed and measured flame temperature as functions of the mass flow rate (right)[65]](image)

![Computed and measured flame stand-off distance as functions of the mass flow rate (left) Computed and measured flame temperature as functions of the mass flow rate (right)[65]](image)

It may be beneficial to revisit the results of the HEX-Combustor here [46]. Since it was not possible to observe the location and shape of the flame in the HEX-Combustor, only the temperature of the products along the centreline was measured. The results showed that at low mass flow rates, the maximum flame temperature was measured very close to the porous flame holder, whereas at high mass flow rates it was far from the porous flame holder, at approximately 6 mm. As can be concluded from the previous studies, it is necessary to investigate flame location with varying equivalence ratio, mass flow rates and reactants temperature. In particular, there appears to be no study in the literature showing the effect of the reactants temperature on the flame location.

### 2.3.6 Flame instabilities

Heat loss from the flame to the burner plate, fluctuations and changes in both the incoming flow velocity and the equivalence ratio may cause flame instabilities.
Chou et al. [92] explained the reason for flame instabilities in micro combustors as the following; flame-flow and flame-structure interactions and heat loss induced high-frequency extinction-re-ignition may lead to flame instabilities in micro combustors.

Clarke and McIntosh [93] investigated the effect of the heat loss from the flame to the burner plate on the flame response of perforated plates. They found that due to heat loss from the flame to the burner plate the flame stand-off distance changes with the location of the flame front. McIntosh and Clarke [94] also compared models to find the relation between the stand-off distance and the temperature of the flame. They also developed an analytical model to examine the response of planar burner stabilized flames due to the heat loss mechanism. McIntosh’s model predicts the response of burner stabilized flames to oscillatory heat loss to the burner plate. It can be applied to flat flame in which the incoming flow velocity has to match with the burning velocity. However, Altay et al. [95] extended the planar perforated-plate stabilized flame model considering both the effect of flame area oscillations and the heat loss oscillations.

El-Hamdi et al. [96] investigated a variety of pulsating instabilities of flames stabilized on top of perforated plates. They presented the stability boundaries for the occurrence of different pulsating modes at a fixed pressure as a function of mass flow rates and equivalence ratios.

Blackshear and Mapp [97] observed the oscillations in rich, light hydrocarbon-air and lean, heavy hydrocarbon-air low pressure flames. The observed oscillation frequencies ranged from 15 to 65 Hz with a stainless steel porous plug burner. The intensity of the flame was measured by imaging the flame on a photodiode. The frequency of oscillation was determined by displaying the time series of the intensity on a storage oscilloscope and measuring the period.

Margolis [98] performed a theoretical study of oscillation of a flame stabilized on a porous plug burner and predicted that the instabilities of the steady-state solution is always enhanced by a low burner surface temperature, larger activation energy, a slow mixture velocity and nonadiabatic burned temperatures.

Yuuki and Matsui [91] numerically investigated the stable structure for a range of mixture flow rates and the time varying behaviour of stoichiometric methane-air flames on porous metal burners at atmospheric pressure. The comparison with experimental data
confirmed that the model gives quantitative agreement. The study confirmed that the flame intrinsically oscillates due to the time lag of the temperature disturbance and its instability is enhanced by a large flame stand-off distance. It was found that the premixed laminar methane-air flame on porous plug burner of flame temperature less than 1550 K, which corresponds to the incoming mixture velocity being lower than 1 cm/s, is unstable on the burner at any surrounding conditions. Margolis [99] also found similar results that when the incoming flow velocity is sufficiently less than the adiabatic flame speed an unstable region becomes feasible. Margolis investigated the one-dimensional stability of a burner stabilized premixed flame assuming a one step chemical reaction.

These discussions show that non-adiabatic combustion occurs in flat flame burners, thus flame instabilities are unavoidable.

### 2.3.7 Emissions

Since reduction of NO\textsubscript{X} emissions from flames is one of the requirements for clean energy and a clean environment, some studies also investigated the influence of fluctuations of equivalence ratio or hydrogen enrichment on NO\textsubscript{X} emissions [100]. Darabiha performed both experimental and numerical studies on the effect of fluctuations of equivalence ratio on flame temperature and NO\textsubscript{X} emissions. In the numerical study, a one dimensional burner stabilized flame was considered and simulated by two detailed mechanisms. One of those involved 50 species and 235 elementary reactions which included detailed prompt and thermal NO\textsubscript{X} reactions. The other one involved 17 species and 46 reactions which included only thermal NO\textsubscript{X} reactions.

The experimental burner consisted of a 20 mm diameter quartz tube and a horizontal stainless steel screen flameholder. The temporal fluctuations of equivalence ratio was provided by the injection of methane through an oscillating poppet type valve. Temporal equivalence ratio was measured by a non-intrusive optical technique based on infrared absorption. All the calculations were presented by Darabiha et al. [100] at reactants temperature of 300 K and atmospheric pressure. The results showed that for an unsteady flame, temporal equivalence ratio fluctuations diminish the maximum temperature and the mean value of NO\textsubscript{X} emissions compared to a steady flame.

One of the approaches to achieve lower NO\textsubscript{X} emissions is hydrogen enrichment in natural gas. This extends the lower flammability limits in fuel-lean conditions where NO\textsubscript{X}
emissions are significantly reduced. Coppens et al. [101] investigated the effects of composition on both the burning velocity and nitric oxide formation in premixed flames of CH₄+H₂+O₂+N₂ since hydrogen enrichment leads to higher burning velocities whereas dilution by nitrogen leads to the reduction of the burning velocity and NOₓ emissions. Both experimental and numerical studies showed that in lean flames enrichment by hydrogen has little effect on the concentration of nitric oxide, whereas in rich flames, the concentration of nitric oxide decreases with hydrogen enrichment significantly. Dilution by nitrogen decreases nitric oxide concentration at any equivalence ratio. The Konnov mechanism, which consists of 1200 reactions among 127 species was used for modelling with the burner-stabilized flame option of the Chemkin-II code.

Bouma and De Goey [71] studied combustion of a lean premixed methane air mixture stabilized on a ceramic foam burner which was developed by the Netherlands Energy Research Foundation and was produced by ECO Ceramics. The ceramic foam burner was developed for domestic heating systems, small industrial furnaces and drying equipment. The ceramic foam burner pore sizes are 0.4 mm and has a volumetric porosity of 90% with dimensions of 114x114x11 mm³. The temperature and concentration profiles of the major combustion species were computed by a skeletal mechanism for lean methane oxidation and the NOₓ emission was computed with a NOₓ post processor using the output of the flame calculation as input.

Bouma et al. [72] also performed both numerical and experimental studies on NOₓ emission of flat premixed methane-air on a ceramic foam burner. They investigated at two thermal load cases; lower and higher thermal loads. At lower thermal loads the premixture incoming gas velocity is lower than the adiabatic burning velocity thus a flat flame stabilizes very close to or even partly in the burner. While at higher thermal loads, the premixture incoming gas velocity is higher than the adiabatic burning velocity. Bouma et al. called the mode at low thermal loads the ‘radiation mode’ since the flame is cooled by conductive heat losses to the burner and this energy loss of the flame is radiated to the surroundings by the burner surface. In this mode, the gas flow and the combustion phenomena can be assumed to be one-dimensional. On the other hand, they called the mode at high thermal loads ‘blue-flame mode’ since at this mode Bunsen type flames appear. In this mode the combustion phenomena is three-dimensional. It will be beneficial to recall the experimental results of the prototyped HEX-Combustor. At high mass flow rates the maximum temperature was measured far from the porous plate, which was utilized as a flameholder. It was assumed that a lifted flame
occurred at these high mass flow rates [46]. One of the objectives of the present study is to understand the flame behaviour and shape at varying mass flow rates.

2.4 The effect of the reactants temperature on burning velocity

The main focus of this study is to investigate the effect of preheating the reactants on the flame stability and combustion characteristics, therefore it is important to show how burning velocity changes with reactants temperature. In this section, the studies of the effect of the reactants temperature on the burning velocity and the empirical relations between the reactants temperature and burning velocities is presented.

Andrews and Bradley [102] investigated the dependence of burning velocity on reactants temperature empirically for methane/air flames at atmospheric pressure. They obtained the formula for stoichiometric methane/air flames as follows

$$S_L = 10 + 0.0003717 T_u^2, \quad 150K < T_u < 1000K$$

(2-6)

where $T_u$ is unburned gas temperature.

Similarly, Coffee et al. [103] also investigated the reactants temperature effect on the overall reaction parameters $A$ and $E$, where $E$ is the activation energy. They obtained the following formula for burning velocity

$$S_L = 10 + (5.532E - 5)T_u^{2.29}$$

(2-7)

The most popular correlation showing the influence of reactants temperature on the adiabatic laminar burning velocity is

$$S_L = S_{L0} \left( \frac{T}{T_0} \right)^\alpha$$

(2-8)

where $T_0$ and $S_{L0}$ are the reference temperature and the burning velocity at this temperature, respectively [104]. Konnov summarized the empirical expressions for the power exponent $\alpha$ for methane-air flames in equation (2-8) as shown in Table 2-2.

In addition to these experimental data, Mishra [105] developed a similar correlation with a power exponent of 1.575 numerically for stoichiometric methane-air flames in order to describe the dependence of reactants temperature on the burning velocity at atmospheric pressure. The reactants temperature range was considered from 300 K to 600 K. This study
clearly indicated that detailed chemical kinetics is essential for the prediction of the effects of reactants temperature on the burning velocities.

Table 2-2 Experimental data and empirical expressions for the power exponent $\alpha$ for methane-air flames from [104]

<table>
<thead>
<tr>
<th>Pressure range (atm)</th>
<th>Temperature range (K)</th>
<th>Range of $\bar{\phi}$</th>
<th>Correlation</th>
<th>$\alpha$ at $\bar{\phi}$=1</th>
<th>Year</th>
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<td>1.88-0.95($\bar{\phi}$-1)</td>
<td>1.88</td>
<td>2005</td>
</tr>
<tr>
<td>1-5</td>
<td>298-498</td>
<td>1</td>
<td>1.653</td>
<td>2007</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>298-418</td>
<td>0.8-1.2</td>
<td>11-14.8$\bar{\phi}$+7.279$\bar{\phi}^2$</td>
<td>1.589</td>
<td>2009</td>
</tr>
</tbody>
</table>

It can be concluded from Table 2-2 and Mishra’s study that the empirical power exponent shows significant scattering but it is always greater than 1, therefore increasing the reactants temperature increases the burning velocity exponentially. As a conclusion, the higher the reactants temperature, the higher the burning velocity. The increase in reactants temperature may widen the flame stability limit and therefore this subject is studied in further detail.

2.5 Premixed laminar flame

In this section, a brief explanation of premixed laminar flames is given in order to help in understanding the phenomena in the results and discussion sections of the present study, in relation to both the experimental and numerical parts.

In premixed flames, the flame consists of four regions. These are cold reactants zone, preflame zone, reaction zone, and products zone or post-flame zone. Concentration and temperature profiles of a one-dimensional, premixed, adiabatic flame is shown in Figure 2-26.

In the detailed structure of the flame, the temperature increases smoothly from the initial state to the final state. The intermediate and product concentrations increase similarly, whereas the fuel and oxidant concentrations show a corresponding decrease as shown in Figure 2-26. The visible part of the flame is located in the reaction zone. The emission is due to electronically excited species, such as CH, CN, and C₂. Heat flows from the boundary of b of
the burned gas to the boundary 0 of the unburned gas, while mass flows in the opposite direction. The flame temperature eventually reaches a constant value when all the fuel has been consumed and reaction has completed. More details about the propagation of premixed laminar flame can be found in references [106, 107].

![Figure 2-26 Concentration and temperature profiles of a one-dimensional, premixed, adiabatic flame[106]](image)

Flat flames are very similar to the stationary flames. In addition, in premixed flames, as well as the flat flames, conical flames, similar to the flame from the Bunsen burner, are also observed. A schematic of a conical flame front is shown in Figure 2-27.

![Figure 2-27 Flame front of a conical flame](image)

The burning velocity is defined as the velocity at which the unburned gases move through the combustion wave in the direction normal to the wave surface [39]. In Figure 2-27, \( S_L \) is the burning velocity, normal to the flame front, \( u \) is the local velocity of the unburned gas, \( \alpha \) is the cone angle which is the angle between flame surface and gas flow. The cone angle changes according to the unburned gas velocity. When the unburned gas velocity is low, the cone angle is higher which means the height difference between the flame tip and flame root is small. On the other hand, when the unburned gas velocity is high, the cone angle becomes
small in order to balance the normal component of the unburned gas velocity with the burning velocity. In this case, the height difference between the flame tip and flame root increases.

2.6 Summary

UMGT and micro combustor research around the world were presented. Each micro combustor design was introduced with their respective shortcomings. Thereby, the gaps in the micro combustion research, outlined in the literature, were presented. This research aims to fill these gaps. Next, flat flame combustion was introduced. Different research topics investigated on flat flames were detailed. Furthermore, the studies on the effect of the reactants temperature on the burning velocity and the empirical relations between the reactants temperature and burning velocities were presented. Lastly, details of the premixed laminar flame were introduced briefly.
3 EXPERIMENTAL APPARATUS AND METHODOLOGY

In this chapter, the experimental setup, equipment and the methodology used for the experimental work is presented.

3.1 Flat flame combustor

A test rig, which enables the observation of both the flame shape and location, was developed in the Thermodynamic Laboratory of the University of Auckland. The new test rig also provides the ability to change the flame holders and to control the reactants temperature. A drawing and a photo of the combustor and mixing chamber are shown in Figure 3-1.

![Figure 3-1 Drawing and photo of the test rig](image)

A stainless steel mixing chamber was inserted at the bottom of the combustor to obtain homogeneous uniform premixed fuel-air. Fuel was supplied from a fuel cylinder, the mass flow rate of which was controlled and measured by a Sierra Mass flow controller, and from there it entered the bottom of the mixing chamber. Air entered the mixing chamber through two pipes after being heated by two Omega T type air process heaters. On top of the mixing chamber, a machinable ceramic part was used as a base for the combustor, which helped to reduce the heat loss from the flame to the mixing chamber. A quartz tube was chosen as the combustor wall since it facilitated observation of the flame. A second concentric quartz tube was used in order to minimize the heat loss from the flame. The inner diameter of the first quartz tube is 46 mm with a 1.5 mm wall thickness. The whole system was assembled together with stainless steel
connectors. Graphite sealants were used between the flame holders, quartz tubes and flame holder base in order to prevent leakage problems.

3.2 Flame holders

Alumina ceramic porous plates, perforated stainless steel plates and sintered stainless steel plates were used as flame holders. The set-up design allows for easy change of the flame holder. Sintered stainless steel plates were provided by Siperm Tridelta from Germany and alumina ceramic porous plates were provided by FujiChem from Japan. Perforated plates were manufactured at the University of Auckland. The material and geometric parameters of the different flame holders are given in Table 3-1. The sintered stainless steel plates have a 3 mm thickness and average pore sizes of 200 µm and 100 µm, for the R200 and R100 types, respectively. Alumina ceramic porous plates have thicknesses of 1, 2, 3 and 4 mm. The average pore sizes are 130 µm, 230 µm and 580 µm for FA100, FA060 and FA024 type ceramic porous plates, respectively. The porosity of the flame holders used in the experiments was in the range of 43~54%. In addition, a 2 mm thick perforated plate, with a hole diameter of 1 mm and hole center distances of 2 mm was manufactured and tested. Photos of the flame holders are shown in Figure 3-2.
Table 3-1 Specification of porous and sintered flame holders

<table>
<thead>
<tr>
<th>Material</th>
<th>Average pore size (µm)</th>
<th>Porosity (%)</th>
<th>Thickness (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>FA024 Alumina ceramic</td>
<td>580</td>
<td>45~50</td>
<td>2.4</td>
</tr>
<tr>
<td>FA060 Alumina ceramic</td>
<td>230</td>
<td>45~50</td>
<td>1,2,3</td>
</tr>
<tr>
<td>FA100 Alumina ceramic</td>
<td>130</td>
<td>45~50</td>
<td>1,2,3</td>
</tr>
<tr>
<td>R100 Stainless Steel</td>
<td>100</td>
<td>43~58</td>
<td>3</td>
</tr>
<tr>
<td>R200 Stainless Steel</td>
<td>200</td>
<td>49~54</td>
<td>3</td>
</tr>
<tr>
<td>SSFilter (Stainless Steel Filter)</td>
<td>Unknown</td>
<td>Unknown</td>
<td>1.6</td>
</tr>
<tr>
<td>Perforated plate (PP)</td>
<td>1000</td>
<td>21</td>
<td>2</td>
</tr>
</tbody>
</table>

3.3 Mixing chamber

Although a mixing chamber was installed at the bottom of the combustion chamber, initially it did not provide proper mixing of the fuel and air. The flame was observed to settle down on only a small portion of the flame holder surface. Thus, in order to assist mixing of the fuel and air properly, different procedures were investigated. Firstly, foam sponges were installed in the mixing chamber, but this did not improve the mixing. Secondly, stainless steel wool of 30 mm thickness was installed in the mixing chamber between two perforated plates. Unfortunately, this did not help either. Next, the mixing chamber was filled with glass beads, however the outcome was the same as the previous trials. Finally, the air inlets were extended and both air flows were placed symmetrically on either side of the fuel inlet. This final adjustment improved the mixing and flat flames started to cover the whole surface of the flame holder. The photos of foam, stainless steel wool between perforated plates, glass beads and the extended air inlets are presented in Figure 3-3.

Improper mixing of the fuel air mixture was understood from both the shape and the colour of the flame. Photos of flames resulting from improper mixing are shown in Figure 3-4. On the left photo, three different coloured regions were observed. A blue region where lean premixture was available, a green region showing rich mixture and a red region which shows that flame occurred very close to flame holder increasing the flame holder temperature. On the other hand, on the right photo, two coloured regions were observed. On the left half, the flame occurred very close the flame holder, while on the other half, lifted and flickering flames were observed.
Even with the modifications mentioned above, at high mass flow rates, mixing was still insufficient. As a result, the air and fuel inlets were modified. Instead of two air inlets, air entered to the mixing chamber through twelve 3 mm diameter holes. Likewise, fuel also entered the mixing chamber via twelve 1 mm diameter holes. The air and fuel inlets are presented in Figure 3-5. In addition, a 30 mm thick, ceramic porous block was inserted in the mixing chamber in order to further improve mixing. After these modifications, the preliminary experiments showed that this small volume was still not enough to obtain a homogeneous uniform premixed fuel-air mixture. Therefore, the mixing chamber was initially extended by 60 mm and then by 120 mm. With the 120 mm extension to the mixing chamber, flat flames were finally obtained.
Since the main aim of this project is to develop a methane-fuelled micro combustor, 99.99% pure methane and New Zealand pipeline natural gas, whose main constituent is methane, were used as fuels. The reasons for choosing methane as a fuel can be explained as follows:

- The abundance of methane and the ease of storage.
- To help reduce carbon emissions, which is possible by using the least carbon content.
- To assist in reducing the emissions from animal farming and thereby contribute to a more sustainable use of energy resources and the environment.
3.4.1 Natural gas

In this study New Zealand pipeline natural gas was mainly used as a fuel. The composition of natural gas is listed in Table 3-2. The composition of the New Zealand pipeline natural gas was provided by Ben Smith from the company Vector Limited. It was informed that the composition very rarely changes. Before being fed in to the combustor, the natural gas was compressed and filled in cylinder bottles. Although the combustion tests were performed at atmospheric pressure, the inlet pressure of the natural gas before passing through the mass flow controller was kept higher than 4 bar. This was required in order to compensate for the pressure loss through the mass flow controller.

New Zealand natural gas can be written as $C_{1.18}H_{4.12}O_{0.11}$ from the chemical compositions presented in Table 3-2. (In the chemical formula of natural gas, the component of N is not shown, because N has a very small value compared to other main components, which is 0.08502). Molecular mass is calculated as 20.22 kg/kmol while the lower heating value of the New Zealand natural gas is found as 42.87 MJ/kg from these compositions. The calculations are explained in Appendix A1.

Table 3-2: Molar gas composition of New Zealand natural gas in Auckland (July/2012)

<table>
<thead>
<tr>
<th>Gas components</th>
<th>% Mole fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>82.02</td>
</tr>
<tr>
<td>Ethane</td>
<td>7.39</td>
</tr>
<tr>
<td>Propane</td>
<td>3.13</td>
</tr>
<tr>
<td>n-Butane</td>
<td>0.59</td>
</tr>
<tr>
<td>I-Butane</td>
<td>0.54</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>0.09</td>
</tr>
<tr>
<td>I-pentane</td>
<td>0.12</td>
</tr>
<tr>
<td>Hexane</td>
<td>0.06</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0.43</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>5.63</td>
</tr>
</tbody>
</table>

3.4.2 Methane

Some of the experiments were performed using 99.99% pure methane. Although the main constituents of New Zealand natural gas is methane, pure methane tests were performed
in order to elucidate any discrepancy on the combustion characteristics due to the H/C differences.

3.5 Mass flow controllers

Air was provided from the line and a pressure regulator was used to keep the inlet pressures constant. The air flow rate was controlled by Sierra Smart Trak 100L mass flow controller (Model number: C100L-DD-13-OV1-SV1-PV2-V1-S0). Fuel was provided from a compressed cylinder and the pressure regulator was used to adjust the pressure above 4 bars. The fuel flow rate was controlled by a Sierra Smart Trak 100M mass flow controller (Model number: C100M-DD-14-OV1-SV1-PV2-V1-S0). The accuracy and the repeatability of both Sierra mass flow controllers are ±1% and ±0.2% of full scale. The most important part of controlling fuel to air ratios was provided by the set values on the mass flow controllers. However, there was no setting for natural gas in the fuel mass flow controller. Therefore, in addition to Sierra mass flow controller, a Micro Motion mass flow meter was used. Both the mass flow controller and the mass flow meter were connected in series. In this study, although the control of the fuel flow rate was conducted by the Sierra mass flow controller, the equivalence ratios were determined from the exhaust emissions.

The working principles of the Sierra mass flow controller and the Micro Motion mass flow meter are totally different. The Sierra mass flow controller is a thermal mass flow controller, while the Micro Motion mass flow meter is a Coriolis mass flow meter. The working principles of these are explained in Appendix A2 and A4.

In the Micro Motion mass flow meter, changes in fluid parameters such as temperature, pressure, density, viscosity, and conductivity have no effect on the mass of the fluid being measured.

The Sierra mass flow controller was provided with manufacturer’s calibration data with air. However, for natural gas, a conversion factor was used to convert the actual readings. The conversion factor calculations are given in Appendix A3.

Furthermore, Micro Motion mass flow meter was also calibrated with the amount of water passing through the mass flow meter in an elapsed time. The water flowed from a higher location and passed through the mass flow meter. With the help of a valve, a stopwatch and an Ohaus balance, as shown in Figure 3-7, the mass flow rate was calculated. The calculated mass flow rates were compared with the Micro Motion mass flow meter readings. A comparison
with the mass flow rates obtained with water are presented in Figure 3-8. A smaller range of the measurements is also shown in the right figure in more detail. As can be seen from these plots, the Micro Motion mass flow meter is able to measure accurately at the lower limit of its range.

![Figure 3-7 Micro Motion mass flow meter calibration set-up](image)

![Figure 3-8 Calibration of Micro Motion mass flow meter with water](image)

### 3.6 Flame stability limit

By controlling the air and fuel mass flow rates and observing the flame and temperature values, the flame stability limit was obtained. Mass flow controllers set the air and fuel mass flow rates, heaters provided control of reactants temperature, and extinction and blow off
conditions were determined, both through direct observation and exhaust gas emission measurements.

3.7 Flame visualization

The experiments were performed under atmospheric pressure and room temperature. Ignition was supplied by a pilot flame.

The location and shape of the flame was observed through the quartz wall of the combustor. Since flat flame burners provide a flame front in which the areas of the shadow, schlieren, and visible fronts are all the same [108], in this study the flame was photographed and recorded by a Canon PowerShot SX210 IS digital camera.

Initially, visualization of the flame was conducted under normal room and daylight conditions. However, it was quickly understood that observing the flame in the dark makes the flame easier to observe with the naked eye. Therefore, in order to observe the flame better, a black cylinder with a hole was manufactured, as shown in Figure 3-9. This improved the observation of the flame, but still it was difficult to see the flame particularly at the very lean side of the stoichiometric when the flame was very weak. In order to solve these observation problems, the test rig was moved into a dark test cell in the Thermodynamic Laboratory. In the dark room, it was possible to observe both the flame and the flame holder colours without any external assistance.

![Figure 3-9 Observing flat flame with the help of a black cylinder](image)

3.8 Pressure measurements

Pressure values were measured by a 2100 Meriam smart gauge pressure transducer and a Digitron manometer. The calibration of the transducers was performed using a Betz micromanometer and a U-tube manometer. Pressure drop measurements were performed in the non-reacting flow case. The pressure transducer was used to measure the pressure at the upstream side of the flame holder as shown in Figure 3-10. As the downstream side was
exposed directly to atmospheric pressure, the pressure drop value through the flame holder could be determined readily. The test rig incorporates the ability to easily change the flame holder and therefore obtain the pressure loss measurements of different flame holders.

Figure 3-10 a) Sintered stainless steel flame holder b) View of quartz tube combustor

A photo of the pressure transducers and Betz micromanometer and U-tube manometer calibration instruments is shown in Figure 3-11. The accuracy of the pressure transducers and Betz micromanometer are listed in Table 3-3.

Table 3-3 Accuracy of the pressure transducers and Betz micromanometer

<table>
<thead>
<tr>
<th>Instrument</th>
<th>2100 Meriam smart gauge</th>
<th>Digitron 2082P pressure transducer</th>
<th>Betz micromanometer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Accuracy</td>
<td>±0.05% Full scale</td>
<td>±0.1% Full scale</td>
<td>±0.04% Full scale</td>
</tr>
</tbody>
</table>

Figure 3-11 Pressure transducers, Betz micromanometer and a U-tube manometer
3.9 Emission measurements and combustion efficiency

Emission measurements were performed using the gas analysers available in the Thermodynamic Laboratory. CO, CO\textsubscript{2}, O\textsubscript{2}, NO\textsubscript{X} and unburned hydrocarbon were measured at different mass flow rates, and equivalence ratios. From the measurement values, combustion efficiency and equivalence ratios were calculated. The calculations are explained in detail in Chapter 4.

3.9.1 Exhaust gas analyzers

Different test analyzers were employed for exhaust gas concentrations of CO\textsubscript{2}, CO, O\textsubscript{2}, NO\textsubscript{X} and unburned hydrocarbon (UHC). For the measurement of CO\textsubscript{2} and CO, a Signal multi gas analyzer, which is based on the NDIR absorption technique, was used. For the measurement of O\textsubscript{2}, a Signal 8000 series gas analyzer was employed on a working method of paramagnetic detector. For the measurement of NO\textsubscript{X} and UHC, Signal 4000 series and Signal 3000 series gas analyzers were used on a working method of chemiluminescent and flame ionization detector, respectively. The range and accuracy of the analyzers are given in Table 3-4.

<table>
<thead>
<tr>
<th>Gas</th>
<th>CO\textsubscript{2}</th>
<th>CO</th>
<th>O\textsubscript{2}</th>
<th>NO\textsubscript{X}</th>
<th>UHC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analyzer</td>
<td>Signal Multi gas analyzer</td>
<td>Signal Multi gas analyzer</td>
<td>Signal 8000 Series</td>
<td>Signal 4000 Series</td>
<td>Signal 3000 Series</td>
</tr>
<tr>
<td>Range</td>
<td>0 to 20%</td>
<td>0 to 10%</td>
<td>0 to 25%</td>
<td>0-10000 pm</td>
<td>0-4000 ppm</td>
</tr>
<tr>
<td>Accuracy and repeatability</td>
<td>±1% span</td>
<td>±1% span</td>
<td>±0.01% O\textsubscript{2}</td>
<td>±1% span</td>
<td>±1% span</td>
</tr>
<tr>
<td>Condition</td>
<td>Dry</td>
<td>Dry</td>
<td>Dry</td>
<td>Wet</td>
<td>Wet</td>
</tr>
</tbody>
</table>

The sample passed through a heated line by a Signal oven. The temperature of the oven was kept at 190 °C in order to prevent heavy hydrocarbons from condensing out and blocking the sample capillary and other critical paths. The heated line fed to the NO\textsubscript{X} and UHC analyzers while for CO\textsubscript{2}, CO and O\textsubscript{2} the sample was passed through a chiller and a water trap in order to remove the majority of water content. Therefore, the emission data gathered by CO\textsubscript{2}, CO and O\textsubscript{2} analyzers were on a dry basis.

The details of the working principles of these analyzers can be found in reference [109]. Calibration of these analyzers was performed prior to each testing session.
Firstly, the emission probe was inserted 60 mm above the flame holder surface, as shown in Figure 3-12a. But after performing some experiments with different equivalence ratios, it was found that at both lower and higher equivalence ratios, the flame did not settle down on the flame holder. Instead, at low equivalence ratios it was lifted and unstable (Figure 3-12b). On the other hand, at higher equivalence ratios, in addition to a flat flame a cone shaped red coloured glow (Figure 3-12c) was also observed. Therefore, the exhaust chimney was extended and the emission probe was installed 300 mm above the flame holder surface. Thus, any obstruction by the probe to the flame was prevented. However, at high equivalence ratios, due to exposure to high temperatures, inserting the probe in the quartz walled combustor caused the melting and consequent dripping of the probe tube on the flame holder. In Figure 3-12d, it can be seen that dripping of the probe left deposits on the flame holder, which in turn affected the flame. Around the deposit an orange glow could be observed.

Furthermore, emission measurements with long and short chimneys showed that with the short chimney, $O_2$ concentration was higher than that of the long chimney. This shows that air entrainment from the exit to the inside of the combustor tube occurred. Therefore, the exhaust chimney was extended in order to prevent air entrainment effects at sampling position and the emission probe was installed in the middle of the extension tube. Thus, both the intrusion on the flame by the probe and air entrainment were prevented. The photos of the extended exhaust chimney and emission probe location are shown in Figure 3-13a. The photos of the Signal oven and gas analysers in the rack are also presented in Figure 3-13.

![Figure 3-12](image-url)  
*Figure 3-12* a) Emission probe 60 mm far from the flame holder surface, b) flame at low equivalence ratio, c) flame at high equivalence ratio, d) deposits from the melting of the emission probe affecting the flame
3.10 Temperature measurements

In the experiments it was expected that high flame temperatures would be achieved, but nevertheless these should be lower than the adiabatic flame temperature. This is because there is heat loss from the flame to the burner, which is the mechanism for the stabilization of flat flames, in addition to the heat loss to the environment. In addition to the exit gas temperature of the combustor, the temperature of the flame should also be known in order to choose the combustion material. Since this combustor is designed to operate in ultra micro gas turbines, the turbine inlet temperature is one of the important issues in terms of cycle and system efficiency. Because of these reasons, the temperature of the flame and the reactants should be measured.

Furthermore, one of the objectives of this study is to show both the stabilization of flat flame and widening of the flame stability limit through preheating the reactants. Therefore, measuring and controlling the reactants temperature was an important part of this research. The preheating of the air was provided by two T type Omega heaters. The reactants temperature was measured with a K type thermocouple before passing through the flame holder.

In addition to 0.25 mm and 0.5 mm diameters K type thermocouples, a 0.0254 mm diameter S type Medtherm fine wire thermocouple, which was designed for gas temperature
measurements in internal combustion engines, was used to measure the flame temperature. A drawing of the fine wire thermocouple is shown in Figure 3-14, including tip details of the thermocouple. Thermocouples were connected to Campbell Scientific CR850 Logger and data logger was connected to a computer.

It was very difficult to measure the flame temperature since the thermocouple was exposed to very high temperatures. In order not to affect the flame, very thin thermocouples were selected. A 0.0254 mm diameter K type Medtherm fine wire thermocouple and a couple of 0.25 mm diameter unshielded K type thermocouples were broken very quickly when they were exposed to the flame.

Figure 3-14 a) Schematic of Medtherm fine wire thermocouple b) Tip detail (G. Luft from Medtherm Corporation, email to author, January 27, 2012)

A cone shaped thermocouple holder was manufactured in order to hold the thermocouple while keeping the resin at the top of the thermocouple from exposure to high temperature. Furthermore, a very thin tube was used to try and keep the thermocouple rigid. A photo of the thermocouple with the cone shaped holder is shown in Figure 3-15a. The cone shaped thermocouple holder helped in the protection of the thermocouple resin, by keeping it from melting. In Figure 3-15b, a photo of a perfect very thin flat flame obtained at air mass flow rate of 0.22 g/s with an equivalence ratio of 0.60 with a thermocouple for measuring the flame temperature is shown. From this photo, it can be seen that thermocouple was very close to the flame, and visually no intrusion of thermocouple on the flame was observed. However, the thermocouple shook significantly when it was moved to downstream and it was not possible
to obtain a stable temperature reading. Therefore, the use of a more stiff and robust thermocouple holder was decided upon and consequently manufactured. A photo of the robust thermocouple holder is shown in Figure 3-16a. A vertical traverse was used to measure the flame temperature vertically. The precision of the vertical traverse is 0.1 mm. In order to keep the fine wire thermocouple safe, water cooling was installed at the top of the thermocouple, around the resin. A photo of the water cooling is shown in Figure 3-16c.

![Thermocouple with the cone shaped holder, thermocouple very close to the flame](image1)

**Figure 3-15** a) Thermocouple with the cone shaped holder, b) thermocouple very close to the flame

![Thermocouple with robust holder, vertical traverse, water cooling for fine wire thermocouples](image2)

**Figure 3-16** a) Thermocouple with robust holder, b) vertical traverse, c) water cooling for fine wire thermocouples

Calibration of the K type thermocouples was performed by using a reference thermometer, ISOTECH Jupiter 650B dry block high temperature calibrator. The accuracy of calibrator is ±0.3 °C. Calibration results and uncertainty calculations are shown in Appendix A5.
S type thermocouple was not able to be calibrated since the tip was very delicate. After communications with Dr. White from Measurement Standard Laboratory of New Zealand, we found that it is not possible to calibrate this very delicate thermocouple. Medtherm, which is the supplier of fine wire thermocouples, informed us that these fine wire thermocouples have an ANSI standard limits of error.

Temperature measurements error due to the radiation was calculated and the calculations are explained in Appendix A6.

3.11 Summary

In this chapter, the experimental set-up and specifications of the equipment were presented. The modifications and improvements of the test rig were explained.
4 EXPERIMENTAL RESULTS AND DISCUSSION

This chapter presents the results of the experimental work, performed on the test rig explained in the previous chapter, and discusses the findings in terms of developing a flat flame combustor for UMGT applications. The results include the pressure loss through the flame holders, the effect of preheating on the flame stability limit and the usability of different materials as flame holders for flat flame combustion. The effect of preheating the reactants on the flat flame formation are presented. Thus the relationship between the incoming flow velocity and burning velocity for obtaining flat flame combustion is shown. A new correlation for flat flame burners is proposed. The flame behaviour, exhaust emissions and combustion efficiencies with varying equivalence ratios are presented. Since the equivalence ratios were obtained from the exhaust emissions, the equivalence ratio calculation from the emissions are presented.

4.1 Pressure loss through flame holders

One of the requirements of micro combustors for UMGT application is to keep the pressure loss to a minimum. Ideally the combustor pressure loss should be less than 5% of the operating combustor pressure [24, 25, 31]. In flat flame combustors, most of the pressure loss occurs through the flame holder. Therefore, the structure of the flame holder such as the pore size and the thickness become very important in terms of pressure loss.

Since flame holders are used for flat flame combustion, and one of the conditions for flat flame combustion is that the incoming flow velocity be less than the burning velocity, the pressure loss values were therefore measured up to a maximum incoming velocity of 2 m/s. This value was calculated by taking into consideration the preheating of the reactants, since the burning velocity $S_L$ increases with the increase of the reactants temperature. In the present test, New Zealand natural gas was used as a fuel, the main constituent being methane. Therefore, the burning velocities of methane were considered in the calculations. The effect of the initial reactants temperature $T_u$ on burning velocity for methane/air flames at atmospheric pressure was calculated by equation (4-1) provided by Andrews and Bradley [102].

$$S_L = 10 + 0.0003717T_u^2 \quad 150K < T_u < 1000K$$ (4-1)

The frictional pressure loss through the quartz and stainless steel tubes at the top of the combustion chamber was calculated and found to be very small compared to the pressure loss values through the flame holders; therefore it was ignored in the measurements.
Pressure loss values plotted against incoming velocities up to 2 m/s are shown in Figure 4-1. In Figure 4-1, the thickness of the flame holders are shown as a suffix to the label of the materials. For example, t1 represents a thickness of 1 mm. Pressure loss values were very low through the perforated plate thus, their values are not shown in Figure 4-1.

As can be seen from Figure 4-1, both pore size and thickness have an effect on the pressure loss. Since the porosity percentage of the porous and sintered materials are very close to one another, approximately 43~54 %, the effect of porosity on the pressure loss was not taken into consideration. Pressure loss increases in a quadratic form of the incoming flow velocity. The quadratic form is consistent with the Forchheimer equation which is the most widely used relation for describing the pressure drop in porous media [110]. The Forchheimer equation is given by

\[ \frac{\Delta P}{L} = \frac{\mu}{K} V + \rho C V^2 \]  

where \( \Delta P \) is the pressure drop, \( L \) is the length of the porous medium in the flow direction, \( \mu \) is the fluid viscosity, \( \rho \) is the fluid viscosity, \( C \) is a form drag coefficient and \( K \) is the permeability.

![Figure 4-1 Pressure loss vs incoming velocity with different flame holders](image-url)
Maximum pressure loss occurs through the sintered stainless steel R100 flame holder with a thickness of 3 mm. On the other hand, the minimum pressure loss occurs through the alumina ceramic porous FA024 flame holder with a thickness of 2 mm. This result was expected since R100 has the minimum average pore size of 100 µm while FA024 has the maximum average pore size of 580 µm. When the flame holder gets thicker the pressure loss increases, this can be easily seen from Figure 4-1 with flame holders of FA060, FA024 and FA100. It can be also concluded from Figure 4-1 that, the pore size has an influential effect on the pressure loss, and this can be seen with flame holders having the same thickness. For example, although R200t3 and R100t3 have the same thicknesses, R100t3, with a pore size half that of R200t3, has pressure losses more than four times that of R200t3.

Plots of percentage of pressure loss to ambient pressure versus incoming flow velocity, with different flame holders, are shown in Figure 4-2. From this figure, it can be concluded that except for sintered stainless steel R100 and alumina ceramic porous F100 with flame holder thicknesses of 2 and 3 mm respectively, all others have a pressure loss of less than 5% throughout the whole range of incoming flow velocities. This indicates that they are suitable candidates as flame holders for a flat flame combustor. It should be noted that the measurements of pressure loss were performed for the non-reacting case and also at room temperature. Therefore, when the reactants are at room temperature, the burning velocity of methane-air mixture at atmospheric pressure is around 0.36 m/s, in which case all the flame holders that were tested satisfied the less than 5% pressure loss criteria. All the flame holders achieved pressure losses of less than 5% up to an incoming velocity of 1.2 m/s.

Based on the experimental results of Marbach and Agrawal [111], the pressure loss due to combustion is not included in the 5% pressure loss criteria. Marbach and Agrawal performed pressure drop measurements through different porous mediums for both surface combustion and interior combustion. They performed the experiments with both cold flow and combustion. With the flat flame combustion on the surface of the porous media, pressure loss increased very slightly (around 0.05%) compared to the pressure loss with cold flow. On the other hand, with interior combustion pressure loss increased more than a factor of 2. Since in this experimental study, only surface combustion occurs, the pressure loss due to combustion would be very low compared to the pressure loss through the flame holder, therefore it is neglected in the 5% pressure loss criteria.
It was observed that flat flame may be obtained on varying flame holders, but that the stability of the flame can change slightly with different flame holders.

The experiments were performed in the air mass flow rate range of 0.19 g/s to 0.94 g/s for equivalence ratios varying from 0.53 to 0.98. It was observed that thin, blue, flat flame combustion was not possible to be achieved in all the cases. The envelope of the flat flame combustion with different flame holders may be shown by the encircled blue line as presented in Figure 4-3. On this plot, the lowest equivalence ratio values represent the lean blow off limit and these values display slight differences with the use of different flame holders. It can be seen from this figure that flat flame combustion was obtained at low air mass flow rates, indicating low incoming flow velocities. Between the lean blow off limit and the bottom of the flat flame combustion envelope, the flames were not in a flat shape even though some part of the flames were settled down on the surface of the flame holder.

When the equivalence ratio was increased up to 0.80, the colour in the centre of the flame holder became red. At first it was assumed the combustion occurred inside the flame.
holder but reviews of the video footage of the experiments showed that although the flame holder colour had turned red, a blue flat flame, very close to the flame holder surface, was present. Furthermore, the measurement of the reactants temperature before passing through the flame holder showed that when the centre of the flame holder became red, the reactants temperature started to rise. This rise was sometimes very high. For instance, when the equivalence ratio was very close to stoichiometric, and with low mass flow rates, reactants temperatures of up to 490 K were measured. This may be explained by the effect of preheating the reactants via the flame holder. When the equivalence ratio increases, the heat release rate increases and the flame front moves closer to the flame holder. Then the temperature of the flame holder increases and the colour of the flame holder turns red at the centre since the heat loss at the centre is minimal. As the flame holder is at a high temperature when it is red, the heat transfer from the flame holder to the reactants is also much higher, and increases the temperature of the reactants significantly.

![Figure 4-3 Operating conditions for different flame holders showing the region in which flat flame combustion occurred](image)

When the equivalence ratio was increased, in addition to the flat flame, a red coloured cone shaped glow was also observed. The flame shape and behaviour at different equivalence ratios will be explained in detail in Section 4.6.
Because of the limitations of the measurement system, the minimum natural gas mass flow rate was 0.0088 g/s. Thus, at low air mass flow rates, it was not possible to perform the experiments at low equivalence ratios.

4.3 The usability of different plates as flame holders for flat flame combustion

A number of plates of different materials and structure were investigated for their usability as flame holder for flat flame combustion. These included alumina ceramic, sintered stainless steel, stainless steel perforated plates.

Alumina ceramic flame holders were unfortunately found to be very fragile and suffered from structural damage. After some time being exposed to the flame, and repeated heating and cooling, small cracks formed on the flame holder surface, resulting in uneven lifted conical flames on top of the cracks. At the design stage of the combustor, the possibility of such structural damage resulting from thermal effects was not taken into consideration. This was because of experience from a previous work with flame holders made from the same material FA060, which was used for tens of hours within the HEX-Combustor [46], with no noticeable crack being observed. The difference in performance might be explained by the size effect. The flame holder diameter of the HEX-Combustor was only 14 mm, whereas that of the present combustor is 46 mm. Larger temperature gradients may cause the cracks on the present larger sized flame holder.

Figure 4-4a shows a smooth very thin blue flat flame settled on top of the 2 mm thick FA060 flame holder at an air mass flow rate of 0.38 g/s and an equivalence ratio of 0.75. The red spots are the burning points of thin graphite sealant between the quartz tube wall and the flame holder. On the other hand, after the crack formed on the flame holder, a few uneven mm sized lifted conical flames were observed only where the crack occurred. In the remaining part of the flame holder, a smooth blue flat flame occurred, as can be seen from Figure 4-4b.

The same cracking problem was observed with all the alumina ceramic flame holders. It is thought that the thickness of the flame holders were very thin compared to its diameter. While not pursued in the present study, an optimization study of the thickness of alumina ceramics should be performed in order to enable the usage of alumina ceramics as a flame holder. It is also important to recall that increasing the thickness of the flame holder also
increases the pressure loss. Therefore, any optimization study should also take into account the pressure loss.

![Image of flat flame combustion](image)

**Figure 4-4 Blue flat flame combustion on the surface of FA060 alumina ceramic flame holder: air mass flow rate of 0.38 g/s, equivalence ratio of 0.75, a) before crack and b) after crack**

When the perforated plate was used as a flame holder, without an extension tube to the mixing chamber, it was possible to obtain flat flames over the whole surface of the flame holder, as illustrated in Figure 4-5. But, when the extension tube was installed to the mixing chamber in order to obtain a uniform premixture at higher mass flow rates, an acoustic interference was observed which made it very difficult to perform combustion tests. Therefore, the preliminary tests for the operating conditions of perforated plates were conducted utilizing the initial mixing chamber without an extension. The acoustic interference, which was observed with only a perforated flame holder, is an interesting topic to be elucidated in the future.

![Image of flat flame combustion](image)

**Figure 4-5 Flat flame combustion on the surface of perforated plate flame holder: air mass flow rate of 0.22 g/s, equivalence ratio of 0.66**

Figure 4-6 shows the effects of flame holder pore size on the flat flame. In this figure, the flame holders were made of sintered stainless steel. The average pore size of R100 and R200 flame holders are 100 µm and 200 µm, respectively. However, the average pore size of the flame holder SS filter is unknown. Looking at the appearance of the SS filter flame holder,
it can be inferred that the average pore size is similar to the R100. In Figure 4-6, the flat flames shown were obtained at an air mass flow rate of 0.22 g/s and an equivalence ratio of 0.66. As can be seen from Figure 4-6, smooth flat flames were observed on the surface of the three flame holders, although on the surface of R200 flame holder, the flat flame consisted of very tiny distinctive conical flames. This was thought to be due to the unevenness of the pore sizes. Similar smooth flat flames were observed on the surfaces of SS filter flame holder and R100 flame holder confirming that both flame holders have similar average pore sizes.

By increasing both the air and fuel flow rates, the distinctive conical flames became more definite, and more distinctive conical flames formed on the surface of R200 flame holder, this will be shown in Section 4.6.

![Tiny distinctive conical flames](image)

**Figure 4-6 Flat flame combustion on the surface of a) SS filter flame holder, b) R100 flame holder and c) R200 flame holder at an air mass flow rate of 0.22 g/s and Ø=0.66**

There are three main findings obtained from utilizing different flame holders. The first one is that the utilization of alumina ceramics as a flame holder is limited due to the crack formation. With smaller diameter combustors, alumina ceramics can be used as flame holder, however for larger combustors, a few mm thick alumina ceramic flame holder is not suitable. In order to prevent crack formation, the thickness should be increased. But this may result in high pressure loss through the flame holder. Thus, a thickness vs diameter optimization study with alumina ceramic may clarify this problem. The second finding is the acoustic interference associated with the use of a perforated plate. In the future, different hole configurations may help to solve this problem. For example, a hexagonal configuration of holes may be tried, thus conserving the uniformity of the flow. Finally, at high mass flow rates or incoming flow velocities, flat flame burning method is not convenient, because it requires a larger surface area. In applications such as UMGT, where size is very important, the flat flame burning method can be applied only at low mass flow rates.
4.4 The effects of preheating the reactants on the flame stability limit

The flame stability limit with R200 sintered stainless steel flame holder, using New Zealand natural gas when the reactants temperature was both at room temperature, and 600 K, is presented in Figure 4-7. This plot shows only the lean blow off limit and not the blue flat flame stability limit.

The flame stability limit measurements were performed between air mass flow rates of 0.38 g/s to 1.34 g/s. Figure 4-7 shows that when the reactants were at room temperature, blow off occurred at around an equivalence ratio of 0.53, while increasing the reactants temperature up to 600 K, this limit decreased to around an equivalence ratio of 0.40. These results show that preheating the reactants widened the flame stability limit.

Prior to flame blow off, as the fuel/air ratio was decreased, the flame gradually moved further from the flame holder surface, thus the reactants were not heated unless the heaters were on. On the other hand, when the fuel/air ratio increased, the flame formed very close to the flame holder, heating it, thereby heating the reactants and increasing their temperature. With the help of the heaters it was possible to keep the reactants temperature constant.

![Figure 4-7 Flame stability limit of natural gas-air mixture for reactants at room temperature and 600 K](image-url)
4.5 The effects of preheating the reactants on the flat flame stabilization

The effect of preheating the reactants on the stabilization mechanism of flat flame combustion is shown in Figures 4-8, 4-9 and 4-10. In these figures, the flame on the surface of sintered stainless steel R200 flame holder at an air mass flow rate of 0.38 g/s and equivalence ratios of 0.57, 0.62 and 0.68 are shown when the reactants temperature are at room temperature and 600 K.

In flat flames, the flame stabilizes on the flame holder surface because of the mechanism of preheating of the reactants from the flame. Therefore, even though an external heat source is not used to heat the reactants, the reactants are heated naturally from the flame holder which is heated from the flame. The preheating of reactants from the flame holder in this manner is described as “naturally heated” in this thesis. While the preheating of reactants by an external heater is stated as “heated”. When the heaters are used in order to increase the reactants temperature, the preheating from the flame still exists and the amount of heating depends on the air fuel ratio and closeness of the flame to the flame holder.

The flame shape with changing equivalence ratio will be presented in detail in the next section.

At an equivalence ratio of 0.57, there was a flickering, with a lifted flame a few centimetre from the flame holder surface, as shown in Figure 4-8a. It was unstable and consisted of many big conical shaped flames. Since the flame was lifted, there was no natural heating from flame to the reactants, the reactants were at room temperature. The unstable flame might show cellular flame characteristics since for methane cellular flame behaviour can occur at the very lean side of stoichiometric and close to the flammability limit [107]. However, the flame shape was different than the cellular flames obtained by Konnov and Dyakov [112] and Yu et al. [113] on the surface heat flux flat flame burner.

By keeping the air/fuel ratio constant and only heating the reactants up to 600 K, the flame started to settle down on the surface of the flame holder except around the boundary wall. At the quartz wall boundary, lifted conical flames of a few centimetre height were still observed due to the heat loss. On the other hand, a flame, settled down on the flame holder surface, consisting of a few millimetre lifted distinctive conical flames was observed, as shown in Figure 4-8b.
Keeping the air mass flow rate constant at 0.38 g/s, and increasing the equivalence ratio up to 0.62, the flames obtained at three different reactants temperatures are shown in Figure 4-9. Figure 4-9a shows the flame when the reactants were at room temperature which was photographed just after ignition. Compared to the flame at an equivalence ratio of 0.57, the flame had a bright blue colour and moved closer to the flame holder. However, the flame was still unstable and flickering. At this equivalence ratio, since the flame was close to the flame holder, natural heating of the reactants from the flame was observed. The reactants were naturally heated up to 343 K and the flame at this reactants temperature is shown in Figure 4-9b. With natural heating the bigger sized lifted conical flames started to settle down on the flame holder surface, apart from the quartz wall boundary. By keeping the air/fuel ratio constant and heating the reactants by external heaters up to 600 K, the flame settled down more on the surface of the flame holder and a flat flame, consisting of very tiny (approximately 2 mm in diameter) distinctive conical flames, was observed, as shown in Figure 4-9c. These distinctive conical shaped flames were only observed from the top view, from the side view it was not possible to see any height difference, and thus the flame appeared flat and very close to the surface of the flame holder. The distinctive tiny conical shapes may be due to the unevenness of the pore sizes. At the centre of the flame holder, a slightly reddish colour was observed, indicating that the flat flame was very close the flame holder, thereby heating the flame holder to a high temperature.
A similar preheating effect was also observed at an equivalence ratio of 0.68 and is shown in Figure 4-10. At this equivalence ratio, flames can be observed when the reactants were at room temperature in Figure 4-10a, when the reactants were naturally heated up to 360 K in Figure 4-10b, and finally when the reactants were heated by external heaters up to 600 K in Figure 4-10c. At an equivalence ratio of 0.68, the reactants were naturally heated up to 360 K and the flame completely settled down on the flame holder surface except for near the combustor wall, where a few mm high lifted, flickering conical flames were observed. By increasing the reactants temperature up to 600K, the distinctive conical flames reduced in size, and the flame moved closer to the flame holder increasing the flame holder temperature, which was observed from its very red colour, particularly at the centre.

![Figure 4-10 Flame photos at an air mass flow rate of 0.38 g/s and an equivalence ratio of 0.68 when the reactants are at a) room temperature, b) 360 K, and c) 600 K](image)

The effects of equivalence ratio on the stabilization of the flat flame can be seen in Figures 4-9b and 4-10b. In Figure 4-9b, the flame lifted a few centimetres when the equivalence ratio was 0.62. On the contrary, upon increasing the equivalence ratio up to 0.68, the flame settled a little bit more and lifted only a few mm with smaller conical flames compared to the flame obtained at an equivalence ratio of 0.62. Although increasing the equivalence ratio helps the stabilization of flat flame, the stabilization of flat flame combustion was also obtained by preheating the reactants. Particularly at the very lean side of the stoichiometric, which is the intended design point for ultra micro gas turbine applications, it is important to have stabilized flat flame combustion.

At higher mass flow rates, the effect of preheating on the flame stabilization was also investigated. However, at high mass flow rates, even though the flame settled down on the surface of the flame holder, no flat flame was observed. Instead, a few mm high lifted higher cone angled flames, like jet flames, were observed. Figure 4-11 shows the flame obtained at an air mass flow rate of 0.76 g/s and an equivalence ratio of 0.64 when the reactants were at room temperature (Figure 4-11a) and 600 K (Figure 4-11b). At this mass flow rate, the incoming
flow velocity becomes higher than the burning velocity. Thus, many conical flames form in order to balance the normal component of the incoming flow velocity with the burning velocity.

When preheating the reactants up to 600 K at an air mass flow rate of 0.76 g/s and an equivalence ratio of 0.64, a 100% increase in NO\textsubscript{X} formation was observed compared to the NO\textsubscript{X} formation obtained when the reactants were at room temperature. Therefore, it may be concluded that at high mass flow rates although preheating helps the flame stabilization, it causes an increase in NO\textsubscript{X} emissions. Thus, the flat flame burning method is not convenient for higher mass flow rates.

![Flame photos at an air mass flow rate of 0.76 g/s and an equivalence ratio of 0.64 when the reactants are at a) room temperature, b) 600 K](image)

Normally, the flame formed very close to the flame holder, thereby heating the flame holder and in turn the reactants. The room temperature measurements were done just after ignition, when the reactants were at room temperature. After waiting a long time (between 10 to 30 minutes depend on the equivalence ratio), the flame holder and the reactants reached a steady temperature, normally this was higher than the room temperature and depended mainly on the air to fuel ratio.

### 4.6 The flame behaviour with changing air to fuel ratio

The flame behaviour was investigated by both visualization of the flame and measurements of the major species concentrations.

The flame behaviour was obtained at varying equivalence ratios, at an air mass flow rate of 0.38 g/s. This mass flow rate was chosen because the preliminary flame tests showed that when the air mass flow rate increased beyond this, no flat flame occurred.

At an equivalence ratio of 0.51, there was no stable flame. The flame was flickering and flapping like a butterfly, after which the flame eventually blew out from the combustor. The reactants were around 303 K, showing that there was little natural heating from the flame.
As can be seen from the photo of the flame just before blow out in Figure 4-12a, the flame was weak with a very light blue colour. When the equivalence ratio was increased to 0.54, the flame was still unstable, flickered a lot and lifted approximately 3 to 4 cm above the flame holder, as shown in Figure 4-12b. Since the flame was far from the flame holder, the reactants were at room temperature. The flames at equivalence ratios of 0.57, 0.62 and 0.68 were discussed in the previous section, therefore they will not be repeated here again.

Figure 4-12 Flame photos at an air mass flow rate of 0.38 g/s and equivalence ratios of a) 0.51 and b) 0.54

When the equivalence ratio was increased to 0.75, a blue flat flame consisting of tiny distinctive conical flames was observed except at the quartz wall boundary. At the quartz wall, a few mm high lifted larger conical flames were present. The flame holder was slightly red indicating that the flame occurred very close to the flame holder. Due to this, the reactants were naturally heated up to 393 K. There were red spots on the flame holder surface and the graphite sealant, which can be seen Figure 4-13a. Further increasing the equivalence ratio up to 0.82, a blue flat flame sitting on a very red flame holder was observed, shown in Figure 4-13b. This shows that the flame holder temperature increased due to both the closeness of the flame to the flame holder and the high heat release because of the higher fuel flow rate. The reactants were naturally heated up to around 430 K.

Figure 4-13 Flame photos at an air mass flow rate of 0.38 g/s and equivalence ratios of a) 0.75 and b) 0.82
At an equivalence ratio of 0.88, in addition to the flat flame, a big cone shaped, slightly red glow started to form along the quartz wall, which can be seen in Figure 4-14a. The redness increases on the flame holder although blue flat flame can be seen on top of the flame holder in Figure 4-14b. The reactants were naturally heated up to around 460 K. Close to the quartz wall boundary, a blue flat flame could be seen as a blue ring from the top view, due to the heat loss to the wall. The flame holder close to the wall was not as red as at the centre, indicating higher temperatures at the centre of the flame holder. Similar to the flame obtained at an equivalence ratio of 0.88, at an equivalence ratio of 0.95, both flat flame and a cone shaped glow were observed, as can be seen in Figures 4-14c and 4-14d. As the equivalence ratio increased further, the glow became more distinctive and extended to the combustor exit. More orange spots formed on the flame holder surface and the graphite sealant indicating very high temperatures. The reactants were naturally heated up to 485 K.

Figure 4-14 Flame photos at an air mass flow rate of 0.38 g/s and equivalence ratios of a) 0.88 side view, b) 0.88 closer view from top, c) 0.95 side view, and d) 0.95 closer view from top

A cone shaped glow was observed on both the lean and rich side of stoichiometric. It started to form a slightly red colour, then increasing input energy with increasing equivalence ratio, its colour changed to a yellowish orange. Further increasing the equivalence ratio, the orange colour turned again to a red colour. The formation of the cone shaped glow with increasing equivalence ratio is shown in Figure 4-15. At equivalence ratios of 1.0 and 1.02, the flame holder had very bright colours and the cone shaped glows were very similar with a reddish orange colour. At an equivalence ratio of 1.06, the glow colour changed to yellowish orange colour and the glow had very distinctive borders. At an equivalence ratio of 1.08, an orange glow could still be seen but the brightness disappeared. Further increasing the equivalence ratio up to 1.14 and then to 1.20, slightly red coloured cone shaped glows were observed.
On the rich side of stoichiometric, the colour of the flat flame changed from blue to green. This can be easily seen from the flame photo obtained at an equivalence ratio of 1.32, (Figure 4-16). In Figure 4-16a, the flame shows that a pale red coloured cone shaped glow formed on top of a green flat flame consisting of very tiny distinctive conical flames. At the wall boundary a few mm high lifted conical flames were observed, as shown in Figure 4-16b. Except for the wall boundary, the flame was flat in spite of distinctive conical flames, which are thought to be a result of unevenness of the pore sizes. The flame holder had a slight red colour, indicating that the flame started to move downstream. Furthermore, the naturally heated reactants temperature also confirmed that the flame had moved downstream a little. The reactants were naturally heated up to 490 K at an equivalence ratio of 1.0, while at an equivalence ratio of 1.32, the reactants temperature decreased to 409 K.
Flame characteristics with changing equivalence ratios were also observed at an air mass flow rate of 0.31 g/s. The flame shapes and colours exhibited similar trends to those exhibited at an air mass flow rate of 0.38 g/s. At an equivalence ratio of 1.30, a totally green flat flame with tiny distinctive conical flames, was observed, similar to the flame which was obtained at an equivalence ratio of 1.32 and an air mass flow rate of 0.38 g/s. The green flat flame obtained with an air mass flow rate of 0.31 g/s is shown in Figure 4-17. The only difference found between the two air mass flow rates was that at lower mass flow rates, the reactants were more naturally heated. This shows that at low mass flow rates, the flame occurred closer to the flame holder compared to the flame formation at higher mass flow rates. Thus, the flame holder temperature rose and the reactants were in turn heated via heat transfer from the flame holder.

The change of flame colour from blue to green is due to the rich fuel/air ratio. The green coloured flame was only observed on the rich side of the stoichiometric. Gaydon stated that fuel rich hydrocarbon flames exhibit green colour [114].

From the flame behaviour exhibited with varying equivalence ratios, it can be understood that the flat flame burning method works very well at the design point of ultra micro gas turbine combustors, namely the lean side of the stoichiometric.
At high mass flow rates, when the incoming flow velocity is high, the flame may stabilize far from the flame holder and the shape of the flame is not flat anymore. At low mass flow rates, generally the flame occurs within a few millimetres from the flame holder. Although the main constituent of New Zealand natural gas is methane, some experiments were also conducted with 99.99% pure methane. The experiments were performed at an air mass flow rate of 0.38 g/s with varying fuel flow rates. Similar flame shapes and stabilization mechanisms were observed utilizing both methane and natural gas.

It was found that with increasing mass flow rate, the flame moved downstream, albeit not in the shape of a flat flame. Instead, many steep conical flames formed with small conical angles. The small conical angles indicating that the normal component of the incoming flow velocity tried to balance with the burning velocity. In these conical flames both the root and tip of the conical flame moved downstream.

Furthermore, numerical simulations of 2D methane-air flames also showed that when the reactants were at a low initial temperature, a conical shaped flame was observed, while increasing the initial temperature, led to a flat flame occurrence.

4.7 The relationship between burning velocity and the incoming flow velocity

In order to understand how preheating the reactants widens the flat flame stability limit, the relationship between the incoming flow velocity and burning velocities was examined.

The incoming flow velocities were calculated by dividing the mass flow rate of the fuel air mixture by the surface area of the flame holder and the density of the premixture at the preheated temperature (equation (4-8)).

The burning velocities were calculated using the correlations given by Stone et al. [115] and Liao et al. [116] for methane-air and natural gas-air, respectively. These correlations include the effects of preheating and the equivalence ratio on the burning velocities.

For methane-air and natural gas-air, the same correlation was used, however different power exponents, $\alpha$, reference temperatures and reference burning velocities were used.

The correlation showing the influence of reactants temperature on the burning velocity is
\[ S_L = S_{L,0} \left( \frac{T}{T_0} \right)^\alpha \]  

(4-3)

where \( T_0 \) and \( S_{L,0} \) are the reference temperature and the burning velocity at this temperature, respectively [104].

For methane-air, power exponent correlation of Stone et al. [115] was used in the calculations, and the reference temperature was 298 K. The reference burning velocities were also described by a quartic equation, dependent on the equivalence ratio, with five coefficients [115]:

\[ S_{L,0} = \left[ S_{L,1}(\phi - 1) + S_{L,2}(\phi - 1)^2 + S_{L,3}(\phi - 1)^3 + S_{L,4}(\phi - 1)^4 \right] \text{ (m/s)} \]  

(4-4)

where the coefficients are given in Table 4-1.

The power exponent correlation is given by

\[ \alpha = 1.42 - 1.98(\phi - 1) \]  

(4-5)

Table 4-1 Burning velocity coefficients of methane-air [115]

| \( S_{L,0} \) | 0.376 |
| \( S_{L,1} \) | 0.151 |
| \( S_{L,2} \) | -2.21 |
| \( S_{L,3} \) | -0.458 |
| \( S_{L,4} \) | 3.58 |

As can be understood from the previous section in which flame behaviours with changing equivalence ratio at an air mass flow rate of 0.38 g/s were summarised, flat flame burning occurred at an equivalence ratio of 0.75, while at an equivalence ratios of 0.62 and 0.68 when the reactants were at room temperature, no flat flame was observed. On the other hand, after naturally heating the reactants via the flame holder, the flame settled down on the surface of the flame holder. After further preheating by an external heater up to 600 K, flat flames were then observed at these compositions. Therefore, the incoming flow velocities and burning velocities were compared at these equivalence ratios.

At an equivalence ratio of 0.75, the reactants temperature was 393 K, and the incoming flow velocity was 0.27 m/s. The reference burning velocity at the reference temperature of 298 K was found to be equal to 0.22 m/s from equation (4-4). Using equation (4-5), the power
exponent was calculated as 1.915. Inserting this value and the reference values into equation (4-3), the burning velocity at an equivalence ratio of 0.75 was found to be 0.38 m/s. As can be seen from the calculated values, the burning velocity is higher than the incoming flow velocity, thus flat flame burning was observed at this equivalence ratio, as shown in Figure 4-13a.

At equivalence ratios of 0.62, and 0.68, the reference burning velocities were calculated as 0.10 m/s and 0.15 m/s at the reference temperature of 298 K, respectively. From equation (4-5), the power exponents were calculated as 2.1724 and 2.0536 for equivalence ratios of 0.62 and 0.68, respectively. At an equivalence ratio of 0.62, when the reactants were at room temperature, the incoming flow velocity was 0.20 m/s, while the burning velocity was 0.10 m/s. At an equivalence ratio of 0.68, when the reactants were at room temperature, the incoming flow velocity was 0.21 m/s and the burning velocity was calculated as 0.15 m/s using equation (4-3). At both equivalence ratios of 0.62 and 0.68, when the reactants were at room temperature, the incoming flow velocities were higher than the burning velocities. Thus, when the reactants were at room temperature, flat flame did not occur at these equivalence ratios, which can be seen in Figure 4-9a and Figure 4-10a.

The reactants were naturally heated up to 343 K and 360 K at equivalence ratios of 0.62, and 0.68, respectively. At an equivalence ratio of 0.62, the incoming flow velocity and burning velocity were calculated as 0.24 m/s and 0.14 m/s, respectively. While, at an equivalence ratio of 0.68, the incoming flow velocity and burning velocity were 0.25 m/s and 0.23 m/s, respectively. As can be seen from these results, at an equivalence ratio of 0.62 when the reactants were naturally heated, the incoming flow velocity was still much higher than the burning velocity, thus the flame was not flat flame. On the other hand, at an equivalence ratio of 0.68, when the reactants were naturally heated up to 360 K, the incoming flow velocity and burning velocity were very close to each other. Although a perfect flat flame was not observed, the flame was settled down on the surface of the flame holder.

Unfortunately, the correlation of Stone et al. was only established for a temperature range between 293 K and 454 K and an equivalence ratio range from 0.6 to 1.4. Therefore, it was not possible to compare the incoming flow velocities and burning velocities at 600 K. With preheating, the incoming flow velocity increases linearly with temperature, but the burning velocity increases exponentially. Thus, preheating the reactants increases the burning velocity more than the incoming flow velocity. Therefore, the burning velocity becomes higher than the incoming flow velocity, resulting in flat flame combustion. From this, it can be concluded that
at a reactants temperature of 600 K, at equivalence ratios of 0.62 and 0.68, the burning velocities became higher than the incoming flow velocities. As a result, flat flame occurred at these equivalence ratios when the reactants were heated up to 600 K, as shown in Figure 4-9c and Figure 4-10c.

A similar burning velocity calculation was performed by using the correlation given by Liao et al. [116] for natural gas-air. The correlation of Liao et al. was established for a narrow temperature range between 300 K and 400 K and an equivalence ratio range from 0.6 to 1.4. Liao et al. used the natural gas, which consists of 93.16 % volume fraction methane, 1.10 % ethane, approximately 0.20 % hydrocarbon components higher than C3, and the remains including carbon dioxide, nitrogen, sulfated hydrogen and water are only 2.56 % [116]. The correlation for the power exponent is given by equation (4-6).

\[
a = 7.98 - 12.15\phi + 5.75\phi^2
\]  
(4-6)

The reference burning velocity of natural gas-air at 300 K at different equivalence ratios can be calculated by using equation (4-7), which is also given in reference [116],

\[
S_{L0} = -177.43\phi^3 + 340.77\phi^2 - 123.66\phi - 0.2297
\]  
(4-7)

When the reactants were at room temperature, the burning velocities were calculated as 0.12 m/s and 0.17 m/s for equivalence ratios of 0.62 and 0.68, respectively. Using the correlation given by Liao et al., the calculated burning velocities increased a little, but were still lower than the incoming flow velocities at that temperature. At a reactants temperature of 343 K, the burning velocity was calculated as 0.17 m/s for an equivalence ratio of 0.62, which was still lower than the incoming flow velocity. At reactants temperature of 360 K, the burning velocity was calculated as 0.27 m/s for an equivalence ratio of 0.68, which was higher than the incoming flow velocity at that reactants temperature. From this, it may be concluded that the correlation of Stone et al. may be fit better for this experiment than the correlation of Liao et al., although correlation of Liao et al. is for natural gas-air flames. When the flame characteristics of both natural gas and methane are taken into account, no definite differences were observed, it may be assumed that the correlation for methane-air can also be used for natural gas-air.

Comparison of the incoming flow velocities and burning velocities against equivalence ratio are shown in Table 4-2.
It can be concluded from the experimental results that flat flame combustion occurs only when the burning velocity is higher than the incoming flow velocity. This will be provided by preheating the reactants at high mass flow rates, thus widening the flat flame stability limit.

### 4.8 The proposed correlation for flat flame burners

In the previous section, it was shown that in order to stabilize a flat flame on the surface of the flame holder, the incoming flow velocity should be lower than the burning velocity. It was also shown that it was possible to stabilize flat flame at higher mass flow rates by preheating the reactants. By taking into account these conclusions, the author proposes a correlation between air mass flow rate, equivalence ratio, initial temperature and burner diameter. With this correlation, it would be possible either to choose a burner diameter according to the power requirement, or to decide on the reactants temperature which will provide flat flame combustion within a known burner diameter. It would also be possible to ascertain how much the flat flame stability will be widened by increasing the reactants temperature.

This correlation is obtained from the relationship between the incoming flow velocity and the burning velocity.

The incoming flow velocity is dependent on mass flow rate, surface area of the flame holder, and density, and therefore the temperature of the reactants.

The incoming velocity can be described as follows

\[
    u_{in} = \frac{\dot{m}}{\rho_{mix}A}
\]  

(4-8)
where $\dot{m}$ is the sum of the fuel mass flow rate, $\dot{m}_f$, and the air mass flow rate, $\dot{m}_a$. $\rho_{mix}$ is the density of the fuel-air mixture, while $A$ is the surface area of the flame holder.

From the ideal gas equation, the density of mixture can be written as follows

$$\rho_{mix} = \frac{P}{R_{mix} T} \quad (4-9)$$

where $P$ is the pressure, $R_{mix}$ is the specific gas constant of the fuel-air mixture, and $T$ is the reactants temperature.

$R_{mix}$ can be calculated as follows

$$R_{mix} = m_{fuel} R_{fuel} + m_{air} R_{air} \quad (4-10)$$

where $m_i$ and $R_i$’s are the mass fractions and the specific gas constants, respectively.

The specific gas constant is described by

$$R_i = \frac{R_u}{M_i} \quad (4-11)$$

where $R_u$ is the universal gas constant, which is 8.314 kJ/(kmol.K) [117], and $M_i$ is the molecular mass.

The mass fractions of the fuel and air can be written as follows

$$m_{fuel} = \frac{m_{fuel}}{m_{fuel} + m_{air}} \quad m_{air} = \frac{m_{air}}{m_{fuel} + m_{air}} \quad (4-12)$$

where $m_{fuel}$ and $m_{air}$ are the masses of the fuel and air.

Since the equivalence ratio, $\phi$, defined as the ratio of the actual fuel/air ratio to the stoichiometric fuel/air ratio, mass of fuel can be written in terms of mass of air as follows

$$m_f = B \phi m_{air} \quad (4-13)$$

where $B = \left(\frac{m_{fuel}}{m_{air}}\right)_{stoichiometric} \quad (4-14)$

Inserting equations (4-11) to (4-14) into equation (4-10), specific gas constant of the fuel air mixture becomes
\[ R_{mix} = \frac{R_u}{B\varnothing + 1} \left[ \frac{M_{air} B\varnothing + M_{fuel}}{M_{air} M_{fuel}} \right] \]  

(4-15)

Inserting equation (4-15) into equation (4-9), and subsequently inserting equation (4-9) into equation (4-8), the incoming flow velocity can then be written as follows

\[ u_{in} = \frac{\dot{m}_{air}}{P \frac{d^2}{R_u T \pi} \left( \frac{d^2}{4} \right)} \left[ \frac{M_{air} B\varnothing + M_{fuel}}{M_{air} M_{fuel}} \right] \]  

(4-16)

where \( d \) is the diameter of the flame holder.

It can be seen from equation (4-16) that the incoming flow velocity is a function of \( \dot{m}_{air} \), \( d \), \( \varnothing \), and \( T \).

The condition for flat flame combustion can be written as follows

\[ u_{in} \leq S_L \]  

(4-17)

As shown in the previous section, burning velocity is a function of equivalence ratio and temperature. From the power exponent correlation of Stone et al., burning velocity can be written in terms of equivalence ratio and temperature as follows

\[ S_L = [0.376 + 0.151(\varnothing - 1) - 2.21(\varnothing - 1)^2 - 0.458(\varnothing - 1)^3 + 3.58(\varnothing - 1)^4] \left( \frac{T}{298} \right)^{1.42-1.98(\varnothing-1)} \]  

(4-18)

Inserting equations (4-16) and (4-18) into equation (4-17), the proposed new correlation between the air mass flow rate, burner diameter, equivalence ratio and reactants temperature can be found as follows

\[ \frac{\dot{m}_{air}}{P \frac{d^2}{R_u T \pi} \left( \frac{d^2}{4} \right)} \left[ \frac{M_{air} B\varnothing + M_{fuel}}{M_{air} M_{fuel}} \right] \leq [0.376 + 0.151(\varnothing - 1) - 2.21(\varnothing - 1)^2 - 0.458(\varnothing - 1)^3 + 3.58(\varnothing - 1)^4] \left( \frac{T}{298} \right)^{1.42-1.98(\varnothing-1)} \]  

(4-19)

This correlation allows calculation of change in mass flow rate with changing reactants temperature. For example, as explained in Section 4.5, at an equivalence ratio of 0.68 and an air mass flow rate of 0.38, flat flame stabilization was observed by heating up to 600 K. With
the proposed correlation, it is possible to find the required reactants temperature in order to obtain flat flame combustion. By applying equation (4-19), at an air mass flow rate of 0.38 g/s and an equivalence ratio of 0.68, on the surface of 46 mm diameter flame holder, a reactants temperature of 393 K is sufficient to stabilize a flat flame.

Furthermore, this correlation shows how preheating widens the flame stability at constant equivalence ratio. For example, at an equivalence ratio of 0.68, by preheating from 298 K to 448 K, this correlation calculates the air mass flow rates, at which flat flame combustion can occur. At room temperature, the air mass flow rate is found as 0.28 g/s, which provides flat flame combustion, but preheating up to 448 K, the air mass flow rate increases to 0.44 g/s, as shown in Figure 4-18.

![Figure 4-18 At an Ø=0.68, air mass flow rates with increasing reactants temperature, when d=46 mm and \( u_{in}=S_L \)](image)

Rearranging equation (4-19), the minimum diameter of the burner required for flat flame combustion can be described in terms of air mass flow rate, equivalence ratio and reactants temperature, as shown in equation (4-20).
On the right side of equation (4-19), the author applied burning velocity equation of Stone et al., since the equation of Stone et al. is valid for a wide range of equivalence ratios, $\varnothing=0.6-1.4$, it is also in good agreement with the present experimental results. Therefore, the application of the equation of Stone et al. on the burning velocity was considered appropriate in the proposed correlation.

4.9 Exhaust emissions

4.9.1 CO$_2$, O$_2$ and CO emissions

For UMGT applications, the main focus is only on the lean side of the stoichiometric fuel/air ratio. However, in this study, in order to obtain the equivalence ratio, exhaust emissions were collected both on the lean and rich side of the stoichiometric fuel/air ratios. Figure 4-19 presents the exhaust gas composition data in mole fractions as a function of fuel/air equivalence ratio at an air mass flow rate of 0.38 g/s. The emission data gathered by CO$_2$, CO and O$_2$ analyzers were on a dry basis. As can be easily seen from Figure 4-19, at the lean side of the stoichiometric, as the equivalence ratio decreased, O$_2$ concentrations increased and reached up to a value of 10.83 % mole fraction at an equivalence ratio of 0.51. On the contrary, CO$_2$ concentrations decreased, and a mole fraction of 6.1 % was measured at an equivalence ratio of 0.51. The maximum CO$_2$ concentration, which was 12.25 % mole fraction, was collected at an equivalence ratio of 1.01. At the lean side of the stoichiometric, at all equivalence ratios, CO concentrations were zero. On the other hand, on the rich side of the stoichiometric, as the equivalence ratio increased, CO concentrations rose steadily, CO$_2$ concentrations dropped, and O$_2$ concentrations were very low and close to zero. CO concentrations increased up to a mole fraction value of 7.71 % at an equivalence ratio of 1.32, and at the same equivalence ratio, CO$_2$ concentrations decreased to a value of 7.61 % mole fraction. From the CO concentrations, it may be concluded that flat flame combustion provides a clean method of burning.
Heywood [118] stated that the CO2 concentration values at a given equivalence ratio are affected by the fuel H/C ratio. He also commented that at stoichiometric mixtures, typically there is 0.5 percent O2 and 0.75 percent CO present. Although the percentages of O2 and CO do not change at stoichiometric mixtures with different H/C ratios, CO2 concentration increases as the H/C decreases. For isoctane (H/C=2.25) CO2 concentration is 13.7 percent at stoichiometric, as the H/C ratio decreases to 2-1.8 for typical gasoline, CO2 concentration increases to 14.2 percent. As the H/C ratio decreases further to 1.14 for toluene, CO2 concentration increases to 16. From this, it can be concluded that for New Zealand natural gas whose H/C ratio is 3.5, CO2 concentration is less than 13 percent and the experimental results of CO2 concentration of 12.25 percent is in agreement with this statement.

Exhaust emissions were also collected at an air mass flow rate of 0.31 g/s. As can be seen from Figure 4-20, similar trends and values were obtained for all CO, O2 and CO emissions at the two different mass flow rates.
Although the main constituent of New Zealand natural gas is methane, the natural H/C is less than the methane H/C ratio which is 4. Therefore, in order to understand the effect of utilizing pure methane as a fuel, emissions of methane air flames were examined at an air mass flow rate of 0.38 g/s at varying equivalence ratios. The emissions profiles are shown in Figure 4-21. Similar to the natural gas emissions data, when methane was used as a fuel, at the lean side of the stoichiometric, as the equivalence ratio decreased, O\(_2\) concentrations increased and CO\(_2\) concentrations decreased, whilst CO concentrations were zero. On the other hand, on the rich side of the stoichiometric, as the equivalence ratio increased, CO concentrations rose steadily, CO\(_2\) concentrations dropped, and O\(_2\) concentrations were very low and close to zero.

In addition, a comparison of CO\(_2\), O\(_2\) and CO profiles obtained at the same air flow rates utilizing methane and natural gas as fuels was carried out and the results are presented in Figure 4-22. As can be seen from Figure 4-22, O\(_2\) and CO values are consistent for the two different fuels but CO\(_2\) values were lower at the same air to fuel ratios when methane was used as a fuel. This result is in good agreement with Heywood’s statement which was explained at the beginning of this section. Due to an increase in the H/C ratio, maximum CO\(_2\) concentration value decreased to a value of 11.2 % mole fraction.
Figure 4.21 CO\textsubscript{2}, O\textsubscript{2} and CO emissions of methane at an air mass flow rate of 0.38 g/s with varying equivalence ratio

Figure 4.22 Comparison of CO\textsubscript{2}, O\textsubscript{2} and CO emissions of methane and natural gas at an air mass flow rate 0.38 g/s with varying equivalence ratios
4.9.2 NO\textsubscript{X} emission

Nitrogen oxides (NO\textsubscript{X}), CO and unburned hydrocarbon (UHC) are the main sources of pollution from combustion. Therefore, the measurement of emissions becomes important. According to the author’s knowledge, no information on CO and NO\textsubscript{X} emissions have been presented for the preliminary UMGT combustors (MIT’s combustors [6, 18, 19, 30, 31, 119] and ONERA’s micro combustors [12]). Therefore, it is not possible to compare the emissions from the combustors for UMGT applications.

The NO\textsubscript{X} emissions at an air mass flow rate of 0.38 g/s over a range of equivalence ratio is presented in Figure 4-23. NO\textsubscript{X} emissions increased with increasing equivalence ratio on the lean side of stoichiometric and reached its maximum value at stoichiometric, which was 26 ppm. Further increasing the equivalence ratio on the rich side of stoichiometric, NO\textsubscript{X} emissions gradually decreased. This is in agreement with El-Sherif who performed a study with Egyptian natural-gas air flames on the surface of a water cooled flat flame burner [120]. El-Sherif showed that NO\textsubscript{X} emissions increased with an increase in equivalence ratio and reached its maximum value at stoichiometric, which was 21 ppm, and decreased in rich flames.

![Figure 4-23](image) Effect of equivalence ratio on NO\textsubscript{X} emissions of natural gas at an air mass flow rate of 0.38 g/s

Figure 4-24 shows the effect of mass flow rate on NO\textsubscript{X} emissions. While keeping the equivalence ratio constant at stoichiometric, the air mass flow rate was gradually increased. NO\textsubscript{X} emissions increased approximately four fold with a corresponding twofold increase in the
air mass flow rate. When the mass flow rate increases, heat release also increases, resulting in a higher flame temperature. Therefore, NO\textsubscript{X} emissions increase with higher mass flow rates. An experimental study of Marbach et al. with methane-air flame, stabilized on the surface of porous inert media made of silicon-carbide coated carbon foam, also observed that increasing the air mass flow rate, thus the incoming flow velocity, resulted in increase in both CO and NO\textsubscript{X} emissions [27]. Although they only performed the experiments up to an equivalence ratio of 0.8, it was easy to observe the increase in NO\textsubscript{X} emissions with an increase in air mass flow rates. Although CO emissions also increased with increasing mass flow rate in their study, in this current study CO emissions did not change with increasing mass flow rate, as shown in Figure 4-20.

![Figure 4-24 Effect of mass flow rate on NO\textsubscript{X} emissions at stoichiometric natural gas-air flame](image)

Although NO\textsubscript{X} emissions increased with increasing air mass flow rate, the recorded reactants temperature, which was collected at a fixed location just before passing the flame holder, showed that the reactants temperature decreased. This does not mean that the flame temperature decreases with increasing mass flow rate. It implies that the flame moves downstream, thereby reducing the preheating of the reactants from the flame. At a higher air mass flow rate of 0.76 g/s, the reactants were naturally heated approximately up to 100 °C. On the other hand, at a lower air mass flow rate of 0.38 g/s, the reactants were naturally heated (from the flame) to more than 200 °C at stoichiometric as confirmed by the flame visualization in Figure 4-15a. At an air mass flow rate of 0.76 g/s lifted steeply pitched conical flames were observed instead of flat flames. The measured reactant temperatures at stoichiometric natural-gas air flames with different air mass flow rates are shown in Figure 4-25.
One of the main focuses of this study is on the flame characteristics at a constant equivalence ratio of 0.68, because at this equivalence ratio, it was possible to observe the preheating effect on the stabilization of flat flame. Therefore, at an equivalence ratio of 0.68, NO\textsubscript{X} emissions were also measured with increasing air mass flow rates. At this equivalence ratio, it was found that NO\textsubscript{X} emissions from naturally heated natural-gas air flames obtained from three different mass flow rates were very low. In particular, these were around 4 ppm and 6 ppm at air mass flow rates of 0.38 g/s and 0.76 g/s, respectively. On the other hand, preheating the reactants up to 600 K with an external heater, the NO\textsubscript{X} emissions increased dramatically. However, the maximum reading was still less than 20 ppm.
Newburn and Agrawal [121] experimentally showed that preheating the reactants has no effect on CO emissions at the same equivalence ratio, however NO$_X$ emissions increase with heating the reactants due to a rise in the flame temperature. They reported that at an equivalence ratio of 0.57 which was the highest equivalence ratio that was studied, a maximum of 17 ppm NO$_X$ emission was recorded without heating, while a maximum NO$_X$ emission of 50 ppm was observed with heated reactants.

A similar trend with varying equivalence ratios was also observed in NO$_X$ emissions in the present study when utilising methane as a fuel. Maximum NO$_X$ concentrations of 21 ppm were recorded at stoichiometric. NO$_X$ concentrations increased with increasing equivalence ratio on the lean side of stoichiometric. On the other hand, on the rich side of stoichiometric, NO$_X$ concentrations decreased with increasing equivalence ratio.

![Figure 4-27](image_url)

**Figure 4-27** Effect of equivalence ratio on NO$_X$ emissions of methane at air mass flow rate of 0.38 g/s

A comparison of NO$_X$ profiles, obtained at the same air mass flow rates using methane and natural gas as fuels, is shown in Figure 4-28. Although both fuels exhibit similar trends, with utilising natural gas, NO$_X$ emissions were higher than those when methane was used as a fuel. The differences between two profiles increase with increasing equivalence ratio.
Figure 4-28 Comparison of NO\textsubscript{X} emission of methane and natural gas at an air mass flow rate of 0.38 g/s with varying equivalence ratios

Since this flat flame combustor is designed for lean combustion, from the experimental results it can be concluded that flat flame burning method provides very clean combustion.

4.9.3 Unburned hydrocarbon emissions

Unburned hydrocarbon emissions were collected at an air mass flow rate of 0.38 g/s at varying equivalence ratios utilizing natural gas and methane as fuels. Figure 4-29 shows the unburned hydrocarbon emissions from both natural gas air flames and methane air flames. As can be seen from this figure, unburned hydrocarbon emissions were very low and within the inherent noise level of the gas analyser. This shows that complete combustion occurred within the 46 mm diameter quartz walled flat flame combustor, utilizing both fuels.

Figure 4-29 Unburned hydrocarbon (UHC) emissions of methane at an air mass flow rate of 0.38 g/s
4.10 Equivalence ratio calculation from exhaust gas constituents

Equivalence ratio was calculated from combustor exhaust gas composition, which was determined by analysing dry samples for CO$_2$, CO, O$_2$ and NO$_X$ and wet samples for unburned hydrocarbon.

The overall combustion reaction can be written as follows

\[ C_{n}H_{m}O_{r} + \frac{n_{O_{2}}}{\theta} (O_{2} + 3.76N_{2}) = n_{p}(\tilde{x}_{C_{n}H_{b}}C_{a}H_{b} + \tilde{x}_{CO}CO + \tilde{x}_{CO_{2}}CO_{2} + \tilde{x}_{O_{2}}O_{2} + \tilde{x}_{N_{2}}N_{2} + \tilde{x}_{NO}NO + \tilde{x}_{NO_{2}}NO_{2} + \tilde{x}_{H_{2}O}H_{2}O + \tilde{x}_{H_{2}H_{2}}H_{2}) \]  \hspace{1cm} (4-21)

where \( \theta \) is the equivalence ratio calculated from the exhaust gas constituents, \( n_{O_{2}} \) is the number of O$_2$ molecules required for complete combustion, \( n_{p} \) is the total number of moles of exhaust products and \( \tilde{x}_{i} \) is the mole fraction of the \( i \)th component.

The equivalence ratio from the combustor exhaust gas composition was calculated by using the equations below provided by Heywood [118] for wet hydrocarbon and dry CO$_2$, O$_2$, CO and NO$_X$ for fuel composition of C$_n$H$_m$O$_r$.

\[ \theta = \frac{2n_{O_{2}}}{n_{p}\tilde{x}_{H_{2}O} + n_{p}(1 - \tilde{x}_{H_{2}O})(\tilde{x}_{CO}^{*} + 2\tilde{x}_{CO_{2}}^{*} + 2\tilde{x}_{O_{2}}^{*} + \tilde{x}_{NO}^{*}) - r} \]  \hspace{1cm} (4-22)

where the wet and dry mole fractions are related by

\[ \tilde{x}_{i} = (1 - \tilde{x}_{H_{2}O})\tilde{x}_{i}^{*} \]  \hspace{1cm} (4-23)

\( \tilde{x}_{i} \) and \( \tilde{x}_{i}^{*} \) denote the wet and dry mole fraction of species \( i \), respectively.

Using the atomic balance for each element the following equations are obtained.

From carbon balance:

\[ n_{p} = \frac{n}{\tilde{x}_{CH_{b/a}} + (1 - \tilde{x}_{H_{2}O})(\tilde{x}_{CO}^{*} + \tilde{x}_{CO_{2}}^{*})} \]  \hspace{1cm} (4-24)

From hydrogen balance and the relationship between CO$_2$, CO, H$_2$O and H$_2$ concentrations:
\( \dot{x}_{H_2O} = \frac{m}{2n} \left[ \frac{\dot{x}_{CO}^* + \dot{x}_{CO_2}^*}{1 + \dot{x}_{CO}^*/(K\dot{x}_{CO_2}^*) + (m/2n)(\dot{x}_{CO}^* + \dot{x}_{CO_2}^*)} \right] \)  

(4-25)

\[ \dot{x}_{H_2} = \frac{\dot{x}_{H_2O}\dot{x}_{CO_2}^*}{K\dot{x}_{CO_2}^*} \]  

(4-26)

From nitrogen balance:

\[ \dot{x}_{N_2} = \frac{3.76n_{O_2}}{\phi n_p} - \left(1 - \dot{x}_{H_2O}\right) \frac{\left(\dot{x}_{NO}^* + \dot{x}_{NO_2}^*\right)}{2} \]  

(4-27)

where \( \dot{x}_{CH_{b/a}} = a\dot{x}_{c_aH_b} \)

In the analyzer propane is used, therefore, in the calculations \( a \) is set to 3 and \( b \) is set to 8.

As shown in Chapter 3, New Zealand natural gas can be written as \( C_{1.18}H_{4.12}O_{0.11} \). Inserting these values to the above equation and ignoring \( NO_2 \) concentration, since Heywood commented that \( NO_X \) is mainly nitric oxide (NO), the above equation becomes

\[ C_{1.18}H_{4.12}O_{0.11} + \frac{2.15}{\phi} \left( O_2 + 3.76N_2 \right) \]  

\[ = n_p \left( \dot{x}_{C_3H_8}C_3H_8 + \dot{x}_{CO}CO + \dot{x}_{C O_2}CO_2 + \dot{x}_{O_2}O_2 + \dot{x}_{N_2}N_2 + \dot{x}_{NO}NO + \dot{x}_{H_2O}H_2O + \dot{x}_{H_2}H_2 \right) \]

(4-28)

There are five unknowns. These are the equivalence ratio (\( \phi \)), total number of moles of exhaust products (\( n_p \)) and the mole fractions of \( N_2 \), \( H_2 \) and \( H_2O \). However, there are four atomic balances and they are inadequate to solve for the five unknowns. This problem is solved by using the water gas constant of \( K \). Heywood suggested using 3.5 as a water gas constant, thus a value of 3.5 is used for \( K \) in solving the above equations. Since the water-gas constant depends on temperature, the effect of changing the value of \( K \) on the calculated equivalence ratio was investigated. At the lean side of stoichiometric, changing the water gas constant did not affect the equivalence ratio. Heywood also mentioned that for lean mixtures, changing the \( K \) value has a negligible effect on the value of equivalence ratio.

Although the main focus of this study is on the lean side of the stoichiometric, in order to find the equivalence ratio, experiments were performed over a wide range of fuel flow rates
including both the lean and rich sides of stoichiometric. The calculated equivalence ratio against the set fuel flow rates are shown in Figure 4-30.

![Equivalence Ratio vs Set Fuel Flow Rate](image1.png)

**Figure 4-30 Equivalence ratio from the exhaust gas emissions versus set fuel flow rate**

A comparison of equivalence ratios calculated from exhaust gas constituents and also calculated from the mass flow meter readings is presented in Figure 4-31. As can be seen from this figure, equivalence ratios calculated from the mass flow meter readings are within normal engineering tolerances. The maximum discrepancy between the equivalence ratios calculated with the two different methods was found as ±5%.

![Comparison of Equivalence Ratios](image2.png)

**Figure 4-31 Comparison of equivalence ratios calculated from exhaust gas constituents and mass flow meter readings**
4.11 Combustion efficiency

The combustion efficiency using New Zealand natural gas as a fuel was calculated using the equation

\[
\eta_{comb} = \left[ 1 - \left( \frac{m_f + m_{air}}{m_f} \right) \left( \frac{\bar{x}_{CO} Q_{HV,CO} M_{CO} + \bar{x}_{UHC} Q_{HV,UHC} M_{UHC} + \bar{x}_{H_2} Q_{HV,H_2} M_{H_2}}{Q_{HV,f} M_b} \right) \right] \times 100 \tag{4-29}
\]

where \(\bar{x}_i\) is the mole fraction of CO, unburned hydrocarbon and H\(_2\). The \(Q_{HV,i}\) are the lower heating values of these species, while the \(M_i\) are the molecular mass. The subscripts f and a denote fuel and air, while b indicates burned gas.

For New Zealand natural gas, the combustion reaction is as follows

\[
C_{1.18}H_{4.12}O_{0.11} + \frac{2.15}{\emptyset} (O_2 + 3.76N_2)
\]

\[
= n_p (\bar{x}_{C_3H_8} C_3H_8 + \bar{x}_{CO} CO + \bar{x}_{CO_2} CO_2 + \bar{x}_{O_2} O_2 + \bar{x}_{N_2} N_2 + \bar{x}_{NO} NO + \bar{x}_{H_2O} H_2O + \bar{x}_{H_2} H_2) \tag{4-30}
\]

Molecular mass of the burned gas was calculated as follows

\[
M_b = \frac{\bar{x}_{C_3H_8} M_{C_3H_8} + \bar{x}_{CO} M_{CO} + \bar{x}_{CO_2} M_{CO_2} + \bar{x}_{O_2} M_{O_2} + \bar{x}_{N_2} M_{N_2} + \bar{x}_{NO} M_{NO} + \bar{x}_{H_2O} M_{H_2O} + \bar{x}_{H_2} M_{H_2}}{\bar{x}_{C_3H_8} + \bar{x}_{CO} + \bar{x}_{CO_2} + \bar{x}_{O_2} + \bar{x}_{N_2} + \bar{x}_{NO} + \bar{x}_{H_2O} + \bar{x}_{H_2}} \tag{4-31}
\]

Heating values of 10.11 MJ/kg for CO, 120 MJ/kg for H\(_2\), and 42.87 MJ/kg for both unburned hydrocarbon and fuel were used in the calculations [118] (the heating value of natural gas was calculated from the compositions, as shown in Appendix A1).

Combustion efficiency of the 46 mm diameter quartz walled flat flame combustor utilizing New Zealand natural gas at an air mass flow rate of 0.38 g/s is presented in Figure 4-32. As can be seen from Figure 4-32, at the lean side of the stoichiometric more than 99% combustion efficiency was achieved at all equivalence ratios. This shows almost complete combustion occurred at this region. On the other hand, increasing the equivalence ratio on the rich side of the stoichiometric, combustion efficiency decreased substantially. At an equivalence ratio of 1.32, combustion efficiency decreased to a value of 60%. Since the main focus of this study is combustion on the lean side of stoichiometric, which is shown in Figure
4-32 by the encircled area, it can be concluded that complete combustion occurs on the surface of sintered stainless steel flame holder at an air mass flow rate of 0.38 g/s. This shows that the small scale flat flame combustor works efficiently.

![Figure 4-32 Combustion efficiency of natural gas-air flames at an air mass flow rate of 0.38 g/s](image)

The same equation was used to calculate the combustion efficiency of methane combustion and a heating value of 50.02 MJ/kg was used for both unburned hydrocarbon and methane.

For methane, the combustion equation is as follows:

\[
CH_4 + \frac{2}{\varphi} (O_2 + 3.76N_2)
\]

\[
= n_p(\tilde{x}_{C_3H_8}C_3H_8 + \tilde{x}_{CO}CO + \tilde{x}_{CO_2}CO_2 + \tilde{x}_{O_2}O_2 + \tilde{x}_{N_2}N_2 + \tilde{x}_{NO}NO + \tilde{x}_{H_2O}H_2O + \tilde{x}_{H_2}H_2)
\]

(4-32)

Combustion efficiency of the combustor using methane as a fuel at an air mass flow rate of 0.38 g/s is shown in Figure 4-33. Similar to the combustion efficiency obtained using natural gas, almost complete combustion was achieved at the lean side of the stoichiometric. On the rich side of the stoichiometric, with increasing equivalence ratio, combustion efficiency dropped significantly. At an equivalence ratio of 1.31, a combustion efficiency of 72.7% was obtained. Taking into consideration the utilization of this combustor on the lean side of the stoichiometric, complete combustion was achieved for both fuels.
4.12 Flame temperature

Flame temperature becomes important when considering the combustor material selection and turbine inlet temperature, which mainly depends on the flame temperature. For UMGТ applications, turbine inlet temperature is generally considered as either 1200 K [8, 33] or 1600 K [30]. Therefore, in order to get an idea of the combustor exit temperature with this configuration (which means including flame holders which allow heat recirculation between the flame and the reactants), the flame temperature measurements were conducted.

One of the main objectives of this study is to widen the flat flame stabilization by preheating the reactants. Therefore, the flame temperature was measured at an equivalence ratio of 0.68 and an air mass flow rate of 0.38 g/s, at which the transition from many unstable conical flames to a single stabilized flat flame occurred by preheating. Flame temperature was measured when the reactants were naturally heated from the flame itself.

The flame temperature was measured with three different thermocouples. The thermocouple specifications were given in Chapter 3, therefore the details will not be repeated here. The maximum flame temperature was measured as 1253 K with the 0.5 mm K type thermocouple, while with the 0.25 mm K type thermocouple the recorded maximum flame temperature was 1335 K. The highest maximum flame temperature was recorded with S type fine wire thermocouple, which was 1529 K. The radiation correction for these three thermocouples was 7 K, 35 K and 54 K for S type and 0.25 mm diameter K type and 0.5 mm
diameter K type thermocouples, respectively. The recording of different flame temperatures with different thermocouples at the same flame conditions may be explained by the conduction effect. Although radiation loss increases with the larger thermocouples, conduction loss becomes higher than radiation loss. Thus, with larger thermocouples, the measured temperature was lower. Also larger diameter thermocouples interfere with the thin flat flame formation.

At an equivalence ratio of 0.68 and an initial reactant temperature of 360 K, the adiabatic flame temperature for methane-air flame is found as 1849 K by CEA2. The recorded flame temperatures were lower than the adiabatic flame temperature due to the heat loss to the flame holder.

![Figure 4-34 Flame temperature at an air mass flow rate of 0.38 g/s and an equivalence ratio of 0.68](image)

**Figure 4-34** Flame temperature at an air mass flow rate of 0.38 g/s and an equivalence ratio of 0.68

### 4.13 Summary

In this chapter, the experimental results obtained with the 46 mm diameter quartz-walled flat flame combustor were presented. Alumina ceramic porous plates, sintered stainless steel, stainless steel filter and perforated plates were used as flame holders for flat flame combustion. Furthermore, their usage as a flame holder candidate was observed in terms of pressure loss through them and flame stabilization. With preheating, the obtaining of flat flame stabilization at varying equivalence ratios were presented. It was shown that flat flames can occur when the incoming flow velocity is lower than the burning velocity. From this relationship, a new correlation between mass flow rate, reactant temperature, air to fuel ratio and the diameter of the micro combustor was developed and proposed. The flame behaviour at
an air mass flow rate of 0.38 g/s with varying equivalence ratios were presented. Exhaust emissions using natural gas and methane were presented and it was found that 46 mm diameter flat flame combustor provides very clean combustion with a combustion efficiency of 99%. Flame temperature measurements showed that the flame occurs very close to the flame holder and the maximum flame temperature is lower than the adiabatic flame temperature.
5 NUMERICAL STUDY

5.1 Introduction and literature review on numerical micro combustion research

In this part, the effects of preheating the reactants on the combustion characteristics and flame stability limit of a 2 mm diameter micro combustor tube are presented.

One-dimensional premixed methane-air flames have been widely investigated numerically since the beginning of the 1980s. However, when combustor size is of significance, two-dimensional modelling of micro combustion has gained importance. Research on the two-dimensional numerical simulation of micro combustion has emerged with the increasing interest in combustion-based micro power generators. Due to its less complex reaction mechanisms when compared to hydrocarbon reaction mechanisms, pioneering two-dimensional micro combustion studies were performed on hydrogen micro combustion [122-124]. There are very few studies performed with two-dimensional numerical modelling of premixed methane-air flames at micro scale [89, 90].

1D simulations of methane-air flame have been widely investigated and validated with experimental data. However, 2D simulations, especially at micro scale, is a new developing area. 2D simulations at micro scale found in the literature used the commercial Computational Fluid Dynamics (CFD) software package ANSYS Fluent. Since it is a new area and has been investigated only in the last decade, this study mainly looked at these previous studies on micro combustion in 2D using ANSYS Fluent and the shortcomings of them. Therefore, before showing the effect of preheating the reactants at micro scale, a background of the previous 2D micro combustion studies are introduced in addition to the presentation of the validation of the new model by a comparison with the available experimental data.

Generally in micro combustors, the flame stability limit has a U shape in terms of mass flow rate (or incoming flow velocity) versus equivalence ratio [125]. At low mass flow rates, heat loss is higher than the heat release rate causing flame extinction. On the other hand, at high mass flow rates, the incoming flow velocity becomes higher than the burning velocity, which in turn results in blow out.

Particularly at higher mass flow rates (or higher incoming flow velocities), increasing the reactant temperature raises the burning velocity and prevents blow out, thus widening the flame stability limit, as shown with the present experimental results in the previous chapter.
Lee et al. [126] showed experimentally the effect of increasing the reactant temperature up to 500 K on the flame stability of micro flames on a micro tube. Li et al. [127] numerically investigated the effect of elevated temperatures up to 500 K on the stability of flames from hydrogen-air, methane-air and propane-air mixtures with a 1D model. It was found that when the reactants temperature increases, the heat loss ratio (defined as the ratio of heat loss from the flame to the heat generation in the reaction zone) drops substantially for these three different fuel-air mixtures. However they neither reported on the species concentrations nor studied the effects of incoming flow velocity. The study focused mainly on heat loss ratio and heat recirculation ratio.

The difficulty of performing experiments at very small scales makes numerical simulation an essential part of micro combustion research. The numerical approach has been widely employed, particularly in micro combustors whose size is less than the quenching distance, which is a few millimetres for hydrocarbon fuels and even smaller for hydrogen.

Verstraete et al. [122] and Hua et al. [123, 124] investigated hydrogen combustion in both a micro tube combustor and the geometry of MIT’s ultra micro gas turbine. However, hydrogen is not a good candidate for small portable devices, as mentioned in Chapter 2.

Lee and Kwon investigated methane-air micro flames on micro tubes of different sizes [128]. Although they investigated the effect of increasing the initial temperature on the flame stability, the results of premixed jet flames were found to exhibit different characteristics to premixed flames inside the micro tube.

Vlachos performed a 2D numerical study of both propane-air [129] and methane-air [89] mixtures with a global one-step reaction mechanism. It was found that the micro combustor dimensions strongly affect thermal stability and wall thermal conductivity is vital in determining the flame stability. Li et al. investigated the effects of the micro combustor size and geometry, inlet velocity profile, and the slip-wall boundary condition on methane-air flame temperatures [90]. In these studies, the predictions of flame temperature and stability mechanisms at micro scale were investigated, with either a one-step reaction mechanism [89, 129] or a skeletal mechanism with a first-order upwind scheme. But they have a major shortcoming in the use of high target residuals ($1 \times 10^{-3}$ for normalised RMS residuals) for convergence, particularly for the chemical species [90, 130].
While previous studies in the area of micro combustors have focused on the effects of design factors and operating conditions, the flame structure and characteristics do not appear to have been investigated fully. These studies [89, 90, 123, 124, 129, 130] have neither reported on major species concentrations in 2D nor on the effects of preheating, and varying equivalence ratio, on the flame characteristics. Lastly, none of the numerical studies to date appear to have conducted a validation for their numerical model, nor investigated the sensitivity of the results to different reaction mechanisms available in the literature.

The main objectives of this study, therefore, are to investigate two dimensional methane-air combustion at micro scale and to study the effects of preheating the reactants on the flame stability and combustion characteristics. A micro tube combustor of a fixed size was chosen for the study.

5.2 Numerical model

The diameter of the micro combustor tube was selected as 2 mm which is smaller than the quenching distance of stoichiometric methane-air flame at atmospheric pressure [131]. The length of the micro combustor was 12 mm. Figure 5-1 shows the geometry of the micro combustor considered here. A micro combustor of similar size was also investigated numerically by Li et al. [90], so the present simulations allow a comparison of the results.

The commercial CFD software package ANSYS Fluent 13, which is a finite volume code, was employed to simulate mass, momentum, energy and heat transfer [132]. A pressure based solver was used for the simulations with a laminar viscous model given that the Reynolds numbers are low for the flow conditions. A SIMPLE algorithm was used for pressure-velocity coupling and a 2D segregated solver using under relaxation factor was used to solve the governing equations. A second-order upwind scheme was used to discretize the governing equations and the target for the scaled residuals for convergence are set to $1 \times 10^{-6}$ for continuity, energy and species concentration.

![Figure 5-1 Schematic diagram of the micro combustor tube](image-url)
The mixture gas density was calculated using the ideal gas law while the specific heat of the mixture was calculated by mixing law [132]. The viscosity and thermal conductivity of the mixture were calculated as a mass fraction-weighted average of all species.

The specific heat of each of the species was calculated using a piecewise polynomial fit of temperature [132], while the thermal conductivity and viscosity of each species were calculated using kinetic theory. Thermo-chemical properties of the gas species as a function of temperature and transport properties are imported from the CHEMKIN thermodynamic database [133].

The study utilised skeletal and detailed reaction mechanisms for methane-air, which were imported from CHEMKIN-CFD [135] provided by Reaction Design for ANSYS Fluent. In the literature that was reviewed, it was found that some studies have been performed with a global one step reaction mechanism [89, 129]; however, in order to provide more accurate predictions, skeletal and detailed reaction mechanisms were used in the present study.

The skeletal mechanism of methane oxidation that was used is provided by Correa [136, 137], and consists of 16 species and 41 reactions, as listed in Appendix A7. The effects of different reaction mechanisms on combustion characteristics are compared in Sections 6.3 and 7.2. For comparison, in addition to Correa’s 41 reaction mechanism, the GRI 3.0 mechanism [138] consisting of 50 species and 309 reactions and the mechanism of Lu et al. [139] consisting of 17 species and 73 reactions (listed in Appendix A8) were also employed in the study. However, while the GRI 3.0 mechanism has more than 50 species, Fluent only has the capability of using 50 species, therefore the GRI 3.0 mechanism consisting of 50 species provided by CHEMKIN-CFD (listed in Appendix A9) was employed in the simulations. In this thesis, the 41 reaction mechanism is presented as SK16, and the 73 reaction mechanism and the GRI 3.0 mechanism are presented as SK17 and GRI, respectively. Except for Sections 6.3 and 7.2, all the results are obtained by employing the SK16 reaction mechanism.

The ignition of the mixture was achieved by imposing an initial 2000 K temperature to the entire computational domain. In the simulations, only half of the axisymmetric plane of the micro combustor tube is considered in order to reduce computational cost.

A uniform mesh was used in the model. A mesh sensitivity analysis was performed with 250gridsx50grids, 300gridsx30grids, 350gridsx50grids, 500gridsx50grids and 500gridsx100grids in the axial and radial directions. A mesh density of 350 gridsx50 grids was
decided upon for the simulations, since a higher mesh density did not change the results while a lower mesh density was unable to capture the peak values of the thermal properties.

The numerical results obtained with an adiabatic wall and non-adiabatic wall are explained in Chapters 6 and 7, respectively.
6 NUMERICAL RESULTS AND DISCUSSION: ADIABATIC CASE

This chapter presents the numerical simulation results of the two-dimensional premixed methane-air flame within a 2 mm diameter micro combustor tube with the adiabatic wall. It might be thought that obtaining an adiabatic wall is not possible in reality. However, in order to develop a model for the non-adiabatic case, applying an adiabatic case is an initial step. Furthermore, the adiabatic case provides the comparison of the model with the available experimental data. Also, the adiabatic case simulates a channel at the centre of a combustor consisting of clusters of micro tubes. Thus, numerical simulations with an adiabatic wall were performed.

6.1 Boundary conditions

![Schematic diagram of the micro combustor tube](image)

The boundary conditions used in the simulations are as follows. At the inlet, a fixed uniform velocity and temperature were used while the CH$_4$ and O$_2$ mass fractions were specified according to the equivalence ratios ($\bar{Ø}$). Symmetry boundary conditions are applied at the centreline, no diffusion flux and zero convective flux exist across the symmetry plane. At the wall, no-slip boundary condition and no-species flux conditions were applied. At the combustor exit, a fixed pressure of $1.013 \times 10^5$ Pa was specified. The material of the combustor wall was chosen as stainless steel. The uniform inlet temperature was varied from 300 K to 800 K with 100 K increments. The uniform inlet velocity was chosen as either 0.3 m/s or 1 m/s. 0.3 m/s represents the low incoming flow velocity, while 1 m/s represents the high incoming flow velocity. It should be noted that for stoichiometric methane-air flame, the burning velocity is 0.36 m/s [140] at atmospheric pressure and 298 K.

It might be thought that an 800 K initial reactant temperature is very high and that flashback may have therefore occurred. However, the experimental results of the HEX-Combustor showed that preheating, from the recirculation of both the combustion products and the simulated turbine exit gas, up to around 800 K was recorded and no flashback occurred.
Flashback is expected when the inlet passage of the micro combustor has enough space to auto ignite. However, when the inlet passage is very small compared to the quenching distance flashback cannot occur.

### 6.2 Validation of the model

The validation of two-dimensional modelling was verified by comparing the adiabatic flame temperature and species concentrations with available experimental data, as well as the results obtained using the NASA-Glenn Chemical Equilibrium Program CEA2 [141].

It is not possible to compare the results of the present two dimensional model with experiments performed with the same size geometry, since there are none available. However, in the literature, some experimental data were found for a one-dimensional flame geometry with a stoichiometric methane-air mixture [142-144]. Bechtel et al. experimentally obtained temperature and species concentration profiles of a stoichiometric, premixed laminar methane-air flame at atmospheric pressure from laser Raman scattering [144]. The details of the burner that was used can be found in [142, 143, 145].

The centreline major species and temperature profiles obtained with an initial reactant temperature of 300 K, an incoming flow velocity ($u_{in}$) of 0.3 m/s and an equivalence ratio of 1.0 by employing the SK16 skeletal mechanism of methane-air are shown in Figure 6-2 and Figure 6-3. Although the simulations were performed with a 12 mm long micro combustor, the results are shown only over the first 4 mm from the inlet since the combustion occurred over a very short distance from the inlet and furthermore, data in the literature is presented only for the first 3 to 4 mm.

Figure 6-2 shows that the centerline temperature profile along the combustor as predicted from the numerical simulations employing the SK16 skeletal mechanism, has very good correlation with the experimental data. The rapid rise of temperature obtained from numerical modelling matches the experimental data very well. However, it can also be seen from Figure 6-2 that, at a distance beyond 3 mm from the beginning of temperature rise, the experimentally obtained temperatures are somewhat lower than those predicted with numerical modelling. This is believed to be due to the presence of lateral heat losses inherent in the experiment, but which is not present in the numerical model due to the use of an adiabatic boundary condition for the side walls.
Figure 6-2 Temperature profile for stoichiometric methane-air flame. Experimental data extracted from Bechtel et al. [143]

Figure 6-3 Temperature and major species profiles for stoichiometric methane-air flame. $\phi=1.0$, $u_{in}=0.3 \text{ m/s}$, $T_0=300 \text{ K}$ Experimental data extracted from Bechtel et al. [144]

Figure 6-3 shows streamwise plots of the species concentrations obtained from numerical model along with the experimental data from the literature. As can be seen from Figure 6-3, the initial rapid rate of change of the mole fraction of all the species is very well matched between the present numerical model predictions and the experimental data. Also, in the case of H$_2$ and CO, the maximum mole fraction and the location for this as predicted by the numerical model are in good agreement with experiments. For CH$_4$, its mole fraction profile is matched very well to the experimental data, while for O$_2$, there is reasonable agreement between the numerical model and experiments. However there appears to be some differences between the mole fractions for H$_2$O, especially in a region just beyond the point at which the
temperature profile changes its slope, that is, between approximately 0.8 mm and 2.5 mm from the inlet. For the H₂O experimental data [32], no error information was given, however it was stated that in all the cases the precision was better than ±0.02 mole fractions [142]. A similar difference was also observed with predictions from the 1D modelling of Bechtel et al. [144]. Taking the experimental technology in the early 1980s into account, this may be considered as an experimental issue perhaps in regards to the measurement method. In spite of these, there is good general agreement between the numerical and experimental results.

In conclusion, these results show that the two dimensional numerical model with the SK16 skeletal reaction mechanism predicts the temperature and species concentration profiles very well compared to the experimental data. This provides validation and much confidence in the numerical model.

6.3 Comparison of chemical reaction mechanisms

The temperature, and species concentration profiles of methane-air flame, obtained by employing three different reaction mechanisms with a two dimensional model, were compared at micro scale. The reaction mechanisms consist of one detailed and two skeletal reaction mechanisms. Furthermore, the results obtained from the two dimensional model were also compared with a one dimensional model from the literature [146] and CEA2 calculations for the adiabatic condition. The comparison is performed at an initial temperature of 300 K, an incoming flow velocity of 0.3 m/s, and an equivalence ratio of 1.0.

Figure 6-4 presents the temperature, velocity and CH₄ mass fraction contour plots for stoichiometric, methane–air flame, at an incoming flow velocity of 0.3 m/s and initial reactant temperature of 300 K, employing the GRI, SK17 and SK16 reaction mechanisms. The predicted maximum flame temperature is 2212 K employing the GRI mechanism, 2198 K employing the SK17 and 2142 K using the SK16 mechanism. The adiabatic flame temperature of stoichiometric methane-air is 2225 K according to CEA2 and 2222 K according to the study of Friedman and Levy [147]. These indicate that the three reaction mechanisms predict the flame temperature rather well. The GRI mechanism predicts the flame temperature with an error of 0.6% relative to the adiabatic flame temperature, whereas the SK17 and SK16 mechanisms predict with errors of 1.2% and 3.7%, respectively. The small error levels show that any of these three reaction mechanisms can be applied to predict methane-air flame characteristics at atmospheric pressure.
Figure 6-4 Temperature, velocity and CH$_4$ mass fraction contours for methane-air flame at atmospheric pressure. $\phi=1.0$, $u_\text{in}=0.3$ m/s, $T_u=300$ K. These figures are not to scale. (d=2 mm, L=12 mm)

Figure 6-5 CO$_2$, CO and H$_2$O mass fraction contours for methane-air flame at atmospheric pressure, $\phi=1.0$, $u_\text{in}=0.3$ m/s, $T_u=300$ K (d=2 mm, L=12 mm)

Similar to the flame temperature, the predicted maximum velocity obtained by employing the GRI mechanism is the highest at 4.47 m/s. For the SK17 and SK16 mechanisms the maximum velocity predictions are, 4.45 m/s and 4.36 m/s, respectively. This is expected since the GRI mechanism predicts the highest temperature. Density therefore becomes lower and thus results in higher velocity relative to the SK16 and SK17 velocity predictions. From the predicted CO, CO$_2$ and H$_2$O mass fraction contours, which are shown in Figure 6-5, it can be concluded that the SK16 mechanism predicts the formation of products far from the inlet, which is in contrast to the results of the GRI and SK17 mechanisms.

In addition to the accuracy of the solution, the computational cost needs consideration as well, in any numerical based work. In the present study, it was found that the simulation with the SK16 mechanism takes 2-3 days to complete with a quad core computer. With the SK17 mechanism, it takes over 4-5 days to obtain a convergent result, while with the GRI mechanism it takes approximately a month to obtain a convergent result. When taking into account time and cost, it is concluded that the SK16 mechanism predicts a sufficiently accurate solution in the shortest amount of time.
Figure 6-6 presents the predicted centreline temperature, velocity and major species concentration profiles for stoichiometric methane-air flame at atmospheric pressure, obtained with the three different reaction mechanisms.

The predictions with the SK17 and SK16 mechanisms display the same trend in the first 0.8 mm in which the flame occurs. However after 0.8 mm, the SK17 mechanism exhibits the same trend as the GRI mechanism. As can be seen from the predicted species concentration profiles, for the three reaction mechanisms, there is a delay in the flame computed from the GRI mechanism results. Based on the very good agreement between the results of the SK16 mechanism and experimental data presented in the previous section, it can be concluded that the delay in the flame computed from the GRI mechanism could also relate to the larger number of steps in the GRI mechanism requiring a separate mesh configuration. Given that this mechanism was already very computationally expensive, no merit could be seen in pursuing a mesh sensitivity analysis with the GRI mechanism, especially when the SK16 mechanism was validated already.
Table 6-1 presents the predicted flame temperature, flame thickness and location, as well as species peak mole fractions by employing the GRI, SK16, SK17 mechanisms in addition to Smoot’s [146] 1D predictions and equilibrium mole fractions from CEA2 calculations. The flame thickness was defined as the distance for the CH$_4$ concentration to decrease from 99% to 1% of its original value [146, 148]. The flame location is defined as the location where the mean temperature (of the inlet and flame temperatures) occurs.

### Table 6-1 Comparison of reaction mechanisms of stoichiometric methane-air flame at atmospheric pressure

<table>
<thead>
<tr>
<th>Reaction mechanism</th>
<th>GRI-Mech 2D</th>
<th>SK16 (41 reactions) 2D</th>
<th>SK17 (73 reactions) 2D</th>
<th>Smoot (28 reactions) 1D</th>
<th>CEA 0D*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Final Temperature (K)</td>
<td>2212</td>
<td>2142</td>
<td>2198</td>
<td>2157</td>
<td>2225</td>
</tr>
<tr>
<td>Flame thickness (mm)</td>
<td>0.64</td>
<td>0.56</td>
<td>0.56</td>
<td>0.65</td>
<td>-</td>
</tr>
<tr>
<td>Flame distance from the inlet (mm)</td>
<td>0.43</td>
<td>0.33</td>
<td>0.33</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Species

- CH$_3$: 0.21*10^{-2} 0.39*10^{-2} 0.32*10^{-2} 0.99*10^{-2} -
- CH$_3$O: 0.94*10^{-3} 2.2*10^{-3} 1.1*10^{-3} 0.30*10^{-3} -
- CO: 0.49*10^{-1} 0.56*10^{-1} 0.52*10^{-1} 0.37*10^{-1} 0.898*10^{-2}*
- CO$_2$: 0.83*10^{-1} 0.77*10^{-1} 0.81*10^{-1} 0.80*10^{-1} 0.85*10^{-1}*
- H$_2$O: 0.179 0.172 0.177 0.18 0.18283*
- H$_2$: 0.187*10^{-1} 0.199*10^{-1} 0.173*10^{-1} 0.16*10^{-1} 0.358*10^{-2}*
- H: 0.63*10^{-2} 0.84*10^{-2} 0.67*10^{-2} 0.63*10^{-2} 0.039*10^{-2}*
- OH: 0.69*10^{-2} 0.76*10^{-2} 0.69*10^{-2} 0.73*10^{-2} 0.318*10^{-2}*
- O: 0.28*10^{-2} 0.33*10^{-2} 0.26*10^{-2} 0.30*10^{-2} 0.021*10^{-2}*
- HO$_2$: 0.16*10^{-3} 0.228*10^{-3} 0.16*10^{-3} 0.23*10^{-3} -

* Equilibrium mole fractions

The flame temperature obtained by the GRI mechanism is very close to the adiabatic flame temperature calculated by CEA2. Flame thickness of 0.64 mm is predicted by employing the GRI mechanism which is very close to Smoot’s prediction which is 0.65 mm. With the SK17 and SK16 mechanisms, the same flame thickness is predicted and the value of which is 0.56 mm. A luminous flame region of 0.46 mm was measured experimentally by Bechtel and Teets [143]. For all reaction mechanisms the flame thickness is less than 1 mm. Furthermore, flame location is predicted as 0.33 mm by both the SK16 and SK17 mechanisms and 0.43 mm by the GRI mechanism in 2D.
It can be concluded from Sections 6.2 and 6.3, that two-dimensional methane-air flames at micro scale can be simulated by ANSYS Fluent by importing skeletal or detailed chemical mechanisms through CHEMKIN-CFD successfully.

When the cost and time of the calculations are taken into account, the SK16 mechanism predicts the flame temperature and species concentration rather accurately. Therefore, the continuation of this study was performed by employing the SK16 mechanism.

6.4 Effect of initial temperature and incoming flow velocity

6.4.1 Effect of initial reactant temperature

In order to obtain efficient and clean micro combustion, the combustion on the lean side of stoichiometric is considered. Therefore an equivalence ratio of 0.9 is chosen to further this study. The equivalence ratio of 0.9 would make it easier to compare the results with the numerical results of Li et al. [90] which was performed in a similar geometry using 0.9 as an equivalence ratio. Furthermore, the flame behaviour at an equivalence ratio of 0.9 with preheated reactants temperature up to 800 K will elucidate the flame obtained in the prototyped HEX-Combustor [46] at a high mass flow rate, where both the flame shape and location were not able to be observed.

In Chapter 1, the importance of heat loss and small residence time in micro combustion was emphasised. When increasing the residence time is not possible, complete combustion may be achieved by preheating the reactants. Therefore, in this section the effects of preheating the reactants of lean methane-air mixture on the combustion characteristics and its stability at micro scale will be shown.

Figure 6-7 presents the temperature, velocity, and CH₄ mass fraction contour plots obtained at an equivalence ratio of 0.9 and an incoming flow velocity of 0.3 m/s, with initial temperatures from 300 K to 800 K. As the initial temperature increases, the flame occurs closer to the inlet and tends towards a flat flame. At an initial temperature of 300 K, the flame shape is conical and with an increasing initial temperature it flattens. Only at an initial temperature of 300 K, is a conical shaped flame obtained. As expected, the flame temperature increases with an increasing initial temperature. A maximum flame temperature of 2094 K is predicted with an initial temperature of 300 K. On the other hand, the predicted maximum flame temperature is 2447 K for an initial temperature of 800 K. CH₄ mass fraction contours show that CH₄ is consumed in a short distance (i.e. over a few millimetres) from the inlet. As
observed with the flame temperature, CH₂ consumption and CO₂ and H₂O production (shown in Figure 6-8) also exhibit the same trend, all have a conical shape, with an initial temperature of 300 K.

![Figure 6-7 Temperature, velocity and CH₄ mass fraction contours of methane-air flame at an incoming velocity of 0.3 m/s and equivalence ratio of 0.9 with increasing initial temperature (d=2 mm, L=12 mm)](image)

![Figure 6-8 CO₂, CO and H₂O mass fraction contours of methane-air flame at an incoming velocity of 0.3 m/s and equivalence ratio of 0.9 with increasing initial temperature (d=2 mm, L=12 mm)](image)

6.4.2 Effect of increasing incoming flow velocity

In this section the effect of increasing the incoming flow velocity on the flame stability and combustion characteristics will be presented. Keeping the equivalence ratio constant at 0.9, the incoming flow velocity was increased to 1 m/s and the results are shown below. With an incoming flow velocity of 1 m/s, at initial temperatures of 300 K and 400 K, the flame cannot be sustained within a 2 mm diameter combustor even with an adiabatic wall. At an initial temperature of both 300 K and 400 K, the flames blow out since the incoming flow velocity is much higher than the burning velocity of methane-air at an equivalence ratio of 0.9, which is 0.29 m/s and 0.49 m/s for initial temperatures of 300 K and 400 K [149], respectively. The blow out was observed by checking the flame location and the flame temperature with an increasing number of iterations. It was clearly observed that the flame gradually moves downstream and finally blows out. This result was expected and the simulations were
performed in order to verify whether the model was working properly. These results show that this model is working very well for deciding the flame stability limit.

Figure 6-9 presents the temperature, velocity and CH$_4$ mass fraction contours obtained at initial temperatures of 500 K and 800 K. At an initial temperature of 500 K, a conical flame occurs at approximately 2 mm from the inlet along the centreline. As the initial temperature increases, flame cone angle decreases and the flame moves upstream towards the inlet. Finally, the flame becomes flat and occurs very close to the inlet as can be seen from the temperature and CH$_4$ mass fraction contours with an initial temperature 800 K.

![Figure 6-9 Temperature, velocity and CH$_4$ mass fraction contours of methane-air flame at an incoming velocity of 1 m/s and equivalence ratio of 0.9 with increasing initial temperature (d=2 mm, L=12 mm)](image)

Figure 6-10 presents CO$_2$, CO and H$_2$O mass fraction contours for the same conditions as Figure 6-9. These contours explain very well exactly where the combustion occurs and the products that are produced at micro scale.

![Figure 6-10 CO$_2$, CO and H$_2$O mass fraction contours of methane-air flame at an incoming velocity of 1 m/s and equivalence ratio of 0.9 with increasing initial temperature (d=2 mm, L=12 mm)](image)

Li et al. [90] investigated the effects of inlet velocity on flame temperature with the same size micro combustor. They found that as the inlet velocity increases, the flame is moved further downstream in the micro combustor. The explanation offered for this was that it is due to the higher mass flow rate and hence the longer heating length for the mixture to be heated up to ignition temperature. However, it does not seem possible to have a flame with an initial temperature of 300 K, at incoming flow velocities of 0.8 m/s and 1 m/s, which are much higher
than the burning velocity of methane-air flames, even at stoichiometric ratios, in a meso scale combustor. Especially in micro scale combustors, these incoming flow velocities do not sustain a flame. The reason for how Li et al. obtained a stabilized flame at higher incoming flow velocities may be explained as follows; both applying a first order upwind scheme for approximating the equations and setting high target residuals (1×10^3 for normalised RMS residuals) for convergence of continuity and species concentrations might lead to a quick solution. Indeed, during the present simulations, the flame front could be seen to move along the tube as iterations progressed well before the solution converged. A solution which is obtained with high target residuals in the case of Li et al. prevents observation of the blow out. Applying both a second order upwind scheme and lower target residuals (1×10^-6 for normalised RMS residuals) as in the present study takes a longer time to obtain a converged solution, but it provides an opportunity to observe both the propagation of the flame through the combustor length and the blow out. Thus, this results in more accurate predictions.

The stabilization of the flame in micro scale combustors is due to the balance between the incoming flow velocity and the burning velocity. Preheating the reactants, either from the combustor wall itself, or from an external heat source, increases the burning velocity. Therefore, even at higher incoming flow velocities, if the burning velocity is higher than the incoming flow velocity, the flame is able to stabilize and sustain itself at micro scales.

When the incoming flow velocity increases, the predicted maximum flame temperatures are lower than that obtained with a lower incoming flow velocity. This can be seen from Figure 6-7 and Figure 6-9. This shows that the micro combustor length chosen for the study is not sufficient to reach the maximum flame temperature.

As the incoming velocity increases, the flame moves downstream and the flame temperature decreases, as can be seen in Figure 6-11. At an initial temperature of 500 K and an equivalence ratio of 0.9, the maximum flame temperature is predicted as 2267 K and 2155 K for incoming flow velocities of 0.3 m/s and 1 m/s, respectively. This shows that the micro combustor length should be longer than 12 mm in order to obtain the adiabatic flame temperature. In addition, with increasing incoming flow velocity the flame shape changes from flat to conical. Figure 6-9 exhibits that CH₄ is consumed totally around 2 mm from the inlet with an incoming flow velocity of 1 m/s. However, with an incoming flow velocity of 0.3 m/s, the CH₄ consumption is completed within the first 0.3 mm, as shown in Figure 6-7. The O₂ concentration profiles display the same trend. Altay et al. also showed that the increase in
incoming flow velocity leads to the flame moving downstream and an increase in the flame angle [74].

![Figure 6-11 Comparison of the effect of incoming flow velocity on flame temperature (left) and \( \text{CH}_4 \) and \( \text{O}_2 \) mole fraction profiles (right) at an initial temperature of 500 K and an equivalence ratio of 0.9]

From the numerical simulation results, it can be concluded that the stabilization of the flame at micro scale depends on the relationship between the incoming flow velocity and burning velocity. When the incoming flow velocity is very low compared to the burning velocity, flat flame burning occurs. On the other hand, when the incoming flow velocity is closer to the burning velocity, a conical shape flame occurs with a higher cone angle. This conical shape occurs due to the boundary wall limitation. The cone angle changes with varying incoming flow velocities, because the normal component of the incoming flow velocity tries to balance with the burning velocity. The cone angle decreases with increasing incoming flow velocity, as shown with an initial temperature of 500 K and incoming flow velocity of 1 m/s. Here, both the root and tip of the conical flame moves downstream. With further increase in the incoming flow velocity, eventually, when the normal component does not balance with the burning velocity, the flame blows out.

### 6.4.3 Effect of equivalence ratio

The effects of equivalence ratio were investigated with equivalence ratios of 0.8, 0.9 and 1.0 at an initial temperature of 300 K and an incoming flow velocity of 0.3 m/s. The temperature contours obtained with increasing equivalence ratio are shown in Figure 6-12. The flame temperature increases as equivalence ratio increases. The laminar burning velocity also increases with increasing equivalence ratio. As can be seen in Figure 6-12 and Figure 6-13, at an equivalence ratio of 0.8 the flame has a conical shape and is located somewhat downstream.
of the inlet. On the other hand, at an equivalence ratio of 1.0 the flame flattens and occurs very close to the inlet. A similar trend is also shown by Altay et al. [74].

![Figure 6-12 Temperature, velocity and CH₄ mass fraction contours of methane-air flame at an incoming velocity of 0.3 m/s and an initial temperature of 300 K with increasing equivalence ratio (d=2 mm, L=12 mm)](image)

![Figure 6-13 CO₂, CO and H₂O mass fraction contours of methane-air flame at an incoming velocity of 0.3 m/s and an initial temperature of 300 K with increasing equivalence ratio (d=2 mm, L=12 mm)](image)

### 6.5 Summary

In this chapter, two-dimensional numerical simulation results obtained with an adiabatic wall within a 2 mm diameter micro combustor tube were presented. The simulations were performed by employing a skeletal mechanism consisting of 16 species and 41 reactions. The numerical predictions showed good correlation with experimental data from the literature, particularly for the flame temperature values. The effect of increasing the reactant temperatures from 300 K to 800 K on the combustion stabilization and species concentration were investigated at two incoming flow velocities. The flat flame and conical flames were observed with varying initial conditions. The flame stabilization in the 2 mm diameter micro combustor tube was achieved by increasing the reactants temperature at high incoming flow velocities.
7 NUMERICAL RESULTS AND DISCUSSION: NON-ADIABATIC CASE

In this chapter, two-dimensional numerical simulation results for methane-air mixtures, within a 2 mm diameter micro combustor with a non-adiabatic wall are presented. The effect of preheating the reactants temperature, incoming flow velocity, equivalence ratio, and heat loss mechanism on the flame stability and combustion characteristics are investigated. Furthermore, a comparison of results obtained with adiabatic and non-adiabatic walls are reported. Finally, the effects of increasing the reactants temperature at a constant mass flow rate on the combustion characteristics are compared.

7.1 Boundary conditions

The same computational model is used, as introduced in Chapter 6, except at the wall boundary, where a non-adiabatic wall is introduced. The geometry of the micro combustor is shown in Figure 7-1.

\[ Q = h_{\text{conv}}(T_w - T_a) + \varepsilon \sigma (T_w^4 - T_a^4) \] (W/m\(^2\)) \hspace{1cm} (7-1)

where the convective heat transfer coefficient, \(h_{\text{conv}}\), and the wall emissivity, \(\varepsilon\), are chosen to be 5 W/m\(^2\)K and 0.2, respectively. The same values were used by Li et al. for micro combustion of methane-air mixture [90]. At the combustor wall, a no-slip boundary condition and no species flux normal to the wall surface are applied.

7.2 Comparison of chemical reaction mechanisms

The temperature and species concentration profiles of methane-air flame obtained from the two dimensional CFD simulation model were compared with a non-insulated wall at micro scale. Three different reaction mechanisms consisting of one detailed and two skeletal reaction
mechanisms were employed in the simulations. The detail of the reaction mechanisms were
given in Chapter 5.

In the adiabatic case (presented in Chapter 6), it was possible to compare the numerical
modelling results with available experimental and 1D numerical data in the literature. Good
agreement was found between combustion characteristics obtained from numerical simulations
employing the SK16 skeletal mechanism and available experimental data in the literature. As
far as the author is aware, there is no available combustion data in the literature for an initial
temperature of 800 K with similar boundary conditions. Therefore, in this section only a
comparison of the three different mechanisms with a non-adiabatic wall is presented.

The comparison of reaction mechanisms is performed at an initial temperature of 800
K, an incoming velocity of 1 m/s, with an equivalence ratio of 0.9. Figure 7-2 presents the
temperature, velocity and CH\textsubscript{4} mass fraction contours for methane–air flame, at this condition
employing the GRI, SK17 and SK16 mechanisms. A cone shaped high temperature zone was
observed with a non-adiabatic wall. In this case, the GRI and SK17 mechanisms predict the
same maximum temperature of 2108 K. The SK16 mechanism predicts the maximum
temperature of 2092 K which is less than the prediction of both the GRI and SK17 mechanisms,
but very close to both predictions and shows only a 0.75% discrepancy. From the predicted
CO, CO\textsubscript{2} and H\textsubscript{2}O mass fraction contours, which are shown in Figure 7-3, it can be concluded
that flat flame occurs at an initial temperature of 800 K with a non-insulated wall. However,
the SK16 mechanism predicts formation of products at a little further from the inlet than is
predicted by the other two mechanisms.

The flame shape is considered to be flat when the CO peak values at the wall and at the
centreline, occur at the same axial distance from the inlet. On the other hand, the flame is
considered to have a conical shape when the CO peak values at the centreline, occur at a greater
axial distance from the inlet, than the axial distance of those values at the wall.

Although the major species mass fraction contours show that a flat flame occurs, this is
however difficult to conclude from the temperature and velocity contours. The maximum flame
temperature was obtained approximately 0.5 mm from the inlet, while maximum velocity was
obtained at approximately 1.5 mm from the inlet. These contours show the effect of heat loss
from the outer wall with a non-adiabatic wall. It can be concluded that the heat loss has no
effect on species concentration but a significant impact on both temperature and velocity
profiles. This will be discussed further in the next section.
Figure 7-2 Temperature, velocity and CH₄ mass fraction contours for methane-air flame at atmospheric pressure at an incoming velocity of 1 m/s, an equivalence ratio of 0.9 and an initial reactant temperature of 800 K (d=2 mm, L=12 mm)

Figure 7-3 CO₂, CO and H₂O mass fraction contours for methane-air flame at atmospheric pressure at an incoming velocity of 1 m/s, an equivalence ratio of 0.9 and an initial reactant temperature of 800 K (d=2 mm, L=12 mm)

Due to the heat loss, the flame temperature drops significantly down to a value of 1090 K at the combustor exit. From centreline temperatures and CH₄ concentration profiles, as shown in Figure 7-4, it can be concluded that the predictions by employing the three different reaction mechanisms are very close to each other. As explained in Chapter 6, simulation with the SK16 mechanism takes shorter time compared to the simulations with the SK17 and the GRI mechanisms. Therefore, when taking into account both time and cost, the SK16 mechanism has been used to obtain accurate solutions in the shortest amount of time, it was employed in the rest of the investigations.

Figure 7-4 Centreline flame temperature and CH₄ concentration profiles at an incoming velocity of 1 m/s, an equivalence ratio of 0.9 and an initial reactant temperature of 800 K
7.3 Comparison between adiabatic and non-adiabatic wall conditions

Figure 7-5 shows the temperature, velocity and CH$_4$ mass fraction contours of methane-air flame at an incoming flow velocity of 1 m/s and an equivalence ratio of 0.9 with adiabatic and non-adiabatic walls. It can be seen that the flame temperature decreases significantly with a non-adiabatic wall, due to the heat loss through the wall via both convection and radiation. The maximum temperature decreases from 2355 K to 2092 K due to the heat loss. In both cases, a flat flame occurs very close to the inlet of the combustor. However, in the non-adiabatic wall case, a cone shaped high flame temperature zone is observed only in a small part of the combustor, after which the flame temperature gradually decreases towards the outlet. On the other hand, with an adiabatic wall, the flame temperature beyond the flame location is observed to gently increase along most of the combustor length. Due to the substantial temperature differences between the adiabatic and non-adiabatic cases, the gas velocities are also different, and in the case of the non-adiabatic wall, it also changes significantly. With the adiabatic wall, a maximum velocity of 6 m/s was calculated, while with a non-adiabatic wall a maximum velocity of 4.5 m/s was obtained. As can be seen from the CH$_4$ mass fraction contours however, heat loss does not affect the CH$_4$ consumption.

Figure 7-5 Temperature, velocity and CH$_4$ mass fraction contours of methane-air flame at an incoming velocity of 1 m/s and equivalence ratio of 0.9 with adiabatic and non-adiabatic wall (d=2 mm, L=12 mm)

Figure 7-6 CO$_2$, CO and H$_2$O mass fraction contours of methane-air flame at an incoming velocity of 1 m/s and equivalence ratio of 0.9 with adiabatic and non-adiabatic wall

From the centreline flame temperature profile comparisons shown in Figure 7-7, it can be seen that combustion occurs at the same location for the two wall conditions. The initial temperature profiles have the same slope although they exhibit different trends after the sudden
temperature rise. With the adiabatic wall, flame temperature continues to increase very slightly. On the other hand, with the non-adiabatic wall, temperature decreases dramatically along the micro combustor length. Although both CH\textsubscript{4} profiles show similar tendencies across the two different boundary cases, other major species profiles show different tendencies after the flame temperature starts to drop.

Figure 7-7 Comparison of predicted centreline temperature, velocity and species concentration profiles with an adiabatic wall and non-adiabatic wall at an initial temperature of 800 K, an incoming flow velocity of 1 m/s, and an equivalence ratio of 0.9

123
With the skeletal reaction mechanism, it was possible to observe the formation of the partial oxidation products, such as CO and OH. On the other hand, this was not possible when utilising the one step-reaction mechanism. With a non-adiabatic wall, CO concentration decreases slowly along the combustor length. With CO consumption, CO₂ production reaches its maximum value, as shown in Figure 7-6. Thus, the difference of the CO concentration between the adiabatic and non-adiabatic wall cases is equal to the difference of the CO₂ concentration between the same two cases. This can be seen from Figure 7-7. These results show that with an adiabatic wall, higher flame temperature causes dissociation of CO₂ and H₂O.

7.4 Effect of initial temperature and incoming flow velocity

7.4.1 Effect of initial reactant temperature

Simulations revealed that at initial temperatures of both 300 K and 400 K, the flame could not be sustained within the 2 mm diameter micro combustor and blow out occurred. The blow out can be observed by comparing the temperature contours with respect to the number of iterations. After ignition, a maximum flame temperature is reached, after which the maximum flame temperature zone starts to move towards the outlet where it finally dissipates. Thereafter, the maximum temperature within the combustor is observed to be the same as the initial reactant temperature. A stable flame could only be observed for initial temperatures of 500 K and higher and these results are discussed next.

Figure 7-8 presents the temperature, velocity, and CH₄ mass fraction contours obtained at an equivalence ratio of 0.9 and an incoming flow velocity of 0.3 m/s, with initial temperatures of 500 K to 800 K. Maximum flame temperature is predicted very close to the inlet for all the initial reactant temperatures. CH₄ consumption is completed within the first few mm. As the initial temperature increases, the maximum flame temperature also increases. The maximum flame temperature is predicted at the same axial distance for all the cases. However, the maximum flame temperature values change with the initial reactant temperature. The predicted maximum flame temperatures are 1882 K, 1928 K, 1976 K, and 2022 K for initial temperatures of 500 K, 600 K, 700 K, and 800 K, respectively.

Although the maximum flame temperature is predicted for an initial temperature of 800 K, a lowest combustor exit temperature also occurs in this condition. The reason for the high temperature decrease along the combustor length is due to the low mass flow rate and
corresponding lower energy input at an initial temperature of 800 K. At this condition, the total heat loss is higher than the energy input and that results in a lower temperature at the combustor exit than the initial reactant temperature of 800 K. On the other hand, with an initial temperature of 500 K, the total heat loss is higher than the total heat loss with an initial temperature of 800 K. However, at an initial temperature of 500 K, the combustor exit temperature is higher than the combustor exit temperature with an initial temperature of 800 K. This is due to the higher mass flow rate and resulting higher energy input for the initial temperature of 500 K. Similar results were also obtained numerically by Jejurkar and Mishra [150] with hydrogen-air flame in an annular micro combustor, in which a hollow tube filled with nitrogen gas was inserted in the combustion zone in order to stabilize the hydrogen-air flame. CO is consumed completely within 8 mm of the combustor length, as shown in Figure 7-9. At low incoming velocity, increasing the initial temperature does not provide any advantage, and instead results in low temperature at the combustor exit with the non–adiabatic wall.

![Figure 7-8 Temperature, velocity and CH₄ mass fraction contours of methane-air flame at an incoming velocity of 0.3 m/s and equivalence ratio of 0.9 with increasing initial temperature (d=2 mm, L=12 mm)](image1)

![Figure 7-9 CO₂, CO and H₂O mass fraction contours of methane-air flame at an incoming velocity of 0.3 m/s and equivalence ratio of 0.9 with increasing initial temperature (d=2 mm, L=12 mm)](image2)
7.4.2 Effect of increasing incoming flow velocity

Keeping the equivalence ratio constant at 0.9, the incoming flow velocity was increased to 1 m/s. With the non-adiabatic wall, at initial temperatures of 500 K and 600 K with an incoming flow velocity of 1 m/s, the flame is not able to be sustained within the 2 mm diameter combustor as blow out occurs. It has been shown already that for the adiabatic case however, the flame can be sustained within the micro combustor at these initial temperatures. The difference is primarily due to the increasing heat loss in the non-adiabatic wall condition through the outer wall via convection and radiation. At initial temperatures of 700 K and 800 K, with an incoming flow velocity of 1 m/s and an equivalence ratio of 0.9, the flame is able to be sustained within the micro combustor, reaching maximum flame temperatures of 2004 K and 2092 K, respectively. The maximum axial velocities are predicted as 5.09 m/s and 4.53 m/s for initial temperatures of 700 K and 800 K, respectively.

As the initial temperature increases, the maximum flame temperature also increases. At both these initial temperatures of 700 K and 800 K, a cone shaped high temperature zone was observed. Although at an initial temperature of 800 K the cone shaped high temperature zone is wider with a higher maximum temperature, the combustor exit temperature is lower. This can be seen from Figure 7-10. Flat flames occur with both these initial temperatures, which can be seen from the major species mass fraction contours, in Figure 7-10 and Figure 7-11. Although both flames are flat, increasing the initial temperature causes the flame to move very close to the inlet.

Similar to the adiabatic case (presented in Chapter 6), preheating the reactants widens the flame stability at higher incoming flow velocities. It can be concluded from this section that, with a non-adiabatic wall, the reactants should be heated to a higher temperature of 700 K in order to sustain a stable flame within a 2 mm diameter micro combustor at a high incoming flow velocity of 1 m/s. However, increasing the initial reactant temperature further does not provide any advantage, and instead results in a lower combustion exit temperature due to the lower mass flow rate and corresponding lower energy input.

At low incoming flow velocities, preheating the reactants contributes neither to the flame stability nor the combustion characteristics. On the contrary, it results in low combustion exit temperature. However, it has a significant contribution on widening the flame stability at high incoming flow velocity.
Figure 7-10 Temperature, velocity and CH$_4$ mass fraction contours of methane-air flame at an incoming velocity of 1 m/s and equivalence ratio of 0.9 at initial temperatures of 700 K and 800 K (d=2 mm, L=12 mm)

Figure 7-11 CO$_2$, CO and H$_2$O mass fraction contours of methane-air flame at an incoming velocity of 1 m/s and equivalence ratio of 0.9 at initial temperatures of 700 K and 800 K (d=2 mm, L=12 mm)

7.5 Effect of equivalence ratio

The effect of equivalence ratio on the combustion characteristics are investigated at an initial temperature of 800 K and an incoming velocity of 0.3 m/s. The equivalence ratio is varied from 0.6 to 1. At equivalence ratios of 0.55 or less showed that the flame could not be sustained within the 2 mm micro combustor as blow out occurs. Although experimentally preheating widens the flame stability up to equivalence ratio of 0.4 within the 46 mm diameter combustor, within the 2 mm diameter micro combustor it was found that it was impossible to reduce the equivalence ratio below 0.6 with an initial temperature of 800 K.

Figure 7-12 presents the temperature, velocity and CH$_4$ mass fraction contours obtained at an initial temperature of 800 K with increasing equivalence ratios. As can be seen from the temperature contours, increasing the equivalence ratio results in an increase in the flame temperature. The maximum flame temperature is 1745 K at an equivalence ratio of 0.6, while a maximum temperature of 2064 K is predicted at an equivalence ratio of 1.0.

Although the flame temperature increases with increasing equivalence ratio, the combustor exit temperature decreases dramatically down to around 600 K across all equivalence ratios. At all equivalence ratios, flat flames occur very close to the inlet. In can be
concluded that, increasing the equivalence ratio does not exhibit any advantage in terms of combustor exit temperature and flame stability.

Figure 7-12 Temperature, velocity and CH$_4$ mass fraction contours of methane-air flame at an incoming velocity of 0.3 m/s and an initial temperatures of 800 K with changing equivalence ratio (d=2 mm, L=12 mm)

7.6 Effect of heat loss

7.6.1 Heat loss via convection only

In the literature, some two-dimensional micro combustion studies assume heat loss through the outer wall to the ambient via convection only. Therefore, a similar study was performed in this research; however in reality it is not possible to ignore radiation heat loss through the outer wall to the ambient.

Norton and Vlachos predicted the flame stability at small scale considering only the heat loss through the outer wall via convection [89]. They used convective heat transfer coefficients of between 1-20 W/m2K. Hua et al. [123] also used a convective heat transfer coefficient of 50 W/m2K, while Li et al. [90] and Verstraete et al. [122] chose a convective heat transfer coefficient of 5 W/m2K in their numerical simulations. A convective heat transfer coefficient of 10 W/m2K was also used by Li et al [151].

In this section, heat loss through the outer wall to the ambient via only convection is considered. The effect of convective heat transfer coefficient on the combustion characteristics is compared. Heat losses from the outer wall to the ambient are given by the convective heat transfer loss, expressed as

\[ Q = h_{conv}(T_w - T_a) \quad \text{(W/m}^2\text{)} \quad (7-1) \]

where the convective heat transfer coefficient, $h_{conv}$, is chosen to be 5 W/m$^2$K, 10 W/m$^2$K and 50 W/m$^2$K.
At an initial temperature of 300 K, an incoming velocity of 0.3 m/s, and an equivalence ratio of 0.9, it has been already established that a flame cannot be sustained within the 2 mm diameter micro combustor when the heat loss occurs through the outer wall via both convection and radiation. However, when heat loss occurs at the outer wall via convection only, as in the study of Norton and Vlachos, the flame may be sustained. While assuming no radiation heat loss, the effects of changing the convective heat transfer coefficient on the stability of the flame are investigated. It is found that with convective heat transfer coefficients of 5 and 10 W/m$^2$K, the flame can be sustained within a 2 mm diameter micro combustor even though the initial reactants temperature is 300 K. On the other hand, with a convective heat transfer coefficient of 50 W/m$^2$K, higher heat loss occurs from the outer wall, resulting in an unsustainable flame. The corresponding temperature, velocity and major species concentrations contours are presented in Figure 7-13 and Figure 7-14.

In both cases, conical flames occur. Increasing the convective heat transfer coefficient results in high heat loss, thus a lower combustion exit temperature is obtained with an approximate drop of 250 K. The increased heat loss does not affect the major species concentrations significantly, as can be seen from CH$_4$, CO$_2$, CO and H$_2$O mass fraction contour plots. No changes are observed in the flame location or its thickness.

![Figure 7-13 Temperature, velocity and CH$_4$ mass fraction contours of methane-air flame: incoming velocity of 0.3 m/s, equivalence ratio of 0.9, initial temperature of 300 K, convective heat transfer coefficients of 5 W/m$^2$K and 10 W/m$^2$K (d=2 mm, L=12 mm)](image)

![Figure 7-14 CO$_2$, CO and H$_2$O mass fraction contours of methane-air flame: incoming velocity of 0.3 m/s, equivalence ratio of 0.9, initial temperature of 300 K, convective heat transfer coefficients of 5 W/m$^2$K and 10 W/m$^2$K (d=2 mm, L=12 mm)](image)
Figure 7-15a shows the unstable moving flame along the combustor tube, at an initial temperature of 300 K, with a convective heat transfer coefficient of 50 W/m²K, with increasing number of computational iterations. Figure 7-15b also shows the centreline outlet temperature versus number of computational iterations profile. As can be seen from the temperature profile, the outlet temperature first jumps to around 3000 K, and this occurs due to ignition. Then with an increasing number of iterations, it drops down to 600 K. This means that combustion does occur initially but due to high heat losses at the outer wall, outlet temperature is low, around 600 K. This temperature can be seen at around 25,000 iterations. Afterwards, the outlet temperature again starts to increase. This increase is due to the moving flame. The flame cannot be stabilized, moves downstream, and finally blows out. After 130,000 iterations, the outlet temperature becomes stable at 300 K which is the initial temperature, indicating the blow out.

Similarly, when the radiation heat loss is ignored, the flame can be sustained at an initial temperature of 800 K and an equivalence ratio of 0.55. However, when both radiation and convection heat loss occurs through the outer wall, the flame cannot be sustained within the 2 mm micro combustor.

Figure 7-16 and Figure 7-17 show the temperature, velocity and major species concentration contours at an initial temperature of 800K, an equivalence ratio of 0.55 and an incoming velocity of 0.3 m/s when the convective heat transfer coefficients are 5 and 10 W/m²K. Similar to the predictions with 300 K, increasing the convective heat transfer coefficient does not affect the major species concentrations significantly, although it does result in lower outlet temperature. An outlet temperature drop of approximately 450 K is obtained with an increasing convective heat transfer coefficient. Flat flames very close to the inlet, occur with both convective heat transfer coefficients.
Figure 7-16 Temperature, velocity and CH\textsubscript{4} mass fraction contours of methane-air flame: incoming velocity of 0.3 m/s, equivalence ratio of 0.55, initial temperature of 800 K, convective heat transfer coefficients of 5 W/m\textsuperscript{2}K and 10 W/m\textsuperscript{2}K (d=2 mm, L=12 mm)

Figure 7-17 CO\textsubscript{2}, CO and H\textsubscript{2}O mass fraction contours of methane-air flame: incoming velocity of 0.3 m/s, equivalence ratio of 0.55, initial temperature of 800 K, convective heat transfer coefficients of 5 W/m\textsuperscript{2}K and 10 W/m\textsuperscript{2}K (d=2 mm, L=12 mm)

7.6.2 Effect of heat transfer coefficient with and without radiation

Section 7.6.1 showed that assuming no heat loss via radiation, a flame can be sustained within a 2 mm diameter micro combustor both at an initial temperature of 300 K and at a low equivalence ratio of 0.55 with an initial temperature of 800 K. In this section, the effect of heat transfer coefficient with and without radiation heat loss on the flame stability and combustion characteristics at an initial temperature of 800 K, an equivalence ratio of 1.0 and an incoming flow velocity of 0.3 m/s is presented. The convective heat transfer coefficients are again chosen to be 5, 10 and 50 W/m\textsuperscript{2}K, whereas the wall emissivity is chosen to be 0 and 0.2, which represent reflective and high polished surfaces, respectively.

Without radiation heat loss, a wide, high temperature zone with a maximum flame temperature of 2221 K is obtained when the convective heat transfer coefficient is 5 W/m\textsuperscript{2}K. By increasing the convective heat transfer coefficient up to 10 W/m\textsuperscript{2}K, the high temperature zone narrows. Further increasing the convective heat transfer coefficient up to 50 W/m\textsuperscript{2}K, a cone shaped high temperature zone is observed with a lower maximum flame temperature.

Due to the heat loss via convection, the flame temperature decreases through the combustor length, resulting in low outlet temperatures. This temperature drop increases with increasing convective heat transfer coefficient. Flame temperature decreases by 550 K with 5 W/m\textsuperscript{2}K convective heat transfer coefficient through the combustor length. When doubling the
heat transfer coefficient, the flame temperature also drops twofold. Using a 50 W/m²K heat transfer coefficient, the flame temperature drops dramatically with a decrease of 1750 K.

Although flame temperature and velocity contours display differences with varying convective heat transfer coefficients, species concentrations do not exhibit dramatic changes. As can be seen from Figure 7-18, CH₄ is consumed completely very close to the inlet with all convective heat transfer coefficients with and without radiation heat loss. In all cases, flat flames occur very close to the inlet. With convective heat coefficient of 5 and 10 W/m²K, dissociation of CO₂ due to the high flame temperature can be seen from the CO₂ and CO mass fraction contours, as shown in Figure 7-19.

Figure 7-18 Temperature, velocity and CH₄ mass fraction contours of methane-air flame: incoming velocity of 0.3 m/s, equivalence ratio of 1.0, initial temperature of 800 K, convective heat transfer coefficients of 5 W/m²K, 10 W/m²K and 50 W/m²K, emissivity of 0 and 0.2

Figure 7-19 CO₂, CO and H₂O mass fraction contours of methane-air flame: incoming velocity of 0.3 m/s, equivalence ratio of 1.0, initial temperature of 800 K, convective heat transfer coefficients of 5 W/m²K, 10 W/m²K and 50 W/m²K, emissivity of 0 and 0.2 (d=2 mm, L=12 mm)
When radiation heat loss is taken into account, outlet temperature decreases to less than the initial reactant temperature for all convective heat transfer coefficients. Similar cone shaped high temperature zones are observed with lower maximum flame temperatures compared to the results obtained whilst ignoring radiation heat loss. Flat flames occur very close to the inlet for all cases. When considering radiation heat loss, major species concentrations are not affected by increasing the convective heat transfer coefficient.

Although the maximum flame temperature decreases a little when taking into account the radiation loss, these results show that with low heat transfer coefficients, radiation loss has a marked effect on the flame temperature. On the other hand, with higher convective heat transfer coefficients, heat loss due to the radiation is very low compared with heat loss due to convection.

Heat loss through the outer wall has a significant effect on the flame temperature and the combustor exit temperature. Therefore, it is strongly recommended that the micro combustor not be exposed to the cold surrounding air directly. The double tube micro combustor of Marbach et al. [27] and Turkeli-Ramadan’s [46, 47] triple tube micro combustor are two good examples of preventing high heat loss from the micro combustor to the surrounding air. In these two designs, the combustion chambers exist at the core of the systems and are encapsulated by the heat exchanger parts. At the same time, they allow preheating of the reactants from the combustion products which improves the flame stability at higher mass flow rates.

7.7 The effect of preheating at the same mass flow rate

In this study, incoming flow velocity is chosen as an input for the model, and therefore in each case the volumetric flow rate is constant. However, preheating the reactants results in changing its density, which also results in mass flow rate changes.

As shown in section 7.4.1, with low mass flow rates at an initial temperature of 800 K, although the maximum flame temperature is obtained with this initial temperature, the outlet temperature is the lowest when compared to those with initial temperatures of 500 K, 600 K and 700 K. In this section, the effects of preheating the reactants on the combustion characteristics while keeping the mass flow rate constant, instead of volumetric flow rate, are presented.
Temperature, velocity and major species concentrations are compared at the same mass flow rate of $6.3742 \times 10^{-7}$ kg/s at an initial temperature of 500 K and 800 K, with an equivalence ratio of 0.9. Both initial temperatures have a cone shaped high temperature zone. The maximum flame temperature is predicted as 1882 K with an initial temperature of 500 K. By increasing the initial temperature up to 800 K, the maximum flame temperature also increases up to a value of 2065 K. With both initial temperatures, flat flame burning occurs very close to the inlet. This is concluded from the major species contours, which are shown in both Figure 7-20 and Figure 7-21. Major species concentrations display similar patterns with a little delay at an initial temperature of 500 K.

As can be seen from Figure 7-21, similar CO contour plots are predicted at initial temperatures of 500 K and 800 K. Furthermore, from these contours, it may be concluded that preheating the reactants does not affect the CO emissions. For both initial temperatures, CO emissions are very low and within the mass fraction range of 0-0.004. Newburn and Agrawal [121] showed experimentally that preheating does not affect the CO emissions. CO$_2$ and H$_2$O contours display the same trends for both initial temperatures, except for slight differences at the outlet.
As can be seen from Figure 7-20, although the maximum flame temperature increases with increasing initial reactant temperature, the outlet temperature remains same for both initial temperatures at low mass flow rates. This means that at higher initial temperature, heat loss increases, since the flame temperature becomes higher. At this condition, the heat loss is higher than the energy input resulting in a lower outlet temperature than the initial reactant temperature. On the other hand, at an initial temperature of 500 K, the heat loss is lower than the energy input and results in a slightly higher outlet temperature than the initial reactant temperature. From these results, it can be concluded that at low mass flow rates (incoming flow velocities) preheating the reactants does not improve the flame stability and combustion characteristics. However, preheating the reactants does improve and widen flame stability at higher mass flow rates (incoming flow velocities).

In this study, conduction through the wall of the combustor was not modelled due to insufficient software resources. This is because including wall conduction increases the size of the elements in the simulations. However, conduction through the wall has two competing effects on the combustion behaviour. On the one hand, the axial conduction provides heat transfer from the post combustion region to the unburned upstream region. This will help to preheat the reactants and widens the flame stability. On the other hand, the radial conduction increases the heat loss via radiation and convection through the outer wall. With wall conduction, the flame can stabilize over a wider range of equivalence ratios and the blow out limit increases because wall conduction enhances preheating, thereby widening the flame stability. At low velocities, it does not affect the flame stability. How much upstream heat transfer occurs through the walls to the unburned upstream region depends on the thermal conductivity of the material and also the wall thickness. For example, with low thermal conductivity material, heat loss through the outer wall decreases, but at the same time preheating the reactants from the wall also decreases. The numerical work in this thesis is a preliminary work for future studies and including the wall conduction in the simulations is the next step for future studies.

7.8 Summary

In this chapter, two-dimensional numerical simulation results of premixed, laminar, lean methane-air flames at atmospheric pressure, formed in a circular micro combustor of 2 mm diameter with a non-adiabatic wall were presented. The flame was investigated by employing a skeletal mechanism consisting of 16 species and 41 reactions. The effect of
preheating the reactants at both low and high incoming flow velocities on the flame stability and combustion characteristics were presented. It was found that preheating the reactants has a significant contribution on widening the flame stability at high incoming flow velocities and/or higher mass flow rates.
8 CONCLUSIONS AND SUGGESTIONS FOR FUTURE STUDIES

In this study, both experimental and numerical investigations were conducted in order to investigate the effects of preheating the reactants on the combustion characteristics of micro combustion.

The main purpose of this research is to develop a micro combustor for an ultra micro gas turbine engine with a high combustion efficiency, wide flame stability, minimum pressure loss and clean combustion. In order to achieve this, preheating the reactants was applied and its effects were investigated in two different parts. In the experimental part, flat flame combustion was investigated at a fundamental level with a 46 mm diameter combustor manufactured in the laboratory. In the numerical part, micro combustion was investigated within a 2 mm diameter micro combustor tube.

The findings and conclusions drawn from both the experimental and numerical research are listed as below.

**Experimental research**

- The experimental results of the flat flame combustor showed that flat flame burning method provides clean, stable combustion with low pressure loss through the used flame holders.
- Preheating the reactants widened the flame stability limit. The flame stability limit measurements were performed between air mass flow rates of 0.38 g/s to 1.34 g/s. With preheating the reactants up to 600 K, flame stability limit decreased from an equivalence ratio of 0.53 to around an equivalence ratio of 0.40.
- At low and high air mass flow rates, and varying equivalence ratios, the flame shape and locations were investigated utilising New Zealand natural gas and 99.99 % pure methane. Flame location and shape changed with mass flow rate. At low mass flow rates, flat flame occurred and the flame was very close to the flame holder. On the other hand, with increasing mass flow rate, the flame moved downstream, albeit not in the shape of a flat flame. Instead, many steep conical flames formed with small conical angles. The small conical angles indicating that the normal component of the incoming flow velocity tried to balance with the burning velocity. In these conical flames both the root and tip of the conical flame moved downstream.
• At a constant air mass flow rate of 0.38 g/s the flame shape and behaviour with varying equivalence ratios were observed and photographed. At the very lean side of the stoichiometric, an unstable flame was observed, while with increasing equivalence ratio, the flame settled down on the surface of the flame holder and flat flames were observed. Close to the stoichiometric on both sides, in addition to the flat flame, a cone shaped glow along the combustor length was observed. It started to form a slightly red colour, then, with increasing input energy due to increasing equivalence ratio, its colour changed to a yellowish orange. With further increase of the equivalence ratio on the rich side of stoichiometric, the colour of the flat flame changed from blue to green.

• Preheating the reactants improved flat flame formation and widened the flat flame stability limit. Flat flame stabilization was investigated at equivalence ratios of 0.57, 0.62 and 0.68 in conjunction with preheating the reactants. At these equivalence ratios, a comparison of flame shape and stabilization was conducted, when the reactants were at room temperature and 600 K. When the reactants were at room temperature, with these equivalence ratios, unstable and flickering flames were observed. On the other hand, by preheating the reactants with external heaters, flame stabilization and flat flame formation were observed. Flat flame stabilization occurred with preheating the reactants thereby increasing the burning velocity. Flat flames occurred when the incoming flow velocity was equal to or less than the burning velocity.

• From the experimental results a relationship between the incoming flow velocities and empirical burning velocities, dependant on equivalence ratio and reactants temperature (from the literature), was presented.

• A new correlation was proposed for flat flame burners. From the relationship between the incoming velocity and burning velocity the new correlation was developed. The correlation was developed between mass flow rate, reactant temperature, air to fuel ratio and the diameter of the micro combustor. With this correlation, it is possible to determine the minimum combustor diameter which is required for stable flat flame combustion. Also, in order to have a stable flat flame at higher mass flow rates, the correlation enables the calculation of the required reactants temperature, and is a major contribution towards the design of micro combustors.

• At high mass flow rates or incoming flow velocities, flat flame burning method is not convenient, because it requires a larger surface area. In applications such as UMGT, where
size is very important, the flat flame burning method can be applied only at low mass flow rates or a cluster of micro combustors should be utilized.

- The equivalence ratios were determined from the exhaust gas emissions. The exhaust emission measurements were performed at both the lean and rich side of the stoichiometric. NOx and CO emissions were very low and over 99% combustion efficiencies were observed for both fuels at the lean side of the stoichiometric, which is the focal point for UMGТ applications. This experimental study showed that flat flame combustor provides very clean, almost complete combustion and is convenient for ultra micro gas turbine applications.

- The effect of using different flame holders were investigated in terms of flat flame formation and its durability. It was found that alumina ceramics are very brittle and are susceptible to crack formation, which prevents flat flame generation. In order to prevent the crack formation, the thickness of the flame holder may be increased, but this may result in high pressure loss through the flame holder. With the use of a perforated plate, acoustic interference was observed. Sintered stainless steel flame holders seem the most promising candidate for flat flame combustors.

- Measurements of pressure loss through different flame holders showed that pressure loss increased approximately with the square of the incoming flow velocity. The pressure loss was affected by both the pore size and thickness of the flame holder. When decreasing the pore size of the flame holder, pressure loss increased. Furthermore, when the flame holder thickness increased, the pressure loss also increased. It can be concluded that all flame holders have pressure losses of less than 5% up to an incoming flow velocity of 1.2 m/s.

**Numerical research**

- The effect of preheating the reactants on the flame stability and species concentrations was investigated two-dimensionally within a 2 mm diameter circular micro combustor tube. The flame was investigated with an adiabatic and non-adiabatic wall. The adiabatic wall case simulates a channel at the centre of a combustor which consists of a cluster of tubes. On the other hand, the non-adiabatic case simulates micro combustion. In addition, the adiabatic case provided the comparison of the results with the experimental data available in the literature, with which, the numerical predictions showed good correlation with, particularly for the values of flame temperature.
• A comparison of flame temperature, flame thickness and major species concentrations obtained by employing two different skeletal reaction mechanisms and a detailed mechanism were presented. This study shows that in CFD calculations, applying a second order upwind scheme and lower target residuals for convergence, are important for acquiring accurate predictions.

• The effect of increasing the reactant temperatures from 300 K to 800 K on the combustion stabilization and characteristics were shown. A comparison of incoming flow velocities of 0.3 m/s and 1m/s on the combustion stability and characteristics was also made. 0.3 m/s represents the low incoming flow velocity, whereas 1 m/s represents the high incoming flow velocity. Although the flame cannot be sustained within a 2 mm diameter micro combustor at an incoming flow velocity of 1 m/s at lower reactants temperature, by increasing the reactants temperature up to 500 K, the flame can be sustained with a conical shape. Further increasing the reactants temperature up to 800 K results in the flame moving upstream and becoming flat. In all the cases studied, the flame thickness was found to be less than 1 mm.

• Increasing the equivalence ratio, was found to increase the flame temperature and flatten the flame.

• In the non-adiabatic case, at low incoming flow velocities, preheating the reactants contributes neither to the flame stability nor the combustion characteristics. On the contrary, it results in low outlet temperature. However, it has a significant contribution to the widening of the flame stability at high incoming flow velocities and/or higher mass flow rates.

• The effects of convection and radiation heat losses through the outer wall, and their contribution to the flame instability at micro scale were also shown. In addition, the effect of the convective heat transfer coefficient was also investigated. Increasing the convective heat transfer coefficient does not affect the major species concentration significantly, although it does result in lower outlet temperature. With low convective heat transfer coefficients, radiation heat loss has a marked effect on the flame temperature. On the other hand, with higher convective heat transfer coefficients, heat loss due to radiation is very low compared with heat loss due to convection.

• This study shows that CFD is an important tool to understand the combustion and heat loss mechanisms at micro scales, when it may be very difficult to measure the flow parameters inside the micro combustor itself.
Suggestions for future studies are listed below:

- Although in the experimental study an external heater was used to preheat the reactants, in UMGT applications, preheating the reactants is recommended by using a heat exchanger, like HEX-Combustor, in which the reactants are heated from both the combustion products and the turbine exit gases.
- In order to use ceramic porous plates as flame holder, a thickness versus diameter optimization study is recommended.
- The acoustic interference phenomenon with the perforated plate flame holder and solutions to remedy this should be studied in more detail. Investigation of the effects of different hole diameter and hole to hole distances on the acoustic interference and combustion characteristics is suggested.
- A lifecycle determination study of the sintered stainless steel flame holder applying SEM (Scanning Electron Microscope) is recommended since continued exposure to the very high flame temperatures may lead to clogging and enlarging of the pore sizes. A further study on the effects of coatings on the extended lifecycle of stainless steel flame holders is suggested.
- In addition to the radiation and convective heat loss, numerical investigation of heat transfer along the axial direction in the wall is recommended.
- An investigation of flame characteristics on the surface of a flame holder in two-dimensions with a skeletal reaction mechanism is suggested.
Appendices

A1 Estimation of molar mass and LHV of natural gas

The composition of New Zealand pipeline natural gas was provided by Ben Smith from Vector Limited Company. The composition was sampled in July 2012.

Table A-1 Chemical compositions of natural gas with the corresponding mole and mass fractions and $Q_{LHV}$ of its constituents

<table>
<thead>
<tr>
<th>Gas components</th>
<th>% Mole fraction</th>
<th>Molar mass</th>
<th>Mass fraction</th>
<th>$Q_{LHV}$ (MJ/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(i)</td>
<td>($y_i$)</td>
<td>($M_i$) [152]</td>
<td>($m_f_i$)</td>
<td>[152]</td>
</tr>
<tr>
<td>Methane</td>
<td>82.0201</td>
<td>16.043</td>
<td>0.651</td>
<td>50.029</td>
</tr>
<tr>
<td>Ethane</td>
<td>7.3924</td>
<td>30.070</td>
<td>0.110</td>
<td>47.509</td>
</tr>
<tr>
<td>Propane</td>
<td>3.134</td>
<td>44.097</td>
<td>0.068</td>
<td>46.334</td>
</tr>
<tr>
<td>n-Butane</td>
<td>0.5891</td>
<td>58.123</td>
<td>0.017</td>
<td>45.699</td>
</tr>
<tr>
<td>I-Butane</td>
<td>0.5366</td>
<td>58.123</td>
<td>0.015</td>
<td>45.699</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>0.0927</td>
<td>72.151</td>
<td>0.003</td>
<td>44.982</td>
</tr>
<tr>
<td>I-pentane</td>
<td>0.1244</td>
<td>72.151</td>
<td>0.004</td>
<td>44.982</td>
</tr>
<tr>
<td>Hexane</td>
<td>0.0551</td>
<td>86.177</td>
<td>0.002</td>
<td>44.763</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0.4251</td>
<td>28.013</td>
<td>0.006</td>
<td>0</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>5.6306</td>
<td>44.010</td>
<td>0.123</td>
<td>0</td>
</tr>
</tbody>
</table>

The mass fraction of each component can be expressed as [117]:

$$m_f_i = \frac{y_i M_i}{M_{NG}}$$  \hspace{1cm} (A1)

where $m_f_i$ is the mass fraction, $y_i$ is the molar fraction and $M_i$ is the molar mass of component $i$. $M_{NG}$ is the molar mass of the natural gas and can be calculated by using the following equation:

$$M_{NG} = \sum_i y_i M_i$$  \hspace{1cm} (A2)

The lower heating value ($Q_{LHV}$) of the natural gas can be calculated by the given equation:
Using the above equations the molar mass and $Q_{LHV}$ of the natural gas are calculated as 20.22 kg/kmol and 42.87 MJ/kg.
A2 Sierra Smart Trak mass flow controller working principle

The working principle of the Sierra Smart Trak mass flow controller is based on heat transfer and the first law of thermodynamics. Gas enters the mass flow controller flow body and splits into two flow paths as shown in Figure A-1a. One of these flow paths passes through the sensor tube and the other through laminar flow bypass (or often called laminar flow element (LFE)). The sensor tube is surrounded by two resistance temperature detector (RTD) coils which direct a constant amount of heat into the gas stream. During operation, the gas carries this heat from the upstream coil to the downstream coil. The temperature difference between the coils is measured by the Sierra Smart Trak microprocessor and from the temperature difference the output signal is calculated. Figure A-1b shows the flow measuring principle of Sierra mass flow controller.

![Figure A-1 a) Flow paths through Sierra Smart Trak 100 Series, b) Flow measuring principle [153]]
A3 K-Factor calculation using Sierra Smart-Trak 2 Series with other gases

Sierra mass flow controllers are programmed for 10 gases. These gases are air, argon, CO₂, CO, helium, hydrogen, methane, nitrogen, nitrous oxide and oxygen. If one of these gases is used, selecting the Dial-A-Gas feature in the Pilot Module, the mass flow controller adjusts the output automatically. However, for natural gas a conversion factor calculation was performed. Sierra Smart-Trak 2 Series 100 instruction manual provides the K-factors and thermodynamic properties of commonly used gases.

Using the following fundamental relationship, a gas other than those mentioned above can be calibrated.

$$\frac{Q_1}{Q_2} = \frac{K_1}{K_2}$$  \hspace{1cm} (A4)

where Q is the volumetric rate of the gas referenced to standard conditions of 0 °C and 760 mmHg, and K is the K-factor. 1 refers to the actual gas and 2 refers to the reference gas.

The K-factor is derived from applying the first law of thermodynamics to the sensor tube.

Sierra Smart Trak 2 Series mass flow meter and controller instruction manual provides the K-factor calculations for only a single gas. However, the New Zealand natural gas consists of many gases. Therefore, K-factor calculations for gas mixtures were found in the Sierra 820 Series Top-Trak mass flow meter instruction manual [154]. Since these two mass flow meters and controllers are working in the same principle, K-factor calculations for gas mixtures from the Sierra 820 Series Top-Trak mass flow meters instruction manual is used in the calculations.

The relationship between the heat applied to the sensor tube and mass flow rate can be written as

$$H = \frac{\dot{m}C_p\Delta T}{N}$$  \hspace{1cm} (A5)

where H is the constant amount of heat applied to the sensor tube, \(\dot{m}\) is the mass flow rate of the gas (gm/min), \(C_p\) is the coefficient of specific heat of the gas (Cal/gm) and is given in the manual Tables (at 0 °C). \(\Delta T\) is the temperature difference between the downstream and upstream coils and N is a correction factor for the molecular structure of the gas given by Table A-2.
Table A-2 Correction factor for the molecular structure of the gas [154]

<table>
<thead>
<tr>
<th>Number of atoms in the gas molecule</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monatomic</td>
<td>1.040</td>
</tr>
<tr>
<td>Diatomic</td>
<td>1.000</td>
</tr>
<tr>
<td>Triatomic</td>
<td>0.941</td>
</tr>
<tr>
<td>Polyatomic</td>
<td>0.880</td>
</tr>
</tbody>
</table>

The mass flow rate can also be expressed by

\[ \dot{m} = \rho Q \quad (A6) \]

where, \( \rho \) is the gas density at standard conditions (g/l) and is given in the instruction manual tables (at 0 °C, 760 mmHg).

The temperature difference, \( \Delta T \), is proportional to the output voltage, \( E \), of the mass flow controller and can be written as

\[ \Delta T = aE \quad (A7) \]

where \( a \) is a constant.

When equations (A6) and (A7) are combined and inserted into equation (A6), the flow rate becomes

\[ Q = \left( \frac{bN}{\rho C_p} \right) \quad (A8) \]

where \( b \) is a constant if the output voltage is constant.

\[ b = H/aE \quad (A9) \]

The ratio of the flow rate for an actual gas to the flow rate of a reference gas can be written as follows by combining equations (A4) and (A8).

\[ Q_1/Q_2 = K_1/K_2 = \left( \frac{N_1/\rho_1 C_{p_1}}{N_2/\rho_2 C_{p_2}} \right) \quad (A10) \]

When the actual gas is a mixture, as in the case of natural gas, the equivalent values of \( \rho, C_p \), and \( N \) for a gas mixture can be calculated as follows:

The equivalent gas density can be written as

\[ \rho = \frac{\sum \dot{m}_i \rho_i}{\dot{m}_T} \quad (A11) \]

where \( \dot{m}_T \) is the total mass flow rate, \( \dot{m}_T = \sum \dot{m}_i \) (gm/min), and \( i \) refers to the gas number.
The equivalent specific heat can also be calculated as

\[ C_p = \sum F_i C_{pi} \quad (A12) \]

where \( F_i = \frac{\dot{m}_i \rho_i}{\dot{m}_T \rho} \)

The equivalent value of \( N \) can be written as

\[ N = \sum \frac{\dot{m}_i}{\dot{m}_T} N_i \quad (A13) \]

It was informed in the manual that when the K-factors calculated from the above equations is used, the inaccuracy of the measurement can range from ±5 to 10% [154].

A comparison of equivalence ratios calculated from Sierra mass flow controller reading against the equivalence ratios calculated from the exhaust emissions was made and presented in Figure A-2. In this figure, a comparison of equivalence ratios calculated from the Micro Motion mass flow meter readings against equivalence ratios from the exhaust emissions is also presented. Sierra mass flow meter readings were corrected using the above equations for K-factor conversion. Applying the K-factor conversions there is a substantial difference between the equivalence ratios. A maximum of around 13 % discrepancy was found between the equivalence ratios calculated from the exhaust emissions and Sierra mass flow meter readings.

![Figure A-2 Comparison of equivalence ratios calculated from mass flow meter and controller readings and exhaust emissions](image-url)
A4 Micro Motion mass flow meter working principle

The Micro Motion flow meter measures fluid mass in motion. The Micro Motion mass flow meter has dual parallel flow tubes and fluid entering the sensor is split with half of the fluid passing through each flow tube. During operation, a drive coil is energized causing the tubes to oscillate in opposition to one another. When fluid is moving through these tubes, coriolis forces are induced in both the inlet and outlet legs of both flow tubes causing the flow tubes to twist in opposition to each other. The amount of twist is proportional to the mass flow rate of fluid passing through the tubes. More information can be found in reference [155].
A5 Uncertainty calculation of the K type thermocouples

A5.1 K type reactants thermocouple

An ice point check was followed by temperature measurements. The true temperature was obtained by adding a correction to the reading.

The curve fit equation of the reactants K type thermocouple is as follows

\[
y = 3.9241 \times 10^{-8}x^3 - 4.9914 \times 10^{-5}x^2 + 1.7290 \times 10^{-2}x + 8.5012 \times 10^{-1}
\]  
(A14)

where \( x \) is the thermocouple reading.

Total uncertainty is calculated by the quadrature sum of the individual uncertainties. These are random residual uncertainty, \( U_{\text{res}} \), variations in the spatial (axial and radial), \( U_{\text{axial}} \) and \( U_{\text{radial}} \), thermocouple inhomogeneity, \( U_{\text{in}} \), and uncertainty due to hysteresis, \( U_{\text{hys}} \),

\[
U_{\text{total}} = \left( U_{\text{res}}^2 + U_{\text{axial}}^2 + U_{\text{radial}}^2 + U_{\text{in}}^2 + U_{\text{hys}}^2 \right)^{1/2}
\]  
(A15)

Thermocouple inhomogeneity can be calculated by the given equation

\[
U_{\text{in}}(T) = 0.15 + 0.0003T + 0.000006T^2
\]  
(A16)

where \( T \) is in Celsius.

Uncertainty due to hysteresis is calculated by the difference between the pre-calibration and post-calibration ice points.

The expanded uncertainty can be calculated by

\[
U_{\text{exp}} = kU_{\text{total}}
\]  
(A17)

where \( k \) is the coverage factor, which is 1.96 at 95% confidence interval.

The uncertainty in the corrected thermometer readings is estimated to be \( \pm 6.06^\circ \text{C} \) with a 95% confidence level, and a coverage factor, \( K \), of 1.96.

A5.2 0.25 mm diameter K type thermocouple

The curve fit equation of 0.25 mm diameter K type thermocouple is as follows

\[
y = 3.87 \times 10^{-8}x^3 - 3.18 \times 10^{-5}x^2 + 9.70 \times 10^{-3}x + 1.29
\]  
(A18)
The uncertainty in the corrected thermometer readings is estimated to be $\pm 5.85^\circ C$ with a 95% confidence level, and a coverage factor, $K$, of 1.96.

**A5.3 0.5 mm diameter K type thermocouple**

Curve fit equation of 0.5 mm diameter K type thermocouple is as follows

$$y = 2.48 \times 10^{-8}x^3 - 2.41 \times 10^{-5}x^2 + 9.72 \times 10^{-3}x + 1.14$$  \hspace{1cm} (A19)

The uncertainty in the corrected thermometer readings is estimated to be $\pm 5.94^\circ C$ with a 95% confidence level, and a coverage factor, $K$, of 1.96.
A6 Thermocouple radiation correction

Measurements error due to the radiation is calculated by the heat balance of the thermocouple bead [156]. The convection from the flame is equal to the radiation to the surroundings. From the below figure, flame temperature can be calculated as follows.

\[ \dot{Q}_{\text{conv}} = \dot{Q}_{\text{rad}} \quad (A20) \]
\[ \dot{Q}_{\text{conv}} = hA(T_{\text{flame}} - T_{\text{TC}}) \quad (A21) \]
\[ \dot{Q}_{\text{rad}} = \varepsilon_{\text{TC}}\sigma A(T_{\text{TC}}^4 - T_{\text{surr}}^4) \quad (A22) \]
\[ h = \frac{2\lambda}{d} \quad (A23) \]

where “TC” denotes thermocouple reading, “surr” denotes surroundings.

The emission coefficient of the bead is approximated as below

\[ \varepsilon = 9.6 \times 10^{-5}T_{\text{TC}} + 0.03 \quad (A24) \]

The flame temperature becomes

\[ T_{\text{flame}} = T_{\text{TC}} + \frac{\varepsilon_{\text{TC}}\sigma d}{2\lambda}(T_{\text{TC}}^4 - T_{\text{surr}}^4) \quad (A25) \]
A7 SK16 reaction mechanism

Skeletal mechanism for methane oxidation by ANSYS Fluent (16 species and 41 reactions) (SK16)

Reaction mechanism rate coefficients in the form \( k_f = AT^\beta \exp(-E_a/RT) \). Units are moles, seconds, Kelvins and calories/mole

<table>
<thead>
<tr>
<th>SPECIES</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂O</td>
</tr>
<tr>
<td>CO</td>
</tr>
<tr>
<td>O₂</td>
</tr>
<tr>
<td>CH₄</td>
</tr>
<tr>
<td>H₂</td>
</tr>
<tr>
<td>OH</td>
</tr>
<tr>
<td>H</td>
</tr>
<tr>
<td>O</td>
</tr>
<tr>
<td>CH₃</td>
</tr>
<tr>
<td>CH₂O</td>
</tr>
<tr>
<td>HCO</td>
</tr>
<tr>
<td>HO₂</td>
</tr>
<tr>
<td>CH₃O</td>
</tr>
<tr>
<td>N₂</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>REACTIONS</th>
<th>( A_k )</th>
<th>( \beta_k )</th>
<th>( E_k )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 H+O₂=OH+O</td>
<td>1.59E+17</td>
<td>-0.927</td>
<td>16874.0</td>
</tr>
<tr>
<td>2 O+H₂=OH+H</td>
<td>3.87E+04</td>
<td>2.700</td>
<td>6262.0</td>
</tr>
<tr>
<td>3 OH+H₂=H₂O+H</td>
<td>2.16E+08</td>
<td>1.510</td>
<td>3430.0</td>
</tr>
<tr>
<td>4 OH+OH=O+H₂O</td>
<td>2.10E+08</td>
<td>1.400</td>
<td>-397.0</td>
</tr>
<tr>
<td>5 H+H+M=H₂+M</td>
<td>6.40E+17</td>
<td>-1.000</td>
<td>0.0</td>
</tr>
<tr>
<td>6 H+OH+M=H₂O+M</td>
<td>8.40E+21</td>
<td>-2.000</td>
<td>0.0</td>
</tr>
<tr>
<td>7 H+O₂+M=HO₂+M</td>
<td>7.00E+17</td>
<td>-0.800</td>
<td>0.0</td>
</tr>
<tr>
<td>8 HO₂+H=OH+OH</td>
<td>1.50E+14</td>
<td>0.000</td>
<td>1004.0</td>
</tr>
<tr>
<td>9 HO₂+H₂=H₂O+H</td>
<td>2.50E+13</td>
<td>0.000</td>
<td>693.0</td>
</tr>
<tr>
<td>10 HO₂+O₂+OH</td>
<td>2.00E+13</td>
<td>0.000</td>
<td>0.0</td>
</tr>
<tr>
<td>11 HO₂+OH=H₂O+O₂</td>
<td>6.02E+13</td>
<td>0.000</td>
<td>0.0</td>
</tr>
<tr>
<td>12 H₂O₂+M=OH+OH+M</td>
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<tr>
<td>13 CO+OH=CO₂+H</td>
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<td>14 CO+O₂=CO₂+M</td>
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<td>15 HCO+H=H₂+CO</td>
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<td>16 HCO+O=OH+CO</td>
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<td>17 HCO+OH=H₂O+CO</td>
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<td>18 HCO+O₂=HO₂+CO</td>
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<tr>
<td>19 HCO+M=H⁺+CO+M</td>
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<tr>
<td>21 CH₂O+O=HCO+OH</td>
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<td>22 CH₂O+OH=HCO+H₂O</td>
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<tr>
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<td></td>
<td>Reaction</td>
<td>Rate</td>
<td>Energy</td>
</tr>
<tr>
<td>---</td>
<td>----------------------------------------------</td>
<td>-------</td>
<td>--------</td>
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<tr>
<td>39</td>
<td>CH$_3$O+OH=CH$_2$O+H$_2$O</td>
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<td>41</td>
<td>CH$_3$O+M=CH$_2$O+H+M</td>
<td>1.00E+14</td>
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</table>
**A8 SK17 reaction mechanism**

Skeletal mechanism for methane oxidation by Lu et al. (17 species and 73 reactions) (SK17)

Reaction mechanism rate coefficients in the form \( k_f = A \exp(-E_a/RT) \). Units are moles, seconds, Kelvins and calories/mole.

<table>
<thead>
<tr>
<th>SPECIES</th>
<th>REACTION</th>
<th>( A_k )</th>
<th>( \beta_k )</th>
<th>( E_k )</th>
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<tbody>
<tr>
<td>H₂</td>
<td>O+H+M=OH+M</td>
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<tr>
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<td>O+CH₂=H+HCO</td>
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<tr>
<td>CH₂</td>
<td>O+CH₂=H₂+CO</td>
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<tr>
<td>CO</td>
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<td>0.0</td>
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<tr>
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<td>47800.0</td>
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<tr>
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<td>O₂+H⁺+CO₂</td>
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<tr>
<td>Reaction</td>
<td>K = $10^x$</td>
<td>$\Delta H^\circ$</td>
<td>$\Delta S^\circ$</td>
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<tr>
<td>---------------------------------------------------</td>
<td>-------------</td>
<td>------------------</td>
<td>------------------</td>
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</tr>
<tr>
<td>$\ce{H+CH2OH=CH2(S)+H2O}$</td>
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<tr>
<td>$\ce{H2+CO(+M)=CH2O(+M)}$</td>
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<tr>
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<td>$\ce{OH+CH2=H+CH2O}$</td>
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<tr>
<td>$\ce{OH+CH2(S)=H+CH2O}$</td>
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<tr>
<td>$\ce{HO2+CH3=O2+CH4}$</td>
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<tr>
<td>$\ce{HO2+CO=OH+CO2}$</td>
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<tr>
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<tr>
<td>$\ce{CH2(S)+N2=CH2+N2}$</td>
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<tr>
<td>$\ce{CH2(S)+O2=H+OH+CO}$</td>
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<tr>
<td>$\ce{CH2(S)+O2=CO+H2O}$</td>
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<tr>
<td>$\ce{CH2(S)+H2=CH3+H}$</td>
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<td>$\ce{CH2(S)+H2O=CH2+H2O}$</td>
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<tr>
<td>$\ce{CH2(S)+CO2=CH2+CO2}$</td>
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<tr>
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<td>$\ce{HCO+M=H+CO+M}$</td>
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## A9 GRI 3.0 reaction mechanism

GRI 3.0 reaction mechanism for CHEMKIN-CFD provided by Reaction Design.

Reaction mechanism rate coefficients in the form $k_f = AT^{\beta} \exp(-E_a/RT)$. Units are moles, seconds, Kelvins and calories/mole

| SPECIES |
|-------------------|-------------------|-------------------|-------------------|
| $H_2$ $O$ $O_2$ $OH$ $H_2$ $O$ $HO_2$ $H_2$ $O_2$ $C$ $CH$ $CH_2$ $CH_2(S)$ $CH_3$ $CH_4$ $CO$ $CO_2$ $HCO$ $CH_2O$ $CH_2OH$ $CH_2(OH)$ $C_2$ $H$ $C_2$ $H_2$ $C_2H_2$ $C_2H_4$ $C_2H_5$ $C_2H_6$ $HCCO$ $CH_2CO$ $HCCOH$ $N$ $NH$ $NH_2$ $NH_3$ $NNH$ $NO$ $NO_2$ $N_2$ $O$ $HNO$ $CN$ $HCN$ $HCN$ $HCO$ $HCN$ $HNO$ $HCCO$ $HNO$ $HCN$ $NCO$ $N_2$ $CH_2CHO$ $CH_3CHO$ |

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<th>$\beta_k$</th>
<th>$E_k$</th>
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157
87 OH+H₂O₂<=>HO₂+H₂O  2.00E+12  0.000  427.0
88 OH+H₂O₂<=>HO₂+H₂O  1.70E+18  0.000  29410.0
89 OH+C<=>H+CO   5.00E+13  0.000  0.0
90 OH+CH<=>H+HCO   3.00E+13  0.000  0.0
91 OH+CH₂<=>H+CH₂O   2.00E+13  0.000  0.0
92 OH+CH₃<=>CH+H₂O   1.13E+07  2.000  3000.0
93 OH+CH₃(S)<=>H+CH₂O   3.00E+13  0.000  0.0
94 OH+CH₃(+M)<=>CH₂OH(+M)  2.79E+18  -1.430  1330.0
95 OH+CH₂<=>CH₂+H₂O   5.60E+07  1.600  5420.0
96 OH+CH₃<=>CH₂(S)+H₂O   6.44E+17  -1.340  1417.0
97 OH+CH₃<=>CH₃+H₂O   1.00E+08  1.600  3120.0
98 OH+CO<=>H+CO₂   4.76E+07  1.228  70.0
99 OH+HCO<=>H₂O+CO   5.00E+13  0.000  0.0
100 OH+CH₂O<=>HCO+H₂O   3.43E+09  1.180  -447.0
101 OH+CH₃OH<=>H₂O+CH₂O   5.00E+12  0.000  0.0
102 OH+CH₃O<=>H₂O+CH₂O   5.00E+12  0.000  0.0
103 OH+CH₂OH<=>CH₂OH+H₂O   1.44E+06  2.000  -840.0
104 OH+CH₃OH<=>CH₂O+H₂O   6.30E+06  2.000  1500.0
105 OH+CH₄<=>H+HCCO   2.00E+13  0.000  0.0
106 OH+CH₄<=>H+CH₂CO   2.18E-04  4.500  -1000.0
107 OH+CH₂<=>H+HCCOH   5.04E+05  2.300  13500.0
108 OH+CH₂<=>CH₂H₂O   3.37E+07  2.000  14000.0
109 OH+CH₂<=>CH₃+CO   4.83E-04  4.000  -2000.0
110 OH+CH₂<=>H₂O+CH₂   5.00E+12  0.000  0.0
111 OH+CH₃<=>CH₃H₂+H₂O   3.60E+06  2.000  2500.0
112 OH+CH₃<=>CH₃H₂+H₂O   3.54E+06  2.120  870.0
113 OH+CH₂CO<=>HCCO+H₂O   7.50E+12  0.000  2000.0
114 2HO₂<=>O₂+H₂O₂   1.30E+11  0.000  -1630.0
115 2HO₂<=>O₂+H₂O₂   4.20E+14  0.000  12000.0
116 HO₂+CH<=>OH+CH₂O   2.00E+13  0.000  0.0
117 HO₂+CH₃<=>O₂+CH₄   1.00E+12  0.000  0.0
118 HO₂+CH₃<=>OH+CH₂O   3.78E+13  0.000  0.0
119 HO₂+CO<=>OH+CO₂   1.50E+14  0.000  23600.0
120 HO₂+CH₂O<=>HCO+H₂O₂   5.60E+06  2.000  12000.0
121 C+O₂<=>O+CO   5.80E+13  0.000  576.0
122 C+CH<=>H+C₂H   5.00E+13  0.000  0.0
123 C+CH₃<=>H+C₂H₂   5.00E+13  0.000  0.0
124 CH+O₂<=>O+HCO   6.71E+13  0.000  0.0
125 CH₂H₂<=>H+CH₂    1.08E+14  0.000  3110.0
126 CH₂H₂O<=>H+CH₂O   5.71E+12  0.000  -755.0
127 CH₂+CH₂<=>H+C₂H₂   4.00E+13  0.000  0.0
128 CH₂+CH₃<=>H+C₂H₃   3.00E+13  0.000  0.0
129 CH₂+CH₄<=>H+C₂H₄   6.00E+13  0.000  0.0
130 CH+CO(+M)<=>HCCO(+M)   5.00E+13  0.000  0.0
131 CH+CO₂<=>HCO+CO   1.90E+14  0.000  15792.0
132 CH+CH₂O<=>H+CH₂CO   9.46E+13  0.000  -515.0
133 CH+HCCO<=>CO+CH₂H   5.00E+13  0.000  0.0
134 CH₂O<=>OH+H+CO   5.00E+12  0.000  1500.0
135 CH₂+H₂<=>H+CH₃   5.00E+05  2.000  7230.0
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<td>Reaction</td>
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<td>Preexponential Factor</td>
<td>Temperature (K)</td>
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<td>HCN + O ↔ CN + OH</td>
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234  HCN+OH <=> NH_2+CO  1.60E+02  2.560  9000.0
235  H+HCN(+M) <=> H_2CN(+M)  3.30E+13  0.000  0.0
236  H_2CN+N <=> N_2+CH_2  6.00E+13  0.000  400.0
237  C+N_2 <=> CN+N  6.30E+13  0.000  46020.0
238  CH+N_2 <=> HCN+N  3.12E+09  0.880  20130.0
239  CH+N_2(+M) <=> HCNN(+M)  3.10E+12  0.150  0.0
240  CH_2+N_2 <=> HCN+NH  1.00E+13  0.000  74000.0
241  CH_2(S)+N_2 <=> NH+HCN  1.00E+11  0.000  65000.0
242  C+NO <=> CN+O  3.30E+13  0.000  0.0
243  C+NO <=> CO+N  2.90E+13  0.000  0.0
244  CH+NO <=> H+NCO  3.12E+09  0.880  20130.0
245  CH+NO <=> N+HCO  2.46E+13  0.000  0.0
246  CH+NO <=> N+HCO  2.46E+13  0.000  0.0
247  CH_2+NO <=> H+HNCO  3.10E+17  0.000  0.0
248  CH_2+NO <=> OH+HCN  2.90E+13  0.000  760.0
249  CH_2+NO <=> H+HCNO  3.80E+13  0.000  580.0
250  CH_2(S)+NO <=> H+HNCO  3.10E+17  0.000  0.0
251  CH_2(S)+NO <=> OH+HCN  3.80E+13  0.000  0.0
252  CH_2+NO <=> H+HCNO  3.60E+13  0.000  28800.0
253  CH_2(NO) <=> H_2CN+OH  1.00E+12  0.000  21750.0
254  CH_2+NO <=> H_2CN+OH  2.20E+13  0.000  0.0
255  HC(NO)O+H+H+H+N_2  2.00E+12  0.000  0.0
256  HC(NO)O+H+H+HCN+NO  2.00E+12  0.000  0.0
257  HC(NO)O+H+H+HCN+NO  1.20E+13  0.000  0.0
258  HC(NO)O+H+H+HCO+N_2  1.20E+13  0.000  0.0
259  HC(NO)O+H+H+HCO+N_2  1.00E+14  0.000  0.0
260  HC(NO)O+H+H+HCO+N_2  1.00E+14  0.000  0.0
261  HC(NO)O+H+H+HCO+N_2  9.80E+07  1.410  85000.0
262  HC(NO)O+H+H+HCO+N_2  1.50E+08  1.570  440000.0
263  HC(NO)O+H+H+HCO+N_2  2.20E+06  2.110  114000.0
264  HC(NO)O+H+H+HCO+N_2  2.25E+07  1.700  3800.0
265  HC(NO)O+H+H+HCO+N_2  1.05E+05  2.500  13300.0
266  HC(NO)O+H+H+HCO+N_2  3.30E+07  1.500  3600.0
267  HC(NO)O+H+H+HCO+N_2  3.30E+06  1.500  3600.0
268  HC(NO)O+H+H+HCO+N_2  1.18E+16  0.000  84720.0
269  HC(NO)O+H+H+HCO+N_2  2.10E+15  -0.690  2850.0
270  HC(NO)O+H+H+HCO+N_2  2.70E+11  0.180  2120.0
271  HC(NO)O+H+H+HCO+N_2  1.70E+14  -0.750  2890.0
272  HC(NO)O+H+H+HCO+N_2  2.00E+07  2.000  2000.0
273  HC(NO)O+H+H+HCO+N_2  9.00E+12  0.000  0.0
274  HC(NO)O+H+H+HCO+N_2  6.10E+14  -0.310  290.0
275  HC(NO)O+H+H+HCO+N_2  3.70E+12  0.150  -90.0
276  HC(NO)O+H+H+HCO+N_2  5.40E+05  2.400  9915.0
277  HC(NO)O+H+H+HCO+N_2  5.00E+07  1.600  955.0
278  HC(NO)O+H+H+HCO+N_2  9.40E+06  1.940  6460.0
279  HC(NO)O+H+H+HCO+N_2  1.00E+13  0.000  14350.0
280  HC(NO)O+H+H+HCO+N_2  6.16E+15  -0.752  345.0
281  HC(NO)O+H+H+HCO+N_2  3.25E+12  0.000  -705.0
282  HC(NO)O+H+H+HCO+N_2  3.00E+12  0.000  11300.0
283  HC(NO)O+H+H+HCO+N_2  3.37E+13  0.000  0.0
<table>
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<th>No.</th>
<th>Reaction</th>
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<th>$E$</th>
<th>$T$</th>
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<td>283</td>
<td>$O + CH_2(OH) \leftrightarrow CH_2(O) + O$</td>
<td>$6.70 \times 10^6$</td>
<td>1.830</td>
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<td>284</td>
<td>$O + CH_3 \leftrightarrow CH_2(O) + O$</td>
<td>$1.10 \times 10^{14}$</td>
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<tr>
<td>285</td>
<td>$OH + HO_2 \leftrightarrow O_2 + H_2O$</td>
<td>$5.00 \times 10^5$</td>
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<td>$OH + CH_2 \leftrightarrow H_2 + CH_2O$</td>
<td>$8.00 \times 10^0$</td>
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<td>$CH + H_2(+)M \leftrightarrow CH_3(+)M$</td>
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<td>$CH_2 + O_2 \leftrightarrow 2H + CO_2$</td>
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<td>$CH_2 + O_2 \leftrightarrow O + CH_2O$</td>
<td>$2.40 \times 10^2$</td>
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<td>1500.0</td>
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<td>$CH_2 + CH_2 \leftrightarrow 2H + C_2H_2$</td>
<td>$2.00 \times 10^0$</td>
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<td>$CH_2(S) + H_2 \leftrightarrow H_2 + CH_2O$</td>
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<td>$C_2H_4 + O_2 \leftrightarrow O + CH_2O$</td>
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<td>$C_2H_4 + O_2 \leftrightarrow HO_2 + C_2H_2$</td>
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<td>294</td>
<td>$O + CH_2(OH) \leftrightarrow OH + CH_3CHO$</td>
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<td>$O + CH_2CHO \leftrightarrow OH + CH_3 + CO$</td>
<td>$2.92 \times 10^2$</td>
<td>0.000</td>
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<td>$O_2 + CH_2CHO \leftrightarrow HO_2 + CH_3 + CO$</td>
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<td>$H + CH_2CHO \leftrightarrow CH_3 + H_2 + CO$</td>
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<td>$OH + CH_2CHO \leftrightarrow CH_3 + H_2O + CO$</td>
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<td>$O_2 + CH_2CHO \leftrightarrow OH + CO + CH_2O$</td>
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<td>$O_2 + CH_2CHO \leftrightarrow OH + 2HCO$</td>
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<td>$H + CH_2CHO \leftrightarrow CH_3 + HCO$</td>
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<td>$OH + CH_2CHO \leftrightarrow H_2O + CH_2CO$</td>
<td>$1.20 \times 10^{13}$</td>
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<td>$OH + CH_2CHO \leftrightarrow HCO + CH_2OH$</td>
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References


